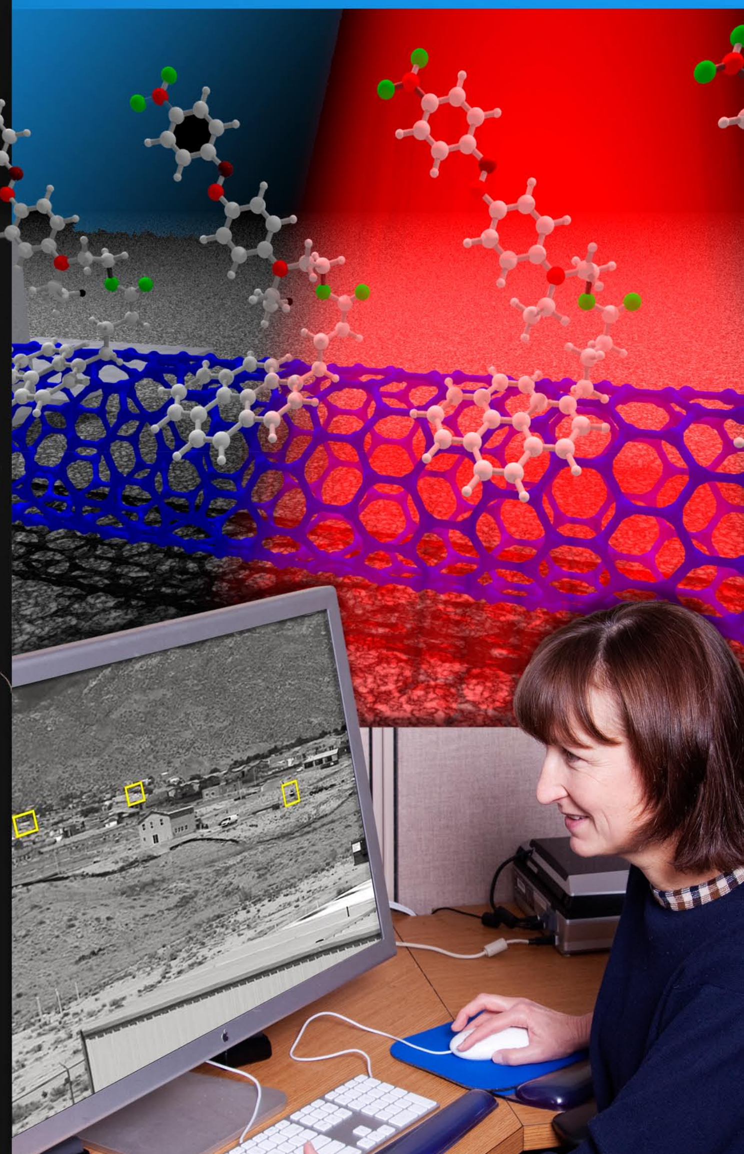
LABORATORY DIRECTED RESEARCH AND DEVELOPMENT

Science, Technology, and Engineering
Mission Technologies
Corporate Investments
Grand Challenges

LDRD

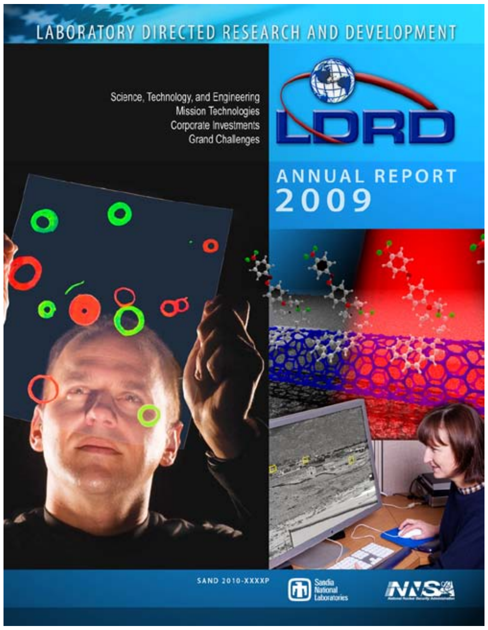
ANNUAL REPORT 2009



SAND 2010-1656P

Sandia National Laboratories

NNSA National Nuclear Security Administration



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Cover photos (top right going clockwise):

1. Artist's conception of an illuminated single-walled carbon nanotube (SWCT), its wall composed of interconnected hexagonal rings of carbon atoms, which in this case, have been chemically modified such that the structure acts as a light sensor. When stimulated with the proper frequency of light, current flow is switched on in the nanotube, which hence functions as a single carbon nanotube field effect transistor. (Project 117835)
2. LDRD principal investigator (PI), Katherine Simonson examines data from a project in which algorithms were devised and written to process the data from remote staring national-security sensors, in order to compensate for jitter effects that would have otherwise rendered the information from such sensors extremely difficult, if not impossible to interpret. (Project 117739)
3. LDRD PI, George Bachand examines tracks made by biological motor proteins as they move biological microtubules labeled with quantum dots along the surface of a glass slide. Employing biological motors as nanomachines could have far-reaching implications in nanoengineering (Project 52531 [FY 03–05] and subsequent DOE Basic Energy Sciences funding).

Abstract

This report summarizes progress from the Laboratory Directed Research and Development (LDRD) program during fiscal year 2009. In addition to a programmatic and financial overview, the report includes progress report from 406 individual R&D projects in 11 categories.

Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin company, for the U.S. Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94-AL85000.

SAND 2010-1656P
March 2010

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Sandia National Laboratories' FY 2009 Laboratory Directed Research and Development (LDRD) Program:

Discretionary Research and Development for the Future of the Labs!

J. Stephen Rottler , Vice President of Science, Technology, and Engineering and Chief Technology Officer

As authorized by Congress, the Laboratory Directed Research and Development (LDRD) program at Sandia National Laboratories (SNL) is critical to maintaining the vitality of our Labs in mission-critical science and engineering (S&E) disciplines. As SNL's sole discretionary R&D program, LDRD enables our technical staff to pursue innovative, high-risk and potentially high-value research and development (R&D) for a range of difficult S&E challenges facing our nation. Through LDRD, the Labs can pursue game-changing S&E, develop the next generation of mission-critical capabilities, and seek innovative solutions for emerging technical surprises. In turn, innovation in each of these arenas is crucial to our overall mission of providing "exceptional service in the national interest."

Often described as the "seed corn" for SNL's future S&E capabilities development, the Lab's LDRD portfolio must be simultaneously at the forefront of science and engineering theory and practice and aligned with our Labs' national security missions. In addition, LDRD supports crosscutting R&D in nuclear, energy, and cyber security arenas to seek innovative technical solutions for these emerging S&E challenges facing our nation in the Twenty-First Century and beyond. These discretionary investments often provide benefits to multiple missions, frequently demonstrating a broader impact, unanticipated in the initial proposal. A robust peer-review process results in a 10-fold down-selection in the process of choosing funded projects from initially submitted ideas, resulting in the selection of only the highest quality R&D projects that are well-aligned with Sandia's national security missions. To maximize impact on national security, LDRD accomplishments are immediately leveraged by management who are actively engaged with direct programs.

The FY 2009 LDRD program sponsored 406 projects costing $148M. This annual report offers an overview of the LDRD projects that were ongoing in FY 2009, highlighting only a few examples to demonstrate the scope of LDRD investments. The program overview and project summaries provide a window into the program's S&E innovation and its potential for impact on national imperatives.

SANDIA FY 2009 PROGRAM OVERVIEW

Sandia National Laboratories' Laboratory Directed Research & Development (LDRD) program has driven innovation for our nation in the form of transformational discoveries and consequential improvements. With 406 projects and a budget of $148M in FY 2009, Sandia LDRD made significant contributions to the nation's security in such mission areas as information technology, defense technologies, renewable fuels development, nonproliferation, nuclear weapons, biological systems, and countermeasures for weapons of mass destruction. Fundamental scientific advancements were made in materials science, quantum computing, cyber security, microelectronics, traditional computer science, and more. Advancements include taking microelectronics from the 2D to the 3D level, bringing quantum computing devices made from silicon closer to fruition, and developing new approaches for solar produced renewable fuels. Through these advancements, the Sandia LDRD program has grown our national technical knowledge base and prepared our nation for an improved level of security in the next decade.

LDRD Program Structure

For nearly twenty years Sandia National Laboratories has been operating a thriving, creative LDRD program. Funded by an assessment on all direct laboratory costs (presently 8%), enforced by statute, and regulated by the Department of Energy, LDRDs have become the seed funds to advance studies "of hypotheses, concepts, or innovative approaches to scientific or technical problems." In addition, they have offered the opportunity to establish "proof of principle" of new ideas and to perform concept development, all of which often leads to funding by DOE or other sponsors to meet the national security needs of the US. Thus LDRD provides a national risk-mitigation path for complex federal research problems, yielding an early down-selection process for DOE/NNSA, DHS and other federal agencies (OFA).

Responsibility for the Sandia LDRD program rests upon the shoulders of the Sandia President, who delegates policy and process authority to the Chief Technical Officer. The LDRD office takes responsibility for on-the-ground program management, process development, final proposal review, monitoring of outcomes, and reporting to the responsible NNSA entities. The LDRD office in turn manages the Senior Steering Committee (SSC), consisting of senior managers who represent each of the five technical Sandia Strategic Management Units (SMU). The SSC directs writing of each Investment Area's Call for Ideas, describing the science and technology interests of their SMU in a representative Investment Area, and directs reviews of submitted ideas and proposals. In addition, the SSC, with recommendation and direction of the LDRD office, helps develop policy to streamline the new-proposal evaluation and continuation-proposal evaluation processes and to help determine techniques for encouraging innovation and the taking of scientific risk in LDRD concept generation.

Sandia's web-based LDRD process allows all regular employees and post-docs to submit proposals at their desktop during the call period. An initial screening of brief 500 word (or 1000 word for large Grand Challenge) Ideas reduces the number of final proposals for review. During FY 2009, 1047 Ideas were submitted, of which 184 were approved for submission of full proposals. As is typically the case, about half of those (91) were accepted as projects. Late start proposals submitted off-cycle yielded an additional 104 new projects. Evaluation of proposals was based upon technical soundness, programmatic alignment with Sandia strategic goals, and the qualifications of the proposal team members.

Sandia chooses to allocate funds strategically, separating out those programs that have more near-term mission needs (<u>Mission Technologies</u>) and those which are producing more foundational knowledge to support longer-term national needs (<u>Science, Technology, and Engineering Foundations</u>). In addition, a relatively small fraction of funds is devoted to Grand Challenges, which address major national problems that require a multidisciplinary approach, and that will have significant impact on both the national scene and on our Laboratory. Finally, a smaller portion of LDRD projects (Corporate Investments) are dedicated to building university collaborations (Strategic Partnerships) and to performing high-risk feasibility studies (Seniors Council) as a risk-mitigation device before entering the regular LDRD stream of projects.

Funding and a breakdown of these Investment Areas follow:

Science, Technology, and Engineering Foundations

- *Nanoscience to Microsystems* — nanotechnology and microelectronics
- *Enabling Predictive Simulations* — computational algorithm and hardware development
- *New Directions* — biological and cognitive science and technology
- *Science of Extreme Environments* — pulsed power studies

Mission Technologies

- *Defense Systems and Assessments* — supporting the needs of the DOD and Intelligence community
- *Nuclear Weapons* — supporting the needs for the nuclear stockpile
- *Energy, Resources, and Nonproliferation* — fuel, water, and global security
- *Homeland Security* —supporting the needs of DHS

Grand Challenges

Corporate Investments

- *Strategic Partnerships* — collaborative university research and partnering for advancing capabilities.
- *Seniors Council* — novel, high-risk, high-impact R&D feasibility projects

Each year the Sandia LDRD office evaluates one aspect of LDRD impact upon our laboratory and its staff. "Expanding Professional Horizons" was a detailed study produced this year, which evaluated the impact of LDRD projects upon employee careers. It found that freedom to pursue new ideas under LDRD has established extensive cross-laboratory, cross-disciplinary partnerships. These have had a long-lasting productive impact not only upon LDRD research, but upon all future research performed by these individuals. As stated in the publication, "Although great ideas are sometimes the product of single individuals, it is perhaps more often the case that the development of truly innovative science and technology flows from the collaboration of researchers who are all working at the leading-edge of a challenge, often from different but complementary directions." The Horizons study also noted that LDRD was clearly attracting high-quality staff to this NNSA national laboratory, who might otherwise not have come. Young scientists and graduate students are intrigued by the early-career flexibility offered by this program and find the cross-disciplinary environment thoroughly exciting.

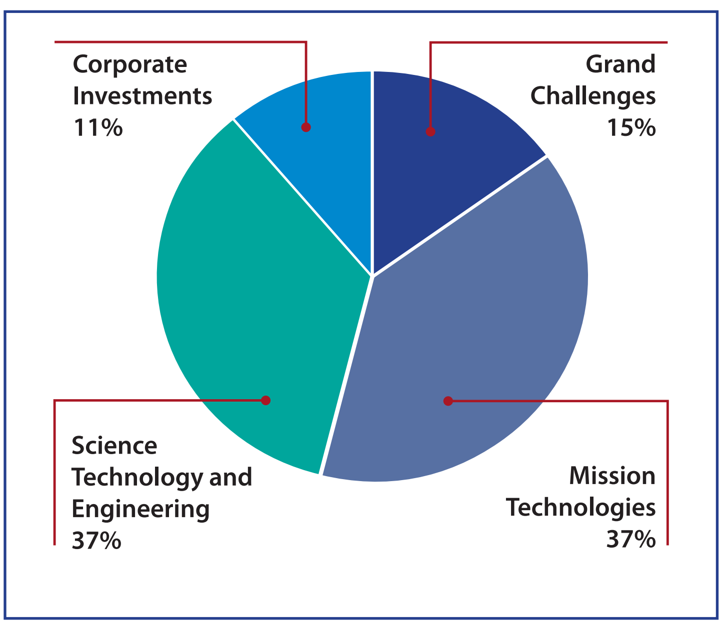


Figure 1: FY 2009 LDRD Investments (based upon a total of $148M)

Innovation is an elusive outcome of sound R&D, of which a central component is level of risk. The guiding LDRD DOE Order 413.2B specifically identifies one program objective as supporting "high-

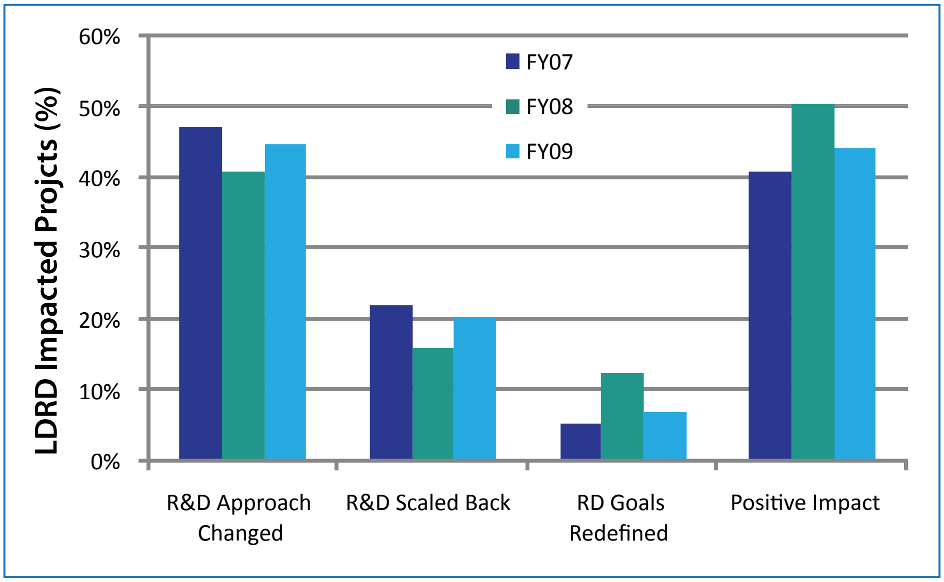


Figure 2: LDRD Program Tolerance for Risk
Many projects were redirected during the scientific process

risk, potentially high value research and development." LDRD risk at Sandia has been taken on by both the project team members as well as the management team in order to permit the technical team members to achieve breakthrough results. Creativity, novelty, and vision can all be stifled by inflexibility and near-term thinking among either the technical staff or management surrounding a project. It has thus become important for the Sandia LDRD program to encourage goals that reach beyond what is easily achievable and to anticipate problems and errors of inadequate questions, incorrect hypotheses, insufficient testing, or poor conclusions. Failures in any of these foundational components of the scientific method may be avoided assiduously via risk mitigation, but if discovered should form the basis of project redirection or redesign under the auspices of Investment Area management. A measure of Sandia's LDRD program flexibility is seen in a survey of the last three years' ending projects (Figure 2) in which project R&D was redirected due to such discoveries. It is a goal of the LDRD program at Sandia to maximize the potential of our scientific staff and to return the most innovative work to our nation as is possible.

LDRD Program Performance

The FY 2009 Sandia LDRD program grew in size over the previous year, proportional to an increase in the Labs' budget, and yielded a plethora of new scientific results. By rolling up our standard metrics for success over the past four years, we note that although the LDRD program only utilizes up to 8% of incoming funds, it returns far more to the laboratory and to the country. Over half of our R&D 100 Awards are derived from LDRDs, over 20% of our publications come from LDRDs, and over a quarter of our patents come from LDRD projects. These figures repeatedly show the vitality of the program and its innovative nature, producing new knowledge for mankind that is reducible to practice.

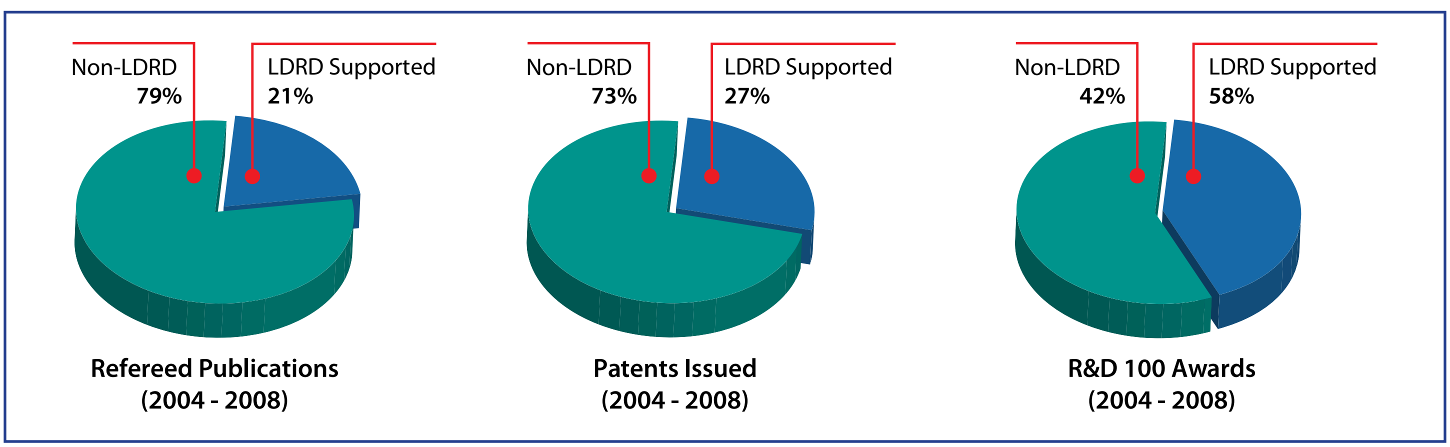


Figure 3: LDRD Program Metrics

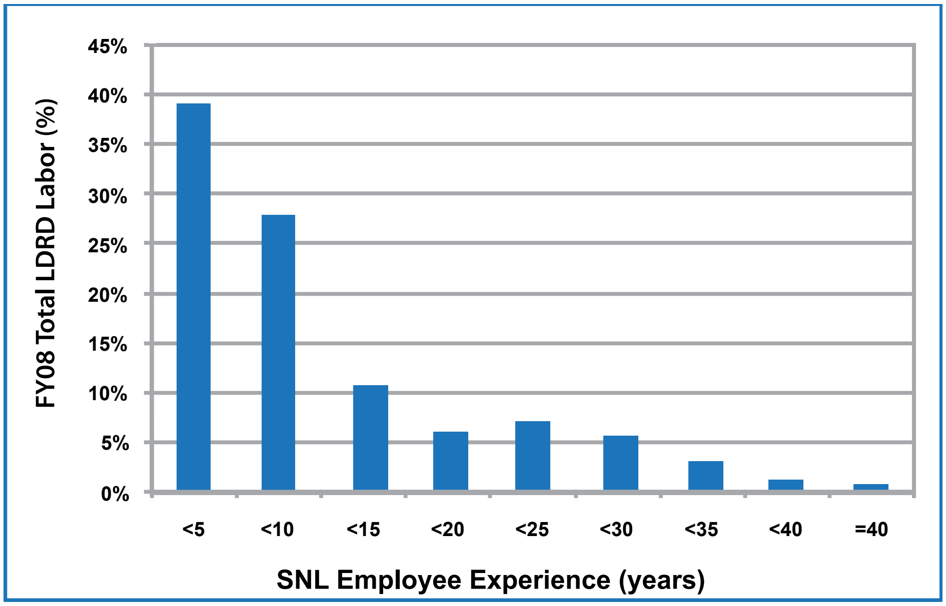


Figure 4: LDRD Participation vs. Employee Experience

Lab vitality is usually measured by the extent of involvement of and attraction to young staff at the DOE national laboratories. LDRD continues to extensively utilize young talent as is seen in Figure 4. Nearly 40% of the individuals working on Sandia LDRD projects are staff with less than 5 years of experience at our laboratory. Over 25% of LDRD workers are staff with 5-10 years of experience. These scientists and engineers are well-mentored by staff with 10-40 years of experience, who are relatively uniformly distributed throughout the LDRD program.

Noting that LDRD is supported by ≤8% of costed programs at Sandia, its impact well-exceeds this modest value. Citations of peer-reviewed published articles are a widely accepted measure of institution credibility in a given technical area. As seen in Figure 5, publications resulting from LDRD efforts typically exceed the number of citations received by all three NNSA labs' publications produced by regular sponsored projects. This suggests that the independence and ability to draw upon employee-suggested ideas yields creative results that are greatly sought after by the general scientific community.

The Sandia LDRD program is continuously fine-tuned to optimize efficiency and increase productivity. How can one permit the broadest exercise of new concepts, while providing the oversight necessary to ensure efforts remain well-focused? The solution applied to this problem is to maintain approximately the same number of projects year to year, even as the overall laboratory budget grows. This has been realized by increasing the average dollar value of LDRD projects, as seen in Figure 6. While the median project size was approximately $350 K in FY08, the median for

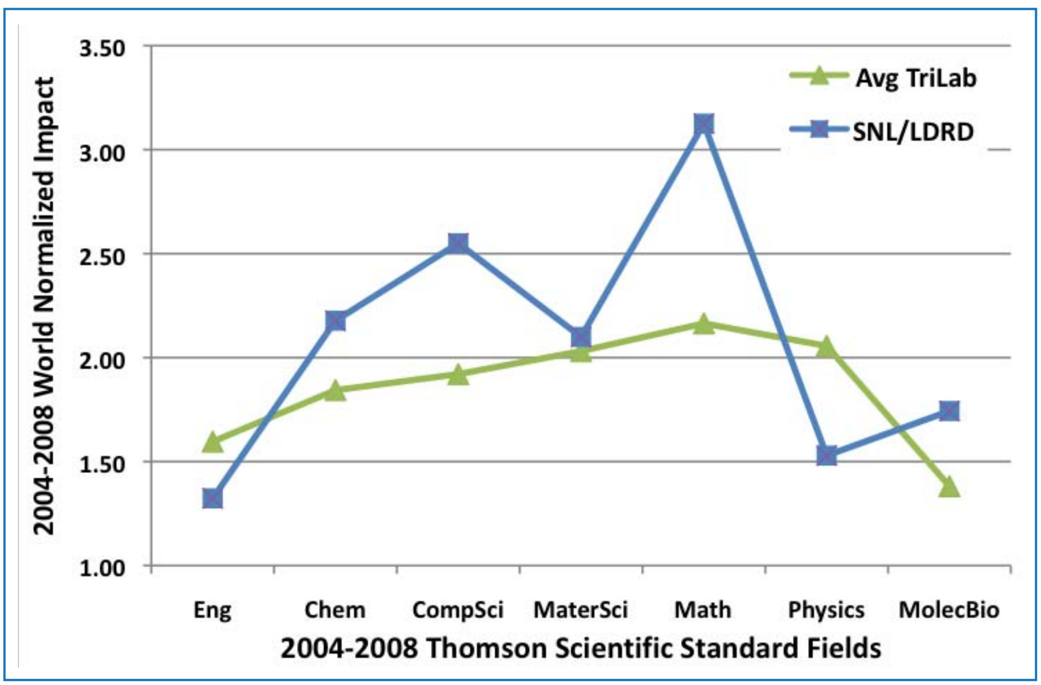


Figure 5: Impact of Sandia LDRD publications as measured by level of citations

FY10 will be $450 K. Such a change yields broader laboratory interaction within each project, and permits coverage of more complex multidisciplinary research problems. The result is to maintain a well-balanced manageable program.

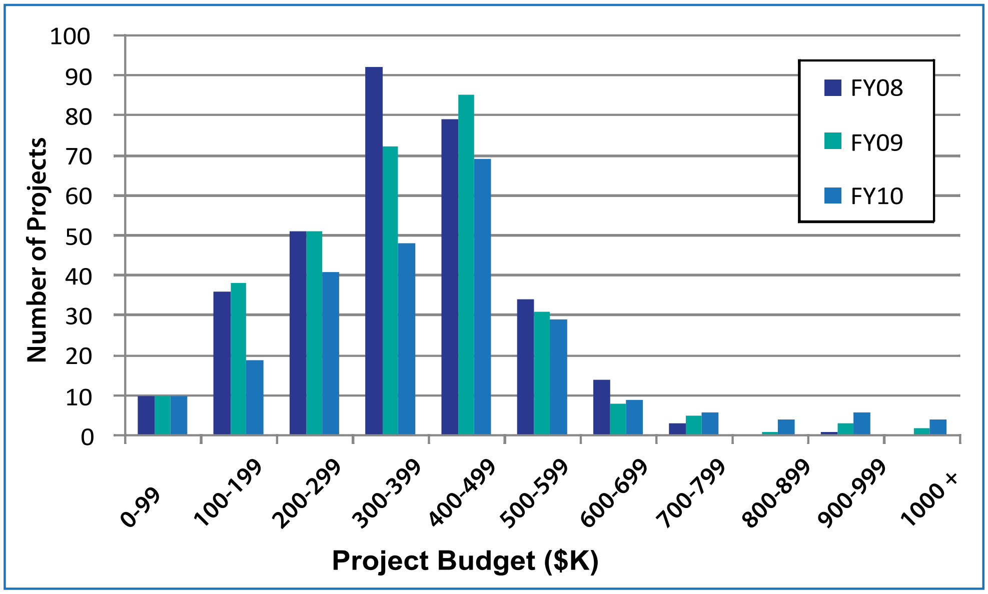


Figure 6: Average LDRD Project Size in the Past Three Years

LDRD Portfolio Profiles

Significant advances were made in many areas of LDRD research, which enriched the science, engineering, and technology base and contributed to a variety of existing and potential applications. The Sandia LDRD program was showcased in August 2009 at the Tri-Laboratory LDRD Symposium in Washington, DC. LDRD efforts from Sandia National Laboratories, Los Alamos National Laboratory, and Lawrence Livermore National Laboratory were highlighted for representatives of multiple US government agencies (NNSA, DOE, DoD, OSTP, and others). America's Infrastructure Security was the focus of the meeting this year, permitting the three NNSA labs and the weapons production labs to describe their LDRD contributions. The Sandia CTO presented our portfolio and referred to the critical infrastructure issues involved in cyber and energy. Posters included ultracapacitors for energy storage and genetic engineering of bacteria for improved ethanol production from fermentation. As an example of FY 2009 LDRD support for infrastructure interests, particular examples will be shown in the areas of energy security, biosecurity (supported under our New Directions and Homeland Security and Defense investment areas), and some of the underlying science and technology related to nanostructured materials. Each area saw contributions from multiple LDRD projects, which demonstrate the breadth of impact one can achieve by staying focused on the technology and solving multiple problems. The projects described below were further represented at Sandia's annual LDRD Day, which displayed the best of the laboratory's FY 2009 LDRD projects to both Sandians and invitees from other laboratories and external sponsors.

Energy Security

America's energy security has been seriously threatened over the past forty years, and is now seeking to generate a plethora of renewable sources to replace oil and coal. Supported by the Sandia Environment, Resources, and Nonproliferation investment area and our Enabling Predictive Simulations investment area, LDRD projects drive new approaches to harnessing solar power, fuel cells, and grid electrical distribution.

Sunshine-to-Petrol is a large Grand Challenge LDRD that seeks to convert solar energy into organic fuels. Focused solar energy heats a mixture of CO_2 and water to 1500 ^{o}C, creating a reactor environment which produces viable hydrocarbon fuels. The renewable fuel consumes CO_2 and later burns to produce CO_2, resulting in a carbon neutral fuel process. In the presence of a metal oxide, the CO_2 splits to form CO, which then combines with water to form volatile hydrocarbons. The process has worked well in the lab, and is being taken to a prototype stage with a small reactor placed at the focus of an eight meter diameter solar reflector. High reactor temperatures stretch the durability of the reactive wall, presenting a significant materials problem. Iron and cobalt oxides have shown themselves inadequate to maintain high efficiency at these temperatures, causing researchers to move towards zirconium and cerium-based oxides. Researchers hope to achieve a 2% conversion efficiency from thermal energy to CO and conclude with a reliable design, capable of being licensed to industry.

A parallel project is developing another renewable energy source, hydrogen in fuel cells. By integrating static fuel cells into a small neighborhood heating, cooling, and electric power plant, modeling results indicate that fuel consumption and CO_2 emissions may be reduced by up to 50%. The project has produced both chemical engineering and techno-economic-environmental models for system optimization. Data was independently validated with data from manufacturers and from the literature.

The incorporation of irregular renewable energy sources (sun and wind) into the national power grid has created serious issues of load balancing. Three Sandia LDRDs are designing new distributed grid systems consisting of local microgrids, which will be capable of adaptive control based on thermodynamic principles. Scalable microgrids offer a pooling of local resources in the event of grid failure and exist in close proximity to power users, limiting transmission problems. Distributed controls yield higher system stability with fast time response, redundancy, security against single point failure, and close management of generation, storage, and loads. Data benchmarking was performed in one case with the Kauai, Hawaii power-generation system to evaluate the impact of added wind power to their grid. Serious power generation instabilities were discovered due to wind intermittency.

Biosecurity

While the 20th century is considered the Atomic age due to the discovery of nuclear fission and fusion, the 21st century is rapidly becoming the biology age, where genetic engineering, bioterror, and improved understanding of how to manipulate living systems are driving significant scientific discoveries. Through the New Directions investment area, Sandia LDRD is leading the development of pathogen diagnostic systems, biofuel production from biomass, and the study of techniques to address various biothreats.

Building upon a decade of Sandia experience in microfluidic analysis of biological samples, a deployable pathogen diagnostic system was designed and built that fit into one's hand. On-chip microfluidic technology permitted sample (blood or saliva) preconcentration, separation, multianalyte processing and presented easily interpreted electropherograms. This device will permit rapid triage of a large population to identify individuals exposed to particular pathogens and to be treated at the earliest time.

In another biosecurity LDRD project, bacteria have been genetically engineered to efficiently ferment biomass into ethanol at higher temperatures than normal. This will permit a one-reactor solution to fuel production, allowing both sugar formation and fermentation to occur at the same high temperature. The *Geobacillus thermoglucosidasius* bacterium was chosen for its ability to withstand high temperatures. Annotation of the entire genome identified relevant sites, and modifications were made to control protein pathways for disruption and to enable it to increase its ethanol yield with no extraneous products.

Maintaining an adequate supply of potable drinking water is becoming an important problem for the 21st century. We must protect against potentially toxic chemicals and pathogenic bacteria and viruses, whether naturally occurring or introduced as a bio-warfare initiative by adversaries. In a ground-breaking LDRD project, the purification of water contaminated with pollutants and viruses was addressed via colloidal capture on a filtering membrane. The idea was to identify and produce a highly efficient colloidal coating, which would trap and precipitate out both toxins and pathogens. Both anionic polyoxometalates and cationic aluminum clusters were combined with surfactants of opposite charge, which resulted in a complex layered chemical structure in water. Using NMR and dynamic light scattering, it was observed that virus particles were removed by a physical-chemical enmeshment within the precipitate. By adding a small percentage of gallium to aluminum clusters, a far superior agent was obtained to remove viruses in particular. Thus a pathway was found for ongoing improvement in water treatment processes.

Science, Technology, & Engineering: Nanostructured Materials

Atomic force microscopes, laser tweezers, and e-beam lithography have all enabled the measurement and manipulation of single atoms in a matrix, giving rise to the field of nanostructured materials. The Sandia LDRD program in collaboration with the joint SNL/LANL Center for Integrated Nanotechnologies (CINT) is actively pursuing nanomaterial research. Recent LDRDs have examined science at grain boundary interfaces in nanocrystalline materials, explored the use of nanomaterials for energy storage in ultracapacitors, and developed techniques to fabricate nanomaterials on the atomic scale. The External Advisory Board for Sandia's Materials Science and Technology Research Foundation lauded LDRD efforts to develop new scientifically engineered materials. They state that, "scientific advancements are needed to understand how materials properties and performance under specified conditions depend on composition, microstructure, and preparation. New materials may be required to replace obsolete or unavailable technologies, meet new system requirements, or provide new functional capabilities." The following examples demonstrate both the microstructural characteristics examined, as well as some of the next generation applications that will be filled by these efforts.

Fundamental materials properties were examined in an LDRD researching the effects of nanostructure on micro- and mesostructural properties in metals. In nanostructured materials, interfaces are more numerous per unit volume of the material, which suggests that they crucially determine the material's properties. Grain boundaries, in particular, are a subset of such interfaces and impact such macro properties as mobility and stiffness. Simulations, high-resolution TEM/SEM, and atom-probe tomography of nickel revealed several unexpected findings. Growth of metastable phases was observed, impacting thermal stability. Further, the formation of lattice defects appears to depend upon an as yet unexplained manner on the scale of the grain structure. Extensive mapping of grain boundary energy levels has further muddied the waters with no clear correlation to parameters usually associated with such energy levels. Much has been learned, but clearly a great deal of further research is required to permit large-scale applications of these materials.

One solution to improving energy storage for electric powertrains or more static situations is the ultracapacitor, a high energy density, high power density device to replace the battery. LDRD has stimulated the study of cylindrical nanostructures as electroactive annular structures, which contain a powerful electrolyte in their center. The extremely short distances (200 µm diam core) permit rapid charge transfer as well as high storage capability. Nanostructures with RuO_2 and Nb_2O_5 have been created showing enhanced proton conductivity. Conductive polymers have been electrochemically deposited into nanopore arrays in anodized aluminum, and models have been used to understand rate limiting behaviors of these devices. They show that ultracapacitors can be fabricated relatively inexpensively by several alternative routes.

Lastly, nanomanufacturing could provide high-performance alloys with strengths and durabilities as yet unseen. Layer-by-layer production of devices using nanomaterials and gamma irradiation has produced "superalloys" with high strength and durability, resistant to both corrosion and high temperatures. In a recent nanomanufacturing LDRD, silver-nickel and palladium-nickel superalloy nanoparticles were created and characterized. Applications for these materials include weapons casings, aircraft parts, gas turbine engines, and membranes for hydrogen storage.

LDRD Awards

LDRD projects are the core of national laboratory innovation and vitality. As such, they typically demonstrate superior performance in publications and awards, as was indicated in Figure 3. In July of 2009, R&D Magazine presented their "R&D 100" Awards to researchers who have developed the year's one hundred most outstanding advances in applied technologies. Sandia received six awards, four of which had been supported fully or in part by the LDRD program. These four projects are reviewed in the paragraphs below.

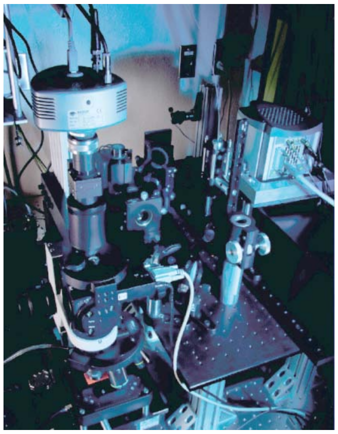


Figure 7: Hyperspectral Confocal Microscope

LDRD projects were the primary support behind development of the **hyperspectral confocal fluorescence microscope**. This instrument rapidly acquires images with diffraction limited spatial resolution of 250 nanometers (nm) in lateral directions and 600 nm in the axial direction. When combined with Sandia's proprietary multivariate analysis algorithms, the system enables the identification of all emitting fluorescence species contained in an image, and the production of relative concentration maps for each species—all without the need for any a priori information about the emitters.

LDRD supported improved fabrication techniques for the **ultra-low-power silicon microphotonic communications platform** that enabled optical data transmission in silicon at nanosecond switching speeds. The system operated with up to 100 times less power consumption and 100 times more bandwidth compared to traditional electronic approaches. Its extremely small size permitted sub-100 fJ/bit data transmission, a hundred times reduction over standard interchip communications.

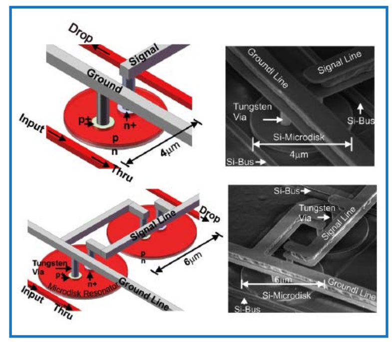


Figure 8: Si-based Microphotonic Communications System

Under LDRD funding, **NanoCoral™ dendritic platinum nanostructures** (Figure 9) were conceived and developed. This innovative nanotechnology for producing platinum catalysts offers unique control over the shape, size, porosity, composition, stability and other functional properties of platinum nanostructures compared with those achieved by existing methodologies. This unique form of platinum is expected to significantly reduce metal usage and thus the cost of platinum catalysts in fuel cells, solar cells, and other applications in the renewable energy sector.

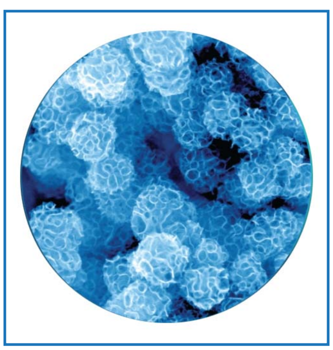


Figure 9: Dendritic Platium Topography

LDRD provided key funding to develop the SMARTMAP approach to data access performance for today's multicore parallel processing applications. This software foundation enabled the creation of the **Catamount N-way Lightweight Kernel** open-source operating system that takes maximum advantage of multicore processors (see Figure 10). Earlier work at Sandia had demonstrated the problems of trying to increase performance via added processors. While each processor could operate rapidly, access to one another's memory significantly limited operating speed. Thus a sixteen-core machine could operate so slowly that it would look like a dual-core machine. High performance computing crucially depends on systems with many cores or "N" cores to solve today's national security problems.

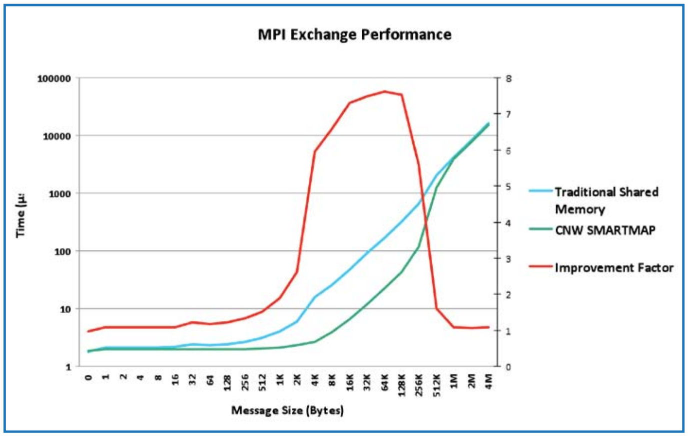


Figure 10:
Speed Enhancement Obtained with the new Catamount N-way Kernal

Catamount attacks this problem at the operating system level, cutting the required memory bandwidth for intra-node message passing in half. It makes processes running on a multicore processor behave as if both processes were running in their own independent address space and as threads that run within a single address space. It enables in-place collective operations, threaded reduction operations, and high-performance, one-sided message passing operations. Together these help preserve the multi-billion dollar investment that has been made in scientific parallel applications.

Conclusion

The LDRD program is a crucial, strategically applied program enabling the security of the nation's future. LDRD is to the NNSA national laboratories as internal R&D investments are to private industry. The national labs would lose their cutting edge capability without this vital injection of innovation and creativity. By virtue of the LDRD program, Sandia maintains its lead in synthetic aperture radar, micro- and nano-electronics fabrication, high-performance computing, solar energy utilization, pulsed power applications, biofuels, and more. As with industrial R&D the modest 8% investment is multiplied three times in its return in publications, patents, and the attraction of new technical staff.

The journal *Science* announced in February 2009 the winners of its 7th annual "Best Places to Work for Postdocs" survey. In a list that included Genentech Inc. of San Francisco, the Whitehead Institute for Biomedical Research in Cambridge, MA and the Novartis Institutes of Cambridge, MA, Sandia National Laboratories ranked fifth. Most postdocs at Sandia are young and are working on LDRD projects, as indicated in Figure 4. This along with supportive benefits and training provide Sandia with a vibrant group of individuals eager to make their mark in their research areas.

External review emphasizes the skills and mastery that Sandia brings to the table in its strategically selected LDRD projects. In a major Grand Challenge LDRD on metamaterials, the project's external advisory board stated, "it is … very beneficial to the field to have the superb materials resources of Sandia brought to bear on metamaterials issues." As one EAB member noted during the session, "If there's a place in the world where metamaterials should be developed, it is Sandia." A solid mix of capabilities, strong mission needs, and innovative staff contributions enhance the value of the LDRD program to both the nation and Sandia.

During FY 2009 the LDRD program produced 406 projects, of which 195 were in their first year, 115 were in their second year, 95 were in their third year, and 1 was provided an extension for a fourth year. The average project size on an annual basis has risen to $450K with a range spanning a low of $24K to a high of $5.4M. Details may be seen in the Appendix. As budgets tighten and the global economy crawls out of today's serious recession, the LDRD program continues to be the "little engine that could," pulling its load, undistracted, pressing for excellence, creating new knowledge, solving critical problems, and investing in our nation's future.

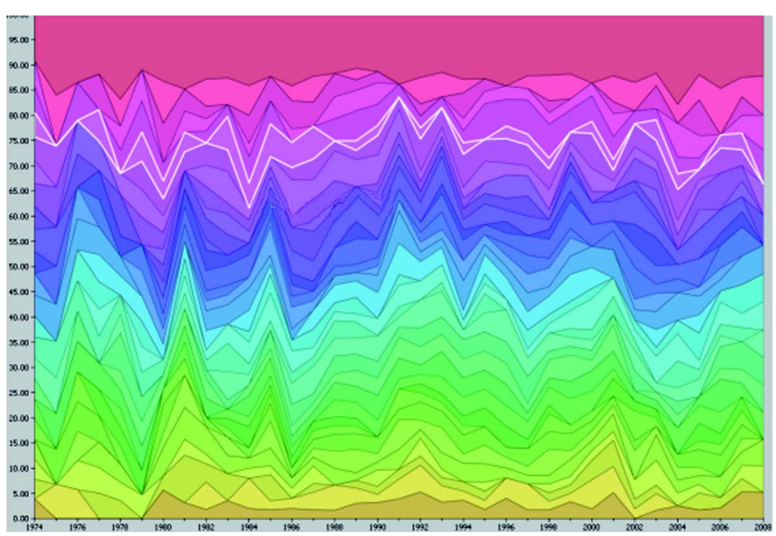
ENABLE PREDICTIVE SIMULATION INVESTMENT AREA

Computational modeling and simulation is the bailiwick of this investment area (IA), funding research into computational activity that has the capability to both confirm and globalize experimental results, as well as to guide future experimentation and scientific intervention into national and global challenges. From predicting the course of epidemics, to models of material failure probabilities, to modeling water systems in semi-arid regions, to clarifying the properties of matter at the nanoscale, to new designs for computational memory, this IA's reach across Sandia's mission areas is quite extensive.

Scalable Solutions for Processing and Searching Very Large Document Collections

Project 117788

This project approaches the dilemma faced by intelligence analysts, namely that, under extreme time pressure, they must make decisions, based on huge quantities of information culled from a diversity of sources — news articles, reports, network traffic, etc. A key task is the determination of the relationships among the persons, entities, and terminology in those information conduits. This project is addressing that dilemma by designing software that, within a text analysis framework, analyzes conceptual relationships among documents, among terms (including named entities) in documents, and among terms and documents, presenting results of this analysis in a convenient visual form. ParaText™ software is available in client-server, web service, and stand-alone versions, and it uses unsupervised natural language modeling based on statistical methods capable of incorporating intelligence analyst expertise, while leveraging existing Sandia tools. It is scalable to different numbers of processors. Network traffic payload analysis provides conceptual document matching and clustering, enabling assessment of emerging cyber threats. It has already demonstrated its value in the area of nonproliferation, capable of extracting meaningful patterns and trends, as well as providing information enabling rapid interpretation of nuclear-forensic signatures.

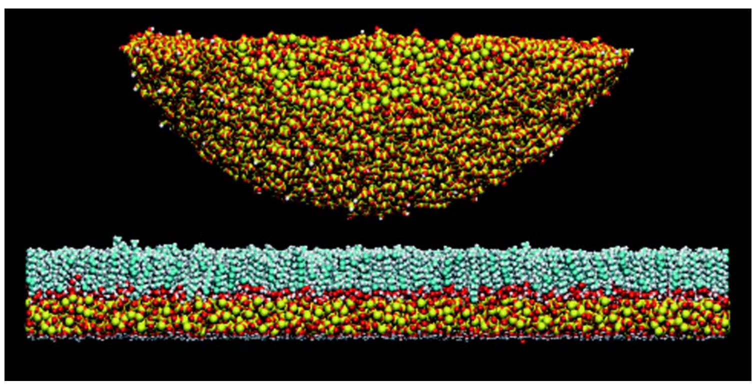


One type of graphical representation depicting temporal relationships among documents.

Nanomanufacturing: Nanostructured Materials Made Layer-by-Layer

Project 130741

Projections are that by 2015, nanomanufacturing will be a one-trillion-dollar industry. Between now and then, there are numerous theoretical and operational hurdles to overcome, for an industry that will need to mass-produce devices such as memory chips, high-brightness LEDs, sensors, flat-panel displays, and photovoltaics. A transformed energy economy depends on such a nanomanufacturing ability. Working with its academic partner, the University of Texas, this project is investigating approaches to ultimate high-throughput nanomanufacturing of these largely multilayered entities. A key part of this initiative is the generation of modeling and simulation capabilities that will scale-up to ultimately impact machine design. A prototype process is step-and-flash imprint lithography (SFIL), which epitomizes nanomanufacturing in terms of its liquid-based coating that is polymerized, imprinted with a pattern, then etched and combined with other layers in a device to be manufactured. Beginning with molecular dynamics and finite-element (FEM) models simulating the molding of a single nanoscale feature, this project team discovered the importance of adhesion and atomistic friction at this scale. At the same time an experimental prototype of imprinting on nanoparticle-laden liquids has laid a groundwork for building an SFIL pattern for nanoparticle-based circuitry templates, which will serve as a proof-of-concept application.



Molecular dynamics analysis of friction and adhesion at the nanoscale

ENABLE PREDICTIVE SIMULATION

Lightweight Storage and Overlay Networks for Fault Tolerance

105799
Year 3 of 3
Principal Investigator: R. A. Oldfield

Project Purpose

Checkpoint-to-disk approaches that account for nearly 80% of the total input/output (I/O) usage on some machines are "bursty" in nature, producing I/O demands that quickly overwhelm the I/O infrastructure for capability-class systems. The trends toward data-intensive applications and petascale systems with tens-to-hundreds of thousands of nodes exacerbate this problem. Checkpoint-to-memory approaches provide an alternative, but require significant memory resources on the compute nodes. Since many large-scale scientific applications (Sandia applications in particular) are already resource constrained on the compute node, these approaches are also unacceptable.

Another perhaps more serious problem is that although many large systems can survive independent component failures, applications still fail if any of the compute-node processors fail. Since the probability of application failure is directly dependent on the number of compute nodes, the application must increase the number of checkpoints to account for the increased risk of job failure. These additional checkpoints add stress to the network and I/O system and severely impact the scalability of the application.

Leveraging our preliminary effort in lightweight file systems, we plan to investigate the use of "lightweight" storage architectures and overlay networks for fault tolerance. Lightweight storage architectures allow secure, direct access to storage, bypassing features of traditional file systems that impose performance bottlenecks. Overlay networks provide processing in the network to offload performance-critical functionality required by compute nodes. Together, these technologies could provide substantial optimization for fault tolerance. For example, intermediate nodes in an overlay network could buffer checkpoint data, enabling the overlap of computation, communication, and disk I/O. Intermediate nodes could format/permute/partition application state to efficiently store and retrieve data from distributed storage devices. Finally, intermediate nodes could cache processor state, allowing restarts without disk I/O or, perhaps, partial application restart.

Summary of Accomplishments

Over the course of this project, we accomplished a great deal of work. In our preliminary investigations, we developed a general analytic model for checkpoint overhead that accounts for network and file system performance. We then revised that model to approximate improvements using lightweight storage and overlay networks to cache checkpoint data in the network. We then designed and implemented a "caching service" that provided the necessary proof to justify our approach. The caching service allowed unmodified parallel applications using Parallel NetCDF (network common data form) to use the caching service to buffer checkpoint operations, leading to a 10× improvement in effective I/O performance.

Significance

This project has relevance to the scientific innovation and discovery mission, and will have a direct impact on applications in virtually all areas of advanced computing. Already, the modeling effort provided a great deal of insight that motivated new funding both internally through other LDRD projects and externally through NSF-funded efforts at the University of Texas, El Paso (UTEP). The caching service work also led to new internal funding for scalable I/O services and led to collaboration with Oak Ridge National Laboratory (ORNL) related to data staging for fusion and climate codes.

Microstructure-Based Approach for Predicting Crack Initiation and Early Growth in Metals

105800
Year 3 of 3
Principal Investigator: L. N. Brewer

Project Purpose

Fatigue fracture is among the most important problems in materials failure, affecting mechanical components from critical welds to solder joints to microelectromechanical system (MEMS) devices. A great deal of experimental and theoretical effort has yielded phenomenological relationships between materials parameters and fatigue life, but we still lack the fundamental materials science understanding at the microstructural level that will allow failure prediction from first principles. Of critical importance is the ability to predict when and where cracks will nucleate in the microstructure and to predict their early growth behavior. These problems are particularly difficult because they are strongly controlled by the microstructure and have not been amenable to standard continuum mechanics approaches or experimental investigation. The ultimate goal is to be able to take a starting microstructure with a loading geometry and accurately predict the crack nucleation and growth behavior to failure. To face this fascinating and yet daunting challenge, we will combine Sandia's world class computational mechanics and structural characterization expertise to develop microstructural models to predict the crack nucleation and early growth. These models will combine the latest in length-scale sensitive crystal plasticity models with novel models using adaptive cohesive zone element and material point method strategies. Experimental deformation and characterization will be performed on the same microstructure as those used by the computational models to allow for model guidance and validation. Novel electron back-scattered diffraction and focused ion beam techniques will be combined to allow characterization of plasticity evolution from fatigue and cracking in both two and three dimensions.

The success of this research will provide the fundamental understanding of plasticity-based crack nucleation and early growth behavior in microstructures necessary for developing robust fatigue failure models. These failure models are critical for Sandia's stockpile stewardship, development of reliable microsystems, and success in the science-based engineering transformation initiative.

Summary of Accomplishments

We developed microscale, in situ techniques for analyzing the deformed microstructures of metals. We designed and built a novel in situ straining stage for the scanning electron microscope which resulted in the submission of an invention disclosure.

We developed a new analytical way to analyze the elastic behavior of triple junctions in polycrystalline microstructures. This analysis discovered both singular and nonsingular stress concentrations at triple junctions, a novel result. This research has been written and submitted in a journal article.

We performed a series of experiments and finite element simulations that examined the importance of detailed microstructural representation on predicting microplastic ratcheting. This work demonstrated that macroscale responses are less sensitive to the details of the microstructural representation while the microscale responses, such as damage accumulation, are quite sensitive to the details of the microstructure. This work has been accepted for publication as a journal article.

We created a set of brass microstructures with systematically altered microstructures (grain sizes and recrystallization textures). These samples were carefully characterized and mechanically tested in order to provide a set of input and validation data for the development of improved polycrystalline plasticity models.

We implement both local and nonlocal polycrystalline plasticity models into a material point method formalism to allow for massively parallel simulations that simultaneously evolve the microstructure and the mechanical state of a microstructure. These results are currently being written into a pair of journal articles.

We combined our work on polycrystalline plasticity with interest in hydrogen embrittlement at crack tips. We also combined simulation codes ARIA and ADAGIO to allow for a couple mechanics-hydrogen transport simulation. These couple simulations have shown that microstructure alone may explain the high stresses hypothesized to exist at crack tips embrittled by hydrogen.

Significance

A microstructural approach to early fatigue life prediction is vital to Sandia's ability to predict critical component life. Thermomechanical fatigue of solder connections in nuclear weapons components is a major area of concern for stockpile reliability. While we currently have continuum-level tools for predicting failure, we do not have the fundamental science necessary to predict the change in component life that would accompany a change in material microstructure.

Refereed Communications

R. Dingreville, C.C. Battaile, L.N. Brewer, E.A. Holm, and B.L. Boyce, "The Effect of Microstructural Representation on Simulations of Microplastic Ratcheting," to be published in the *International Journal of Plasticity*.

Advanced Diagnostics for Full-Scale Fire Experiments: Closure of the Radiation Source Term and Spectral Fire Signatures

105804
Year 3 of 3
Principal Investigator: S. P. Kearney

Project Purpose

Thermal radiation from fire is a primary threat to strategic systems and critical infrastructure and is a key source of infrared signatures detected by battlefield intelligence assets. Fire radiation is dominated by emission by hot soot particles located in submillimeter-scale reaction zones with extreme temperature and concentration gradients. Direct computation of these fine-scale features in fire models of relevant meter-scale size is not feasible even with the largest supercomputers. State-of-the-art fire models predict radiative output using modeled soot-temperature correlations and scalar state relationships, neither of which has ever been validated against experimental values obtained from fires of meaningful size. This R&D is an unprecedented step toward validation of this fire-radiation problem. Advanced laser-based diagnostics will be brought out of the laboratory and applied to full-scale fire-testing in well-controlled fire experiments, which are designed within the context of fire models. The breach between laboratory scale detail and fire size is overcome by Sandia's unique and newly opened FLAME (fire laboratory for accreditation of models and experiments) facility. FLAME is the only research facility in the world that has been specifically designed to accommodate advanced laser-based diagnostics to large-scale fire testing. Coherent anti-Stokes Raman scattering (CARS) and laser-induced incandescence (LII) will be simultaneously applied for joint measurements of temperature, soot concentration, and mixture fraction at the submillimeter length scales, which are needed to resolve gradients in the reaction zones where radiating soot is generated in the fire. The data will be used, for the first time, to validate state relationships and temperature-soot correlations that are predicted by the next-generation fire-radiation models for computation of radiative heat loads to objects. This project will provide Sandia with a capability for computational and experimental fire and large-scale fluid systems research that is truly unique in the world.

Summary of Accomplishments

We have applied CARS and LII for spatially and temporally resolved measurements of gas temperature and soot concentration at length scales that are physically relevant to thermal radiation emission in large pool fires. This work represents the first-ever application of such high-fidelity laboratory combustion diagnostics to fire environments of meaningful size. CARS and LII systems have been constructed at Sandia's FLAME facility for controlled, wind-free fire experiments and are now an integral part of the facility architecture, arguably making Sandia the world leader in large-scale fire-science research. Dual-pump CARS measurements of temperature have been demonstrated in both clean-burning and sooting 2-m-diameter liquid pool fires. CARS temperatures derived from spectroscopy of the nitrogen molecule are accurate to with 1% and precise to within 5% to 7%. We have demonstrated a capability for CARS mole-fraction measurements, presenting quantitative O_2/N_2 mole-fraction ratios, and demonstrating simultaneous detectivity of N_2, O_2, H_2 and CO_2. The single-laser-shot CARS measurements provide a temporal resolution of 10 ns, with a spatial measurement volume of 8×10^{-3} cc, which is needed for subgrid resolution of radiative-emission statistics. Our CARS instrument has been combined with an LII probe for simultaneous detection of soot concentration with the CARS temperature/mole-fraction measurements. Quantitative LII measurements of soot volume fraction have been demonstrated in a 5-mm × 1-mm laser sheet, yielding a time resolution of 10 ns and a spatial measurement volume of 10^{-5} cc. We have demonstrated the ability to perform CARS and LII measurements simultaneously for generation of temperature and soot probability-density-function (pdf) data in pool-fire testing. We are presently working to correlate the CARS/LII results to generate the joint temperature/soot statistics that are required for development of truly predictive fire heat-transfer models.

Significance

The capabilities developed here will vastly improve our understanding of the physics and modeling of large-scale fires, highly relevant to DOE missions in weapon safety, national security and protection of US critical infrastructure. The project represents an unprecedented advance in the measurement science and predictive modeling of large-scale reacting fluid systems, which can benefit DOE energy programs and contributes to DOE's goal to advance efforts at the forefront of science.

Refereed Communications

K. Frederickson, S.P. Kearney, A. Luketa, J.C. Hewson, and T.W. Grasser, "Dual-Pump CARS Measurements of Temperature and Oxygen in a Turbulent Methanol-Fueled Pool Fire," to be published in *Combustion Science and Technology*.

S.P. Kearney, K. Frederickson, and T.W. Grasser, "Dual-Pump Coherent Anti-Stokes Raman Scattering Thermometry in a Sooting Turbulent Pool Fire," *Proceedings of the Combustion Institute*, vol. 32, pp. 871-878, 2009.

T.K. Blanchat, T.J. O'Hern, S.P. Kearney, A.J. Ricks, and D.A. Jernigan, "Validation Experiments to Determine Radiation Partitioning of Heat Flux to an Object in a Fully Turbulent Fire," *Proceedings of the Combustion Institute*, vol. 32, pp. 2511-2518, 2009.

Nanomechanics of Films on Compliant Substrates to Enable New Flexible MEMS and NEMS Devices

105805
Year 3 of 3
Principal Investigator: N. R. Moody

Project Purpose

Deformation and fracture of films on compliant substrates govern performance and reliability of many Sandia systems such as neutron tubes and microelectronic devices, and are critical factors constraining the performance of emerging flexible microelectromechanical system (MEMS) and nanoelectromechanical system (NEMS) devices for medicine, biology, and defense. These systems often contain layers of thin polymer, ceramic, and metallic films and stretchable interconnects where differing properties between adjacent films can induce interlaminar normal and shear stresses. As long as the films and especially metal film interconnects remain substrate-bonded, they may deform far beyond their freestanding counterpart. Once debonded, substrate constraint disappears leading to film fracture. Although there is a large body of mechanics solutions describing deformation and fracture of elastic films on elastic substrates, a basic understanding of substrate compliance, time dependence, and film plasticity effects is lacking. Current fracture modeling efforts are based on classical approaches for steady-state crack growth and do not accurately describe fracture in compliant systems where crack initiation, bulk material dissipation, and geometry effects are important. Moreover, traditional fracture test methods are difficult or impossible to apply at the nanometer scale. As a result, the relationship between deformation and fracture of nanoscale films on compliant substrates is undefined. To address this issue, we are conducting research integrating nanomechanical tests and mechanics-based modeling to define the critical relationship between deformation and fracture of nanoscale films on compliant substrates. The approach involves designing model film systems and developing nanoscale experimental characterization techniques to isolate compliance, rate-dependence, and plasticity effects. Results of the experiments are guiding the development of computational inelastic fracture models to relate deformation to fracture processes. The end result will be a unique capability to model and predict performance of compliant substrate devices.

Summary of Accomplishments

Our study of deformation and fracture of thin hard films on compliant substrates is complete. We deposited tungsten films in several thicknesses on commercial and compositionally pure polystyrene and polymethylmethacrylate substrates under compressive stress states with and without adhesion promoting oxide interlayers. Deposition of these films triggered spontaneous buckle formation in all film systems creating extensive networks of small and large telephone cord blisters accompanied by intense local substrate plasticity along the buckle edges. The small buckles formed with relatively large plastic zones and the large buckles formed with relatively small plastic zones. This resulted in two patterns of behavior, one where growth was deformation limited and another where growth was delamination dominated. Indentation modeling was used to define substrate response to applied loads. Elastic and viscoplastic models accurately described indentation behavior leading to film fracture. In the limit of a vanishingly thin film, we recovered the Hertzian contact response. Surprisingly, large displacement response conformed to the dimensional analysis of plate bending indicating that the effects of film bending remained dominant even for the largest displacements examined. A cohesive zone modeling approach was used to describe interfacial cracking associated with buckle formation. For the sake of simplicity, the effective traction-separation relationship was taken to be triangular with a steep loading segment. The key parameters defining this traction-separation relationship were the interfacial strength and the work of separation/unit area of interface (interfacial toughness). Simulations showed that substrate compliance significantly increased fracture energies especially for small buckles over values obtained using the classical rigid elastic approach. The simulations also showed that substrate compliance markedly altered buckle morphology as observed experimentally. Moreover, the simulations provided a lower bound for seemingly disparate sets of small and large buckle data providing a predictive capability for assessing performance and reliability of compliant substrate devices.

Significance

Many Sandia programs are based on compliant substrate systems, from neutron tube films and microelectronic circuits to multilayer films and hard coatings for MEMS devices. Compliant substrates are also the basis for emerging technologies of electrotextiles, flexible displays, and tactile sensor arrays for medicine, biology, and defense. They are also crucial elements in the development of Sandia designed flexible substrate systems for military and homeland defense.

Refereed Communications

L.M. Hale, X.W. Zhou, J.A. Zimmerman, N.R. Moody, R. Ballarini, and W.W. Gerberich, "Molecular Dynamics Simulation of Delamination of an Elastically-Hard, Body-Centered-Cubic Crystalline Film from a Si Substrate," to be published in the *Journal of Applied Physics*.

T.D. Nguyen, J. Yeager, D.F. Bahr, D.P. Adams, and N.R. Moody, "Nanoindentation of Compliant Substrate Systems: Effects of Geometry and Compliance," to be published in the *Journal of Engineering Materials and Technology*.

X.W. Zhou, N.R. Moody, R.E. Jones, J.A. Zimmerman, and E.D. Reedy, "Molecular-Dynamics-Based Cohesive Zone Law for Brittle Interfacial Fracture under Mixed Loading Conditions: Effects of Elastic Constant Mismatch," *Acta Materialia,* vol. 57, pp. 4671-4686, September 2009.

Crossing the Mesoscale No-Man's Land: Massively Parallel Kinetic Monte Carlo

105806
Year 3 of 3
Principal Investigator: S. J. Plimpton

Project Purpose

Materials inherently interact with their environment at the atomic scale, e.g., via mechanical, chemical, or electrical means. However, their response is usually manifest and observed at the continuum scale. Kinetic Monte Carlo (KMC) is a powerful computational tool for spanning these length and time scales. Critical events, such as diffusive hops or reactions, are defined and rate equations can be specified in terms of external fields, such as electric potential or solute concentration, in order to capture the model's relevant physical underpinnings. Efficient KMC algorithms can then select events, one after another, with the correct probabilities and update the state of the system, without the need to follow detailed atomic motion and spend CPU time waiting for events to occur. However the classic KMC algorithm is inherently serial, and thus KMC has often been limited in the size of systems and timescale of phenomena it can model.

The goals of this LDRD project are three-fold:

1. To develop new parallel KMC algorithms that remove this bottleneck for specific kinds of KMC models.
2. To build a flexible code incorporating these algorithms to enable a suite of KMC models to be implemented.
3. To use the new code to model several systems important for materials science applications at Sandia, at a scale that has not previously been possible.

Summary of Accomplishments

The four main accomplishments of our project were as follows:

1. We wrote a new Monte Carlo code called SPPARKS, which is a framework in which new on-lattice and off-lattice applications can be developed. It has algorithms for performing true kinetic Monte Carlo (KMC) and rejection kinetic Monte Carlo (rKMC) and Metropolis Monte Carlo (MMC) in serial and parallel. It was validated against a second KMC code, MESO. The new code is open-source, freely available for download from the SPPARKS WWW site at www.sandia.gov/~sjplimp/spparks.html.
2. We developed and benchmarked a novel constant-time KMC solver in SPPARKS. It compares favorably with the standard logarithmic-time solvers commonly used for KMC simulations, and scales better in the limit of large problem sizes.
3. We implemented an approximate parallel KMC algorithm in SPPARKS, comparing its accuracy and speed to the exact KMC algorithm. The parallel algorithm works inside sectors within each processor's subdomain while holding boundary information static for short times before communicating. We implemented a heuristic that adjusts this time delay to preserve accuracy while enabling good parallel efficiencies.
4. We developed several on-lattice applications in SPPARKS, for abnormal grain growth, diffusion in nanoporous metals, solid-on-solid surface diffusion, defect formation in erbium hydrides, bubble formation in nuclear fuels, the sintering of a nuclear fuel pin, and thin film deposition and growth. Many of these were run at length and time scales not possible without the parallel options available in SPPARKS.

Significance

Sandia has diverse vested interests in KMC applications, e.g., modeling film growth (chemical vapor deposition, self-assembled quantum dots), annealing (grain growth, recrystallization, sintering, precipitation), chemistry (systems of competing reactions), deposition (field ion beam deposition), phonon transport in microsystems, and atomic mechanisms. These applications span Laboratory missions in defense programs (DP), DHS, and energy and infrastructure security.

Refereed Communications

C.C. Battaile, "The Kinetic Monte Carlo Method: Foundation, Implementation, and Application," *Computer Methods in Applied Mechanics and Engineering*, vol. 197, pp. 3386-3398, 2008.

A. Slepoy, A.P. Thompson, and S.J. Plimpton, "A Constant-Time Kinetic Monte Carlo Algorithm for Simulation of Large Biochemical Reaction Networks," *Journal of Chemical Physics*, vol. 128, p. 205101, 2008.

Predictive Modeling of Microenergetics

105808
Year 3 of 3
Principal Investigator: D. A. Jones

Project Purpose

The development of practical microenergetics has been hindered by current models of energetic material (EM) performance that do not capture the phenomenology necessary for extrapolation to the small scales of microenergetics. The successful development of microenergetics requires a greater understanding of the fundamental processes of EM ignition and reactive wave growth at the mesoscale. This project integrates the disciplines of EM research, shock physics modeling, and microsystems engineering to develop a microenergetic test bed specifically designed to collect experimental data at the small scale necessary to improve our understanding of EM processes at the mesoscale. Important elements of the microenergetic test bed include a microenergetic device, an initiation source, and a new, high-resolution, microelectromechanical system (MEMS)-based pressure transducer array detector (PTAD). The microenergetic device consists of a pentaerythritol tetranitrate (PETN)-filled microchannel measuring 0.5×1×5 mm. Advancements in our thermal vapor deposition process have allowed us to tailor the microstructure of the PETN films to produce functional microenergetic devices. Characterization of these devices by the application of focused ion beam (FIB) nanotomography has provided us an unprecedented view of the three-dimensional microstructure of EMs. Incorporation of these microstructures into shock physics simulations has advanced the state of the art in mesoscale predictive capability. A custom-built explosive-driven flyer has been constructed for initiation of the microenergetic device. The variable intensity of the initiation source in conjunction with our capability to tailor the microstructure of the microenergetic device have allowed us to create a test bed with a protracted shock to detonation transition (SDT), ideal for the study of mesoscale phenomena leading up to detonation. The PTAD, designed to measure pressure (a key state variable) during transition to detonation with unprecedented spatial (50 µm) and temporal resolution (~1 ns), has been designed, fabricated, partially characterized, and demonstrated in test bed experiments.

Summary of Accomplishments

Pentaerythritol tetranitrate (PETN) films were deposited into 1 mm × 8 mm × 0.5 mm microchannels using a physical vapor deposition technique. We demonstrated that the surface morphology and density of these films can be controlled by varying the deposition conditions and may be tuned to optimize the properties of the resultant films. Surface and pore morphology were measured using scanning electron microscopy (SEM) and focused ion beam (FIB) nanotomography, provided a realistic three-dimensional description of the PETN microstructure that was imported into the shock physics code, CTH. CTH mesoscale simulations of shocked three-dimensional microstructures have been demonstrated. This work has advanced the state of the art in materials characterization and mesoscale predictive capability.

The development of an explosively driven flyer initiation system for test bed studies on the shock initiation of deposited explosives has been demonstrated. Initiation of PETN within 2 mm of the flyer impact location has been demonstrated and a consistent method for delayed shock initiation of deposited PETN has been proven. The protracted initiation process demonstrated in this test bed may allow detailed understanding of shock initiation processes in explosives that cannot be studied otherwise due to short SDT distances. Computational models with CTH show flyer morphology issues during launch that agree with framing camera data from experiments.

We have designed, fabricated and tested ultrahigh pressure (GPa) high temporal resolution (ns) pressure transducer array detector (PTAD) in a novel complementary metal oxide semiconductor (CMOS+) MEMS process for characterization of energetic materials. Characterization experiments have been performed which illustrate that the PTAD does respond to high pressure (GPa) loading, although further experiments are needed to fully characterize the useable pressure range and the transfer functions of the PTAD devices necessary for pressure calibration. Test bed experiments show that the PTAD, in its current form, is suitable for high-resolution time-of-arrival applications.

Significance

This work supports Sandia's primary mission to ensure that the US nuclear arsenal is safe, secure, and reliable. Incorporating microenergetic components fabricated by microelectronic methods into weapon systems has the potential to significantly improve their reliability, surety, and safety. This work has significantly improved microenergetic device performance, our mesoscale analytical capabilities for energetic materials (EM), our mesoscale modeling capabilities for EM, and understanding of EM behavior at the mesoscale.

Building More Powerful Less Expensive Supercomputers Using Processing-In-Memory (PIM)

105809
Year 3 of 3
Principal Investigator: R. C. Murphy

Project Purpose

Latency dominates all levels of supercomputer design. Within a node, increasing memory latency, relative to processor cycle time, limits CPU performance. Between nodes, the same increase in relative latency impacts scalability. Processing-in-memory (PIM) is an architecture that directly addresses this problem using enhanced chip fabrication technology and machine organization. PIMs combine high-speed logic and dense, low-latency, high-bandwidth dynamic random access memory (DRAM), reducing local memory access latency. Additionally, PIMs support lightweight threads that tolerate latency by performing useful work during memory transactions. This work examines the potential of PIM-based architectures to support mission critical Sandia applications and an emerging class of more data intensive informatics applications. Results have demonstrated a potential increase in concurrency of two or more orders of magnitude, which a conventional architecture could not support. They have further shown that a PIM-based architecture is significantly improved over Cray MTA-based architectures for informatics applications. This work examines the PIM CPU architecture in the context of two system architectures, by simulating two trans-petaflop scale supercomputer architectures: a PIM-enhanced Red Storm, where PIMs serve as part of the machine's memory system; and an all PIM supercomputer. We are simultaneously developing key compiler algorithms to exploit these architectures. This project will discover a new generation of supercomputers with increased scalability. We do so while retaining the investment in message passing interface (MPI) software, and enabling alternative programming models.

Summary of Accomplishments

We have developed a 3D stacked PIM straw man called X-caliber that combines a multithreaded processor, DRAM, and a silicon photonic network. Using the straw man, we simulated microapplications from the Mantevo LDRD (project 105815), as well as core graph kernels. We have expanded the qthreads application programming interface (API) for multithreaded application development, and used baseline results to test against existing multicore and multithreaded architectures. We are working with Micron on the development of advanced memory technologies.

Significance

This project explores a new computer architecture that directly addresses the problem of high memory latencies experienced by today's supercomputers. For current applications, this will provide levels of computing performance that enhance Sandia's verification and validation ability, confidence level determination, and uncertainty quantification. In addition, the same technology will enable new applications in informatics based on graph theory of critical importance to national security.

Reduced Order Modeling of Fluid-Structure Interaction

105810
Year 3 of 3
Principal Investigator: M. F. Barone

Project Purpose

Reduced order models (ROMs) are numerical models derived from high-fidelity, high-cost numerical simulations that describe the important outputs of the high-fidelity simulations but at a much lower cost. We propose to develop new methods for constructing ROMs for compressible fluid flow interacting with flexible structures. Such models would be applicable to a broad range of engineering applications, including aero-elastic analysis of vehicle control surfaces, aircraft wings, wind turbine blades, and microdevices. The ROM approach begins with collection of data "snapshots" from unsteady fluid/structure simulations at a representative flow condition. From these snapshots, global fluid dynamic modes containing most of the flow energy are constructed using the proper orthogonal decomposition (POD) technique. The governing equations are then Galerkin-projected onto these modes to obtain the fluid ROM, which can then be coupled to a corresponding structural ROM. The number of retained degrees of freedom in the ROM is much smaller than the size of the full simulation used to build the ROM. The major technical challenges include treatment of the fluid/structure interface in the ROM, handling nonlinearities in the fluid dynamics, modeling the effect of neglected low-energy modes, and achieving sufficient robustness and numerical stability of the ROM for use as a predictive tool. Supposing that the ROM can be made accurate and robust for a range of system input parameters of interest, this technology can truly enable predictive simulation by dramatically decreasing the associated computational cost. The ROMs may be used for analysis, shape design, control system design, or fatigue analysis — essentially for any application that requires many solutions over a parameter space. This research is well-suited for LDRD funding, since routine application of ROMs in analysis of engineering systems will require breakthroughs that can only come from a sustained fundamental research effort.

Summary of Accomplishments

We formulated a new reduced-order modeling technique for linearized, compressible flow that addresses major shortcomings of standard techniques. In particular, the new technique is numerically stable and convergent to the exact solution. We implemented this method in a computer code and demonstrated numerical stability and accuracy on several model problems. We then extended this formulation to enable coupling of a fluid ROM to a structural dynamics model, through specification of boundary conditions at the coupling interface that preserve numerical stability. This formulation was used to successfully predict flutter instability of an elastic plate with adjacent supersonic flow. We extended the approach for constructing numerically stable ROMs to nonlinear, viscous fluid flow governed by the compressible Navier-Stokes equations. We employed a symmetrization of the governing equations, along with a "best-points" interpolation technique for handling the nonlinear terms, to propose a novel technique for constructing ROMs that satisfy the second law of thermodynamics. This technique was successfully tested on a one-dimensional convection-diffusion-reaction system of equations.

We also developed a new technique for constructing ROMs of thin, elastic structures with nonlinear in-plane stresses. This technique, based on the method of quadratic components, enabled efficient simulation of nonlinear elastic plate motion that was demonstrated on a model problem and compared favorably to full finite element solutions. We showed how oscillatory limit cycle solutions can be accurately and efficiently calculated directly using this ROM technique.

Significance

This work laid the foundations for a fluid/structure analysis capability, based on reduced-order modeling, that is reliable and accurate. The methods developed have the potential to greatly reduce computational times for analysis of engineering systems of interest. These include modeling of the vibrations of flight vehicles due to fluctuating aerodynamic pressure loading, which is of interest to both the Nuclear Weapons and Defense System and Assessments strategic management units. Another laboratory application that could be impacted is aeroelastic analysis of wind turbines, an important problem for energy security. Reduced-order models provide a possible mechanism for incorporating complex numerical and physical models, such as those contained in computational fluid dynamics models, into computationally affordable engineering predictions of wind turbine dynamics. The methods developed are broadly applicable to many applications within the general S&T community, including any that involve modeling of compressible fluid dynamics, dynamics of thin structures, or the coupling between fluid and structural systems. This work also opens up the possibility of enabling uncertainty analysis with high-fidelity computational tools, using the reduced-order models as affordable surrogates for the more expensive simulations.

Refereed Communications

M.F. Barone, I. Kalashnikova, D. Segalman, and H.K. Thornquist, "Stable Galerkin Reduced Order Models for Linearized Compressible Flow," *Journal of Computational Physics*, vol. 228, pp. 1932-1946, April 2009.

Highly Scalable Linear Solvers for Large Science Simulations on Thousands of Processors

105812
Year 3 of 3
Principal Investigator: J. J. Hu

Project Purpose

This project will investigate and develop a class of novel algebraic multigrid (AMG) algorithms that scale well to tens of thousands of processors. Within many large-scale scientific calculations, it is the solution of linear systems that is the most time-consuming bottleneck and the most challenging obstacle to scalability. This is particularly true with massively parallel multiphysics simulations at Sandia, where the linear systems are very large, but the work per processor is low. Simulations on massively parallel (MP) computing platforms such as Red Storm and BlueGene/L are already taxing current solver technology. For example, recent high-profile MP Z-pinch calculations have revealed the limits of Sandia's current solver capabilities. The algorithms developed in this project will enable predictive simulation and uncertainty quantification on current MP platforms, and position Sandia for future simulations on petascale architectures.

The new algorithms developed in this project will differ significantly from traditional multigrid algorithms in the way that coarse models are processed. Loss of scalability within traditional parallel multigrid algorithms is due to a poor communication to computation ratio (CCR) for coarse resolution processing. This means that during coarse computations the machine is significantly underutilized. The key feature of the new multigrid methods will be significantly more-efficient processing of the coarse resolution problems. This project features two different research strategies that may be combined into a hybrid method. The first, higher risk approach centers on processing coarse resolution meshes in parallel with fine resolution meshes. The second approach focuses on reducing the number of coarse resolution meshes while also improving the CCR on coarse meshes. In both cases, the key to success relies on maintaining optimal numerical convergence properties for the redesigned multigrid cycle.

Summary of Accomplishments

- We established a baseline problem suite to measure weak-scaling (fixed size per processor) and strong-scaling (fixed global size) properties of existing AMG methods in Sandia's multigrid software library, ML. Investigation of AMG weak-scaling behavior for different idealized magnetics simulations led to an unanticipated discovery of algorithmic kernel scaling impediments and a doubling of existing AMG algorithm efficiency at 5832 processors.
- We developed a new fundamental domain decomposition/multigrid capability. Each processor performs an independent multigrid cycle on its subdomain. Key is that subdomain multigrid cycles require no communication. This inner multigrid subdomain solver is a smoother for an outer multigrid solver that requires communication. The key difference is that the outer multigrid method requires many fewer levels (and hence many fewer communication synchronization steps) than standard methods.
- We implemented and profiled a variable block matrix-matrix multiply (MMM) within ML. The dominant cost in AMG setup is forming coarse grid matrices, which requires two MMMs. Profiling showed a core block MMM speedup of 4.5 and overall speedup as high as 2.3×.
- We compared alternative coarsening and smoothing choices to standard multigrid in our scalability benchmark simulations on Red Storm. In Fuego simulations, multigrid improvements yielded a 4×–10× speedup.

- We incorporated Zoltan's hypergraph partitioning scheme into the AMG setup phase and performed scaling tests up to 5800 Red Storm cores. Hypergraph partitioning is intended to address shortcomings in current AMG data distribution.
- We implemented an AMG version of communication-reducing geometric multigrid and analyzed it in context of classic domain decomposition. We found that in some cases it reduces to a traditional two-level additive Schwarz method.
- For multicore architectures we developed an AMG algorithm with internode and intranode communication layers. We tested it on two different architectures. The new algorithm was competitive with existing solvers and in some cases is 10–15% faster.

Significance

The DOE has put considerable effort into developing a petascale computing platform to support simulations in defense, energy, science, and the environment. This project explores scalable algebraic multigrid solution methods that enable future large-scale science calculations in these areas to run effectively and efficiently on next-generation petascale computers. In particular, it is now standard for advanced architectures to have many-core nodes. Solvers such as those developed in this project are necessary to address scaling needs on these architectures.

Massive Multithreading Applied to National Infrastructure and Informatics

105813
Year 3 of 3
Principal Investigator: J. W. Berry

Project Purpose

Large relational datasets such as national-scale social networks and power grids present different computational challenges than do physical simulations. Sandia's distributed-memory supercomputers are well suited for solving problems concerning the latter, but not the former. The reason is that problems such as pattern recognition and knowledge discovery on large networks are dominated by memory latency and not by computation. Furthermore, most memory requests in these applications are very small, and when the datasets are large, most requests miss the cache. The result is extremely low utilization.

We are unlikely to be able to grow out of this problem with conventional architectures. As the power density of microprocessors has approached that of a nuclear reactor in the past two years, we have seen a leveling of Moore's Law. Building larger and larger microprocessor-based supercomputers is not a solution for informatics and network infrastructure problems since the additional processors are utilized to only a tiny fraction of their capacity.

An alternative solution is to use the paradigm of massive multithreading with a large shared memory. There is only one instance of this paradigm today: the Cray MTA-2. Our team has unique experience with and access to this machine. The XMT machine, which is now being delivered, is a Red Storm machine with up to 8192 multithreaded processors and 128 TB of shared memory ("Thread Storm"). For many years, the XMT will be the only way to address very large graph problems efficiently, and future generations of supercomputers will include multithreaded processors. Roughly 10 MTA processors can process a simple short paths problem in the time taken by the Gordon Bell Prize-nominated distributed memory code on 32,000 processors of Blue Gene/Light.

We are developing algorithms for the XMT, and archiving them in an open-source software framework.

Summary of Accomplishments

We have discovered new network community detection algorithms that have greater accuracy than any other published methods when applied to public benchmark instances. These methods depend on computational kernels that can be efficiently computed on massively multithreaded architectures.

We have designed the multithreaded graph library (MTGL), a software framework that supports graph algorithm on various multithreaded platforms. These include the Cray XMT and the Sun Niagara, as well as Intel multicore processors.

We have verified a 2005 conjecture that roughly 10 Cray MTA processors can compute a simple short paths problem in about the same time as 32,000 processors of Blue Gene/Light did in 2005. Such problems are characterized by a small amount of computation, nearly random memory access, and a giant dataset. We did our computations on a 512 processor Cray XMT.

We have designed and demonstrated multithreaded versions of maximum flow problems that enabled the Cray MTA-2 to compute solutions to problems of size roughly 30× larger than those solvable on serial workstations. These implementations do not perform as well on the Cray XMT, and the reasons bear further exploration.

We have begun to analyze a multithreaded algorithm for finding triangles (3-cyles) in a class of power-law graphs. The analysis is statistical, and we have collaborated with professors in the Statistics Department of Iowa State University for this work.

We have presented several talks, including a keynote, at the Institute of Electrical and Electronics Engineers' (IEEE's) "Multithreaded Architectures and Applications" (MTAAP) workshop, establishing Sandia as one of the technical leaders in this area.

Our work has resulted in workshop, conference, and journal publications.

More intangibly, we have learned much about the massively multithreading paradigm. We have remained engaged with Cray as they improve their compiler and runtime system, sometimes as a result of our observations.

Significance

Informatics and high performance computing is a growth area for Sandia. For example, informatics is relevant to cybersecurity, a DOE focus. Sandia has always been a leader in high performance computing for scientific computing (HPC). However, informatics applications place different demands on HPC. There is evidence that traditional platforms will not meet informatics needs efficiently. In this project we explore algorithms and software for the multithreaded Cray XMT.

Practical Reliability and Uncertainty Quantification for Complex Hierarchical Systems

105814
Year 3 of 3
Principal Investigator: P. T. Boggs

Project Purpose

Estimating reliability in complex systems of interconnected components is of great importance. Equally important is calculating the uncertainty of the reliability estimate, particularly in systems where it is impractical or impossible to perform sufficient classical tests to ensure a specified confidence. A key application at Sandia lies in the nuclear weapons testing program, where there is significant pressure to reduce the costs of testing while maintaining the integrity of the stockpile.

We will develop novel mathematical strategies — in particular, structured probabilistic models — for the testing of these systems, rigorously assessing the impact of subsystem- and component-level tests on the overall reliability and its associated confidence. We will also consider the problem of predicting future reliability given time-dependent data. The Bayesian approach of Martz-Waller will be extended to time-dependent systems and to testing regimens where continuous data, e.g., voltage, is collected in addition to simpler "pass-fail" tests. We will also extend this approach to more general Bayesian networks in which certain components may exist in or directly affect multiple systems. Exact or approximate inference algorithms will allow probability distributions characterizing reliability to be updated through and across systems. This is crucial for estimating the uncertainty in the overall system reliability. This construction will, for the first time, enable the formulation of optimization questions concerning the best testing strategies and the relative importance of each individual test on the overall reliability and uncertainty estimates.

Summary of Accomplishments

We accomplished all the major milestones for the third year of this project and made substantial progress on some interesting new directions. The major accomplishments are summarized as follows.

1. First, the underlying mathematical foundations and models have been known, but not well articulated in a single place. In addition, there has been some confusion about certain aspects of the theory. We wrote a detailed SAND report, laying out the details of the theory and the mathematical tools that form the basis for our analyses.
2. Second, we continued the development of the steady-state case, improving the efficiency in the likelihood calculations and developing further techniques for general density estimation and for using "reversible-jump" strategies to predict the order based on test data. These also served as the basis for the much of the work in the time-dependent case.
3. Third, we continued the development, implementation, and testing of the time-dependent case. We formulated an appropriate general model for the underlying stochastic process and considered an initial specific model that captured general time-dependent aspects in a computationally reasonable setting. We extended the steady-state computational procedures, as necessary, to adapt them to the time-dependent case and showed how to do certain computations in parallel to dramatically speed up the calculations.

4. Finally, we did extensive work to formulate the problem of optimal testing strategies. We used Bayesian decision analysis as the fundamental approach and we developed a formalism to choose the best location to test to minimize the Bayesian risk of making a wrong decision. This would require a computationally unreasonable amount of work, so we made appropriate approximations in creating an algorithm.

A separate SAND report is being written on each of the above four topics.

Significance

The project is relevant to the national security mission of DOE in its role to ensure the reliability of the nuclear weapons stockpile. It addresses questions of estimating the reliability of complex, hierarchical systems, such as nuclear weapons, but includes many other complex systems in the DOD and elsewhere. It further addresses the critical question of estimation of the uncertainty, or confidence, in the reliability estimate. The approach is potentially applicable to energy systems.

HPC Application Performance Analysis and Prediction

105815
Year 3 of 3
Principal Investigator: M. A. Heroux

Project Purpose

We propose research and development to accurately model, predict, and improve the performance of Sandia applications on current and future high performance computing (HPC) systems. We will develop tools and analysis techniques that go beyond benchmarking and similar approaches. Specifically, we will focus on four research activities: 1. performance bases that represent the complex performance behavior of key computations on large-scale high performance computers; 2. microapplications and microdrivers that can be used as application proxies on current and proposed architectures; 3. analytic performance models that also use performance bases as part of a numerical model of application performance; and 4. parameterized component models that support study of performance bases using hardware simulators and detailed performance analysis tools.

We will focus our efforts on the Sandia applications found in SIERRA, NEVADA, Salinas, LAMMPS and Xyce, paying special attention to complex computations such as parallel contact detection and distributed unstructured sparse matrix operations, which are both important for optimal performance and challenging to implement well on large-scale parallel machines. We intend to complement and leverage existing efforts, and participate in forums to share our research results with Sandia application developers, for the purposes of informing them of any ideas that may improve their application design and implementation.

Summary of Accomplishments

We have developed a collection of miniapplications that mimic the performance of our key computational science and engineering applications and established the Mantevo Project, an ongoing effort in application performance analysis and prediction.

Initially we studied the performance profiles of key applications in fluid dynamics, structural mechanics and molecular dynamics and identified the most important performance-impacting kernels. Next we developed standalone programs (miniapplications) written in portable C++ that express these important kernels. We then used the miniapplications in collaboration with colleagues who are studying new computer architectures, programming languages and system software designs.

We used the miniapplications to provide insight into design choices, and as prototypes for new application development using new programming models. We performed memory architecture studies to determine how to best utilize multicore memory systems. We rewrote the miniapplications using different parallel programming models and prototyped new software designs that we then used to start redesigning our existing application base.

Significance

A major part of this project was developing a multifaceted team of people who are interested in application performance and starting regular interactions. This team emerged as the Mantevo project, an effort that will continue. We used the results of this project as the foundation for proposals that received funding in FY 2009 for architecture-aware algorithms development and received, in FY 2010, a three-year DOE award for the Extreme-scale Algorithms and Software Institute.

The importance of understanding and improving HPC application performance on HPC systems, and designing and implementing effective future HPC applications and systems cannot be overstated. In the coming years we are challenged to make qualitative advances in predictive simulation. We must be prepared to make key decisions regarding the performance and programmability of future architectures. If successful, our efforts will directly impact our abilities to make informed HPC decisions.

Refereed Communications

M.A. Heroux, "Design Issues for Numerical Libraries on Scalable Multicore," *Journal of Physics Conference Series*, vol. 125, p. 12035, July 2008.

M.A. Heroux, "Software Challenges for Extreme Scale Computing," to be published in the *International Journal of High Performance Computing Applications*.

M.A. Heroux and R.W. Numrich, "A Performance Model with a Fixed Point for a Molecular Dynamics Kernel," in proceedings of the ISC 09 Conference, June 2009.

Model Reduction of Large Dynamic Systems with Localized Nonlinearities

105816
Year 3 of 3
Principal Investigator: D. J. Segalman

Project Purpose

The key nonlinearities in structural dynamics are the load-dependent stiffnesses and energy dissipation associated with mechanical joints. Realistic models for joints now exist and incorporating them in structural dynamics codes yields realistic predictions, but the required computational resources can be prohibitive. The intrinsic difficulties are solving large nonlinear systems of equations with extremely small time steps necessitated by high-frequency responses evoked by slip in the joints.

We propose to develop and combine two new but complementary model reduction strategies to accelerate simulation by one-to-two orders of magnitude and to allow analyses that are not currently feasible. If successful, this new approach could be applied to other nonlinear dynamic systems.

The first strategy is to employ a Galerkin procedure using eigenmodes of a reference linear system augmented by additional basis functions containing appropriate discontinuities in the locations of nonlinearity. This novel approach is motivated by an improved understanding of the source of difficulty in model reduction of systems with localized nonlinearity. It reduces the size of the problem and suppresses extraneous high-frequency resonances, permitting the use of longer time steps. The second strategy is to accelerate component mode synthesis in a massively parallel environment. Component mode synthesis (CMS) decomposes a structure then synthesizes the substructures resolving system dynamics. A new insight is the potential use of various weak formulations to enforce interface conditions thereby dramatically reducing the order of the system and substantially reducing run times. The global response of the system will be retained while possibly sacrificing detailed response at the mechanical interfaces. Also dissimilar meshes can be connected.

These two approaches have not yet been explored in finite element analysis; both their potential benefit and their difficulty of application cannot be fully assessed until implementation is attempted. These methodologies will be fully validated by experiment.

Summary of Accomplishments

A strategy for assembling structures of linearly elastic finite elements that does not cause the proliferation of many small elements where such small elements are not called for on any mathematical or mechanical basis was developed and a mathematical exploration of the preserved accuracy was derived. Perhaps most importantly, this work will greatly facilitate the rapid generation of high-fidelity meshes of complex structures.

A method for extending the method of component mode synthesis (CMS) so that it can be used in a scalable manner to for very fine substructuring of components was brought into mathematical coherence in FY 2009. This technique enables the modeling of very large structures with greater resolution than has been possible previously.

A model reduction method accommodating sharp nonlinearities that both decreases the number of degrees of freedom of the problem, and facilitates much larger time steps than and possible in the base formulation has been developed over the life of this project. Two important developments during FY 2009 have been development of a mathematical statement of system accuracy and the demonstration extraordinary computational speed up on a very large problem.

Significance

Sandia is charged with predicting system level response of weapons and assessing the mechanical loads seen by critical components. To calculate responses out to 50–100 millisecond ranges, accounting for system variabilities, orders of magnitude simulation speed-up of very large finite element models must be obtained. The model reduction explored in this project resulted in the following enabling tools:

- A method of configuring constraints to attach very large, rapidly generated meshes and without loss of accuracy.
- A mathematical strategy for using component mode synthesis (CMS) to reduce the number of degrees of freedom of very large problems, and to do so in a scalable manner.
- Process for reducing yet further the number of degrees of freedom of problems of localized nonlinearity — such as mechanical systems assembled by bolted interfaces and other friction connections. This approach makes possible many simulations necessary to make meaningful statistical statements about the dynamics of weapons systems.

Leveraging Multiway Linkages on Heterogeneous Data

117782
Year 2 of 3
Principal Investigator: T. G. Kolda

Project Purpose

This project's focus is on investigating and developing novel data analysis methods for heterogeneous data because recent experiences with Sandia intelligence analysts have revealed an emerging need to research analytic capabilities for large-scale, complex data. The goal is to be able to combine heterogeneous entities and multiple linkages (i.e., relationships) between them. We are developing a new class of algorithms, emphasizing scalability and robustness, for multiway linkage dimensionality reduction that maps heterogeneous entities into a shared conceptual space. We measure the quality of the mapping according to how well the relationships maintained in the lower-dimensional conceptual space with respect to various problem-dependent quality measures. We are also tackling statistical problems related to combining heterogeneous data. Of important application interest, mapping heterogeneous entities to a shared conceptual space is fundamental to solving a variety of data analysis problems, including entity resolution and disambiguation, link prediction, and anomaly discovery.

Sandia is uniquely positioned to address these challenges because of our expertise in data and graph analysis, matrix and tensor methods, and high performance computing. Our overarching goal is to develop robust and scalable methods for analyzing multiway links on heterogeneous, inaccurate, and incomplete data from real-world applications. Although multiway linkage analysis is of interest to us specifically because of its importance in the intelligence community, there are also applications of this work to social network, bibliometric, critical infrastructure, and complex biological systems analysis.

Summary of Accomplishments

In the past year of this project, we have successfully completed the following milestones: developed algorithms for latent analysis on 3-partite graphs and for multiway graphs, developed algorithms for latent analysis on multiway graphs with one temporal relationship, and extended newly developed methods to temporal link prediction. Our work has resulted in the development of all-at-once optimization methods for tensor decompositions, nonnegative matrix factorization, and the multiway factorizations of direct interest to this project. We have developed MATLAB code for these methods, including a general purpose optimization toolbox called Poblano. We have also developed novel methods for link prediction. We have had only limited success in our goal to discover statistics-based, information theoretic weightings for links, matrices, and tensors, deciding that this problem could not be solved in general.

In this past year, we have written two journal papers (one in print, one to appear in the fall), one journal submission, one refereed conference paper that won the best paper prize, a conference submission, a technical report, two international workshop invited talks plus four domestic invited workshop talks, four minisymposium presentations, and three seminars at leading universities.

Significance

The proposal ties to Sandia's national security mission. Our goals of entity resolution/disambiguation, link prediction, and anomaly detection relate to problems of national security interest because they address data fusion across disparate data sources. Our aims are consistent with Sandia's and DOE's long history of support for the intelligence agencies. Other applications include social network, critical infrastructure, and complex biological system analyses.

Refereed Communications

E. Acar and B. Yener, "Unsupervised Multiway Data Analysis: A Literature Survey," *IEEE Transactions on Knowledge and Data Engineering*, vol. 21, pp. 6-20, January 2009.

T.G. Kolda and B.W. Bader, "Tensor Decompositions and Applications," *SIAM Review*, vol. 51, pp. 455-500, September 2009.

Peridynamics as a Rigorous Coarse-Graining of Atomistics for Multiscale Materials Design

117783
Year 2 of 3
Principal Investigator: R. B. Lehoucq

Project Purpose

The goal of our project is to develop a coarse-graining of finite temperature molecular dynamics (MD) that successfully transitions from statistical mechanics to continuum mechanics. Our coarse-graining overcomes the intrinsic limitation of coupling atomistics with classical continuum mechanics via the FEM (finite element method), SPH (smoothed particle hydrodynamics), or MPM (material point method); namely, that classical continuum mechanics assumes a local force interaction that is incompatible with the nonlocal force model of atomistic methods. Therefore FEM, SPH, and MPM inherit this limitation. This seemingly innocuous dichotomy has far reaching consequences; for example, classical continuum mechanics cannot resolve the short wavelength behavior associated with atomistics. Other consequences include spurious forces, invalid phonon dispersion relationships, and irreconcilable descriptions/treatments of temperature.

We propose a statistically based coarse-graining of atomistics via peridynamics and so develop a first of a kind mesoscopic capability to enable consistent, thermodynamically sound, atomistic-to-continuum (AtC) multiscale material simulation. Peridynamics (PD) is a microcontinuum theory that assumes nonlocal forces for describing long-range material interaction. The force interactions occurring at finite distances are naturally accounted for in PD. Moreover, PD's nonlocal force model is entirely consistent with those used by atomistics methods, in stark contrast to classical continuum mechanics. Hence, PD can be employed for mesoscopic phenomena that are beyond the realms of classical continuum mechanics and atomistic simulations, e.g., molecular dynamics and density functional theory (DFT). The latter two atomistic techniques are handicapped by the onerous length and time scales associated with simulating mesoscopic materials. Simulating such mesoscopic materials is likely to require, and greatly benefit from multiscale simulations coupling DFT, MD, PD, and explicit transient dynamic finite element methods FEM (e.g., Presto). The proposed work fills the gap needed to enable multiscale materials simulations.

Summary of Accomplishments

The project goal of establishing the theoretical groundwork for coarse-graining MD into peridynamics was accomplished during the second year of the funding. This project accomplishment is documented in three related approaches and in three Sandia technical reports. The first approach derives the peridynamic balance of linear momentum from the principles of statistical mechanics. The second approach upscales molecular dynamics into a high order gradient theory, and exploits a relationship between peridynamics and a high order gradient theory. The third approach represents an interatomic multibody potential as a peridynamic material, and then smoothes the resulting heterogeneous peridynamic material model. In recognition of these accomplishments, the project team received a Sandia employee recognition award.

The three coarse-graining approaches described above are synergistic. The first approach, though of significant theoretical value, does not immediately lead to an expedient computational scheme. An important conclusion is that the path from classical statistical to classical continuum mechanics traverses the nonlocal continuum theory of peridynamics. A consequence is that peridynamics can augment, or replace, MD, and AtC coupling can be replaced by PtC coupling (peridynamics to classical continuum mechanics). The second approach is a practical application justifying the contention of the first approach that molecular dynamics can be coarse-grained into peridynamics. In contrast to classical continuum mechanics, peridynamics does capture the short-wavelength behavior associated with molecular dynamics without the need to assume the existence of higher-order derivatives associated with a high-order gradient theory. The third approach represents a sophisticated scheme for generating peridynamic material models by coarse-graining multibody interatomic potentials at the continuum level. The third approach represents a sophisticated scheme for generating peridynamic material models by coarse-graining multibody interatomic potentials at the continuum level.

Significance

Sandia/NNSA has a strong interest in science-based stockpile stewardship, developing nano- and microscale devices, and designer materials for renewable energy production and storage. These three applications can significantly benefit from multiscale materials simulations at the mesoscopic level, which incorporate first principles techniques at the atomistic regime. This project will provide the research and tools to address this critical regime between the atomic and the continuum levels.

Predicting Fracture in Brittle Microscale Structures

117784
Year 2 of 3
Principal Investigator: E. D. Reedy Jr.

Project Purpose

Our goal is to develop a validated failure methodology that can be applied to micron-scale structures made from brittle materials like polycrystalline silicon. The development of such a methodology is especially needed for micron-scale structures that are subjected to high loads (e.g., a chevron thermal actuator, bistable mechanism, etc.). This will require a detailed understanding of how the failure probability for brittle, micron-scale structures depends on flaw distributions, flaw geometry, material microstructure, and regions of intense stress gradients. One source of difficulty in developing such a failure analysis is a consequence of the fact that critical flaw size, grain size, and the region dominated by high stress gradients can all be on the same 100-nm length scale. Note that traditional Weibull statistics-based probabilistic failure modeling approaches are not applicable when flaws and microstructure are not small compared to characteristic specimen dimensions, and when crack-like flaws are present.

In this project, we seek to understand how flaws and microstructure generate probabilistic strength distributions and how regions of high stress gradients affect such distributions. We are performing finite element analyses to determine the effect of crystal properties, flaw geometry, flaw interactions, stress gradients, etc. on fracture mechanics predictions of specimen strength. We are also performing novel microscale tests to elucidate the various factors that generate probabilistic strength distributions. One primary goal is to develop novel on-chip and off-chip testing techniques that will allow us to test on the order of one-thousand nominally identical micron-scale tensile bars so as to define strength distribution tails. These techniques will be used to measure strength distributions of samples with and without stress concentrations (notches). Together, the computational and experimental results will direct the development of a methodology for predicting fracture of brittle micron-scale structures that does not explicitly model its microstructure and edge roughness.

Summary of Accomplishments

An externally actuated sequential tensile test method that enables the rapid collection of very large datasets has been developed and demonstrated. Over 1000 nominally identical tensile bars, which were fabricated using SUMMiT V™ (Sandia ultraplanar multilevel MEMS technology V), were tested in a matter of ~20 hours. The resulting dataset suggests that the three-parameter Weibull model captures the low-strength tail of the strength distribution better than the commonly assumed two-parameter Weibull distribution. We have also successfully demonstrated an on-chip tensile tester that was fabricated using SUMMiT V technology. This device uses a thermal actuator that grips a tensile bar upon heating and pulls on the bar when cooled. This novel tester generates the very large force (~30 mN) needed to fracture polysilicon. Initial measured strength data is in reasonable agreement with that measured with the off-chip tester. The use of two quite different test devices to measure strength distributions allows us to assess the sensitivity of measured strengths to test method.

We have also performed finite element calculations that used a cohesive modeling approach to determine how notch geometry affects the tensile strength of a bar with an edge notch. The edge flaw was parameterized as a generalized ellipsoid and both notch angle and depth were varied. This parameterization is capable of modeling cusp-like cracks, sharp V-notches, and blunted notches. Calculated strengths for cusp-like and sharp V-notches are similar to that predicted by linear elastic fracture mechanics for an edge crack, but differ for the case of a blunted notch.

Finally, we have developed an initial approach for estimating the distribution of controlling edge flaws. This approach uses the polysilicon strength dataset generated by our externally actuated sequential tensile test method; a data set that contains enough points to define extreme values.

Significance

High-performance micron-scale structures will be used in high-risk national security applications only if their structural integrity can be guaranteed. This is particularly true of micron-scale structures made of brittle materials. A validated computational methodology for predicting fracture of brittle micron-scale structures can provide the confidence needed to enable their use in challenging applications. It can also aid in the design effort and guide processing improvements.

Refereed Communications

S.S. Hazra, M.S. Baker, J.L. Beuth, and M.P. de Boer, "Demonstration of an In Situ On-Chip Tensile Tester," *Journal of Micromechanics and Microengineering*, vol. 19, p. 082001:1-5, 2009.

D.H. Alsem, B.L. Boyce, E.A. Stach, and R.O. Ritchie, "Effect of Post-Release Sidewall Morphology on the Fracture and Fatigue Properties of Polycrystalline Silicon Structural Films," *Sensors and Actuators A*, vol. 147, pp. 553-560, October 2008.

B.L. Boyce, R. Balarini, and I. Chasiotis, "An Argument for Proof Testing Brittle Microsytems in High-Reliability Applications," *Journal of Micromechanics and Microengineering*, vol. 18, p. 117001:1-4, November 2008.

B.L. Boyce, "A Sequential Tensile Method for Rapid Characterization of Extreme-Value Behavior in Microfabricated Materials," to be published in *Experimental Mechanics*.

A Lightweight Operating System for Multicore Capability Class Supercomputers

117785
Year 2 of 3
Principal Investigator: K. Pedretti

Project Purpose

Sandia has a long history of fielding capability supercomputers that are among the largest and most scalable in the world. One of the primary reasons for this success has been an in-house developed lightweight kernel (LWK) operating system (OS) that embodies all of Sandia's experience in designing scalable systems. This project will perform the system software research and development necessary to extend this leadership to multicore processors. Industry is focused on lower-end capacity machines and lacks sufficient commercial motivation to develop LWK OS technology for multicore; however, our experience shows that this is an essential ingredient for successful capability supercomputers.

This project will investigate the complex memory hierarchies, advanced on-chip synchronization methods, enhanced hardware virtualization technology, and new programming models that are accompanying multicore processors. To compensate for the expected significant drop in bytes-to-flop ratio, this project will seek out and invent new techniques for reducing per-core memory bandwidth requirements. The insight gained by exploring these topics will be incorporated into the LWK OS system that is developed.

In order to make LWK OS technology more accessible, the software developed by this project will be open-source and publicly available. The proprietary nature of existing LWK OS solutions, their lack of hardware support, and the inaccessibility of capability class testing platforms severely limits their scope. A goal of this project is to mitigate these issues and begin to build a LWK OS research community. If successful, expected benefits are increased proliferation of Sandia's LWK OS technology and increased system software innovation. These benefits would not be achievable using the current model of developing a proprietary LWK OS for each new capability supercomputer.

Summary of Accomplishments

The original proposal outlined two high-level objectives: 1) Design and implement a modern open-source lightweight kernel (LWK) OS that takes maximum advantage of multicore processors, and 2) develop a supercomputing-oriented virtual machine monitor (VMM) that gives individual users the ability to choose the compute node runtime environment. In FY 2009 we continued the work started in FY 2008 on objective 1 and made significant progress on objective 2. FY 2009 accomplishments include:

1. Support for POSIX (portable operating system interface [for Unix]) threads and OpenMP was added to the Kitten LWK, which is being developed by this project. This allows applications to take advantage of threading in a LWK environment. Most experimental programming models for multicore processors are being built on top of POSIX threads and are therefore also supported.
2. The SMARTMAP (simple mapping of address region tables for multicore-aware programming) technique that was developed in FY 2008 was implemented in the Kitten LWK. A paper on SMARTMAP was published at the Supercomputing '08 conference and SMARTMAP was an important component of a winning R&D100 submission.

3. We integrated the Palacios lightweight virtual machine monitor with the Kitten LWK. This enables unmodified guest operating systems to be loaded dynamically by end users. We used the Kitten + Palacios combination to perform native vs. guest OS experiments on a Cray XT system with both Sandia's Catamount and Cray's Compute Node Linux operating systems.
4. Multinode application tests using Kitten as the underlying operating system were performed on Cray XT systems and a four node Infiniband cluster.

FY 2009 communications of results include one SAND technical report, two invited talks, two open-source software releases, and one submitted conference paper.

Significance

The lightweight system software being developed by this project will allow future supercomputers to efficiently utilize multicore processors, scale to unprecedented system sizes, and provide a more flexible environment to end users. National security missions, climate change and cybersecurity in particular, have extreme-scale computing requirements. Experience with the Parallel Ocean Program (POP) climate code has shown that it is very sensitive to collective latency and OS noise. Lightweight system software and novel techniques like SMARTMAP address both of these issues. Cyber projects could utilize the virtualization technology being developed by this project to run unmodified commodity operating systems, such as Windows and full Linux distributions, on capability computing resources and in effect simulate the Internet.

Refereed Communications

R. Brightwell and K. T. Pedretti, "Optimizing Multicore MPI Collectives with SMARTMAP," in *Proceedings of the 38th International Conference on Parallel Processing (ICPP-2009),* September 2009.

Enhanced Molecular Dynamics for Simulating Thermal and Charge Transport Phenomena in Metals and Semiconductors

117786
Year 2 of 3
Principal Investigator: R. E. Jones

Project Purpose

In modeling nonequilibrium thermal transport in solids, classical molecular dynamics (MD) has the primary strength of explicitly representing phonon modes and the defects that scatter phonons. On the other hand, electrons and their role in energy transport are missing. These effects are vital in applications such as laser processing of materials, synthesizing thermoelectric (TE) materials, and estimating heat transport in conducting nanotubes and nanowires. Predictive models of the phenomenology of the interactions between the charge carriers and the atoms represented in MD exist, albeit lacking the phonon-confinement, ballistic transport, defect and grain boundary scattering effects natural to MD. This project will greatly improve the state-of-the-art consisting of a few attempts at adding electronic effects to MD by fully coupling the thermal and electronic transport in a rational framework, extending the regimes of application with new models and rigorously treating defects. We have taken partial differential equation (PDE)-based models of the coupled electron-phonon system and represented the electron transport by finite elements (FE) and the phonon system with MD. By coupling classical MD to FE-based models of the missing physics, we are enabling the simulation of a broad range of physical phenomena from the rapid exchange of heat between the electron and phonon carriers in a lattice through current-induced thermal failure of nanowires. Our approach is intrinsically multiscale and multiphysics. Furthermore, the tight coupling between the MD and FE paradigms utilizes the inherent strengths of each. We will enable predictive simulation for applications such as nanowire lasers, components of integrated semiconductors circuits and superlattice thermoelectrics where the effects of nanosized structures and electronic transport are equally important. Moreover, in the process of developing the methods needed to address electronic transport effects in MD, we anticipate discovering novel means of describing and predicting coupled nanoscale transport.

Summary of Accomplishments

We have developed a drift-diffusion based coupling of the electron flow with the atomic system, which allows for simulation of current-thermal interaction effects like Joule heating. We have also developed thermopower coupling such that thermoelectric effects, where carrier concentration drives thermal current and temperature gradients drive electrical current, can be modeled with the coupled molecular dynamics-finite element code. We have also publicly released our code as part of Sandia's LAMMPS package. Lastly, we have made progress in synthetic material design of superlattice thermoelectric nanowires.

We have presented our work in three widely attended conferences: the fall Materials Research Society conference in Boston, the American Physical Society meeting in Pittsburgh and the spring Materials Research Society conference in San Francisco. In addition we have three manuscripts on our molecular dynamics/finite elements work ready for submission to peer-reviewed journals. The first-principles estimation of electronic transport properties is also nearing a stage where it will go to publication.

Significance

High-efficiency thermoelectrics continue to be part of Sandia's mission and nanoscale powered devices are becoming increasingly so. In general, the design of nanosized devices and simulating the relevant physics has impact on a wide range of energy production, communication, and sensing applications. This project and the enabling simulation it develops will impact the design and understanding of the fundamental behavior of these devices.

Solution Methods for Very Highly Integrated Circuits

117787
Year 2 of 3
Principal Investigator: H. K. Thornquist

Project Purpose

While advances in manufacturing enable the fabrication of integrated circuits containing tens-to-hundreds of millions of devices, time-sensitive modeling and simulation necessary to design these circuits poses a significant computational challenge. Especially true for mixed-signal integrated circuits, detailed performance analyses are necessary for individual analog/digital circuit components and the full system. When integrated circuits have millions of devices, performing a full system simulation is practically infeasible using currently available electrical design automation (EDA) tools.

The proposed research addresses the computational difficulties introduced by these large nonlinear dynamical systems by using model order reduction (MOR) to reduce the overall dynamical system size and generate specialized preconditioners that accelerate the underlying linear system solution computation. Some commercial EDA tools use linear MOR techniques for circuit interconnects, but theory and robust methods for nonlinear MOR are nonexistent. Our goal is to create robust nonlinear MOR techniques, as well as apply linear and nonlinear MOR techniques to the individual devices or logically associated groups of devices in a circuit automatically using the circuit level descriptions. While this approach effectively reduces the overall dynamical system size, efficient and scalable preconditioners are still vital to the feasibility of a full system simulation. We will use information about the dynamical system behavior obtained by the MOR methods to pursue innovative, scalable preconditioning techniques for the reduced or full dynamical system.

Success in this endeavor will provide capabilities for impacting the simulation of sensor systems and other circuit design challenges (e.g., parasitics, environmental/radiation effects). It would also potentially re-vector the EDA industry towards accurate, device-level simulation to help resolve nanoscale design challenges for the larger semiconductor industry. This is an LDRD project because the proposed R&D is leading-edge and the potential advances in circuit simulation will enhance Sandia's ability to address future national security needs.

Summary of Accomplishments

The progress made on this project thus far has mainly addressed the research and development of linear and nonlinear model order reduction (MOR) techniques for generating broadly applicable macromodels. A thorough assessment of the current linear and linear time-varying MOR techniques has been performed and the methods are implemented in Myce, which is a Matlab circuit simulator written at Sandia. Current nonlinear MOR techniques have been assessed, but not fully implemented in Myce. So far, the nonlinear MOR assessment illustrates that the most robust approach was found in the piecewise-polynomial (PWP) method and the most efficient was the empirical interpolation method (EIM).

In the assessment of the current linear and linear time-varying MOR techniques, several deficiencies were identified as unique opportunities for us to impact the applicability of MOR to realistic science and engineering problems:

- The most promising linear MOR method, an optimal H2 approach, was extended to linear time-invariant systems in descriptor form by decoupling the differential algebraic equations (DAEs) into proper and improper portions and then applying the optimal H2 approach to the proper portion.

- Singular-value decomposition (SVD)-based methods, like the optimal H2 approach, have provable error bounds only in terms of the power difference between the original and reduced systems. A somewhat more useful notion of error can be measured in terms of peak amplitude. For this notion of error, we have developed a novel approach that uses L1 norm minimization for MOR.
- We have developed a new approach for linear time-varying (LTV) MOR that circumvents the larger dimension LTV transfer function and, if successful, would be a significant contribution to the MOR community.

Some progress has been made in the area of preconditioning: We have developed a specialized multigrid algorithm for solving linear systems generated by power grids or parasitic networks.

Significance

Discoveries in MOR techniques and preconditioning for large-scale nonlinear dynamical systems will significantly impact the design of very large mixed analog/digital circuits. The ability to simulate highly integrated circuits is of great interest to Sandia, its customers and industrial partners. In a broader sense, this R&D will enable the efficient simulation of circuits at the device level and greatly affect the circuit design challenges that come from the technology drivers of smaller feature scales and higher integration. Thus, not only will this research help provide an efficient design tool, delivered through Sandia's Xyce circuit simulator, and give Sandia a differentiating capability but also potentially re-vector the EDA industry towards accurate, device-level simulation to help resolve nanoscale design challenges for the larger semiconductor industry. Beyond electrical modeling, this research has the promise of leading the way towards new techniques for efficient solution of large-scale nonlinear network problems including such examples as biological systems and national infrastructure problems.

Scalable Solutions for Processing and Searching Very Large Document Collections

117788
Year 2 of 3
Principal Investigator: D. M. Dunlavy

Project Purpose

Intelligence analysts have a big data problem. They answer questions of national security under extreme time pressure, and current tools cannot handle the volume of data they must consider. In addition, they explore data iteratively by testing various "what-if" scenarios. As a result, quick turnaround time for processing, searching, and exploring large document collections is critical. No end-to-end scalable visual text analysis capabilities exist today, and this prevents analysts from exploring, annotating, and analyzing existing petascale document collections. The goal of this work is a suite of independent, scalable capabilities to process and search large document collections for use in data analysis and visualization software that can efficiently leverage parallel algorithms. We will develop exact and conceptual searching methods as well as relevance feedback methods (i.e., active learning methods) for reducing uncertainty inherent in text analysis. Our end-to-end system will serve two purposes: (1) as a production capability, and (2) as an environment for rapid prototyping of algorithms. Initial uses of this new system will include application of existing methods to new problem areas and the development of hybrid algorithms that combine new and existing algorithms in novel ways.

LDRD investment in this project is crucial at this stage of development due to the risk involved (as the first end-to-end fully parallel data and execution text analysis and visualization pipeline) and the need for deeper understanding of the issues and challenges related to coupling text analysis, visualization, and user feedback methods for use in large-scale data analysis.

Summary of Accomplishments

In the past year of this project, we have developed the initial scalable pipeline for the ParaText text analysis engine, developed modular capabilities for text analysis in the new Algebraic Engine software library components, completed the initial version of the LSAView software application, investigated and developed ensemble machine learning capabilities for text analysis, and investigated unsupervised methods for information extraction. Within the scope of ParaText and the Algebraic Engine, we have developed and tested several alternatives for distributed document reading, term dictionary creation, and term-document matrix creation to better understand the challenges associated with a fully scalable text analysis pipeline. With the initial version of LSAView, we have demonstrated how visual analysis can be used to identify optimal parameters in our text analysis capabilities for use in solving real world problems (i.e., text document clustering). In FY 2008, we developed a software system for creating, tuning, and evaluating ensemble models for data classification. This system, called HEMLOCK, is targeted for open source release toward the end of FY 2009.

Also in this past year, we have one invention disclosure, one refereed conference paper, one conference paper submitted, four SAND reports, eight presentations, and one open-source software library scheduled for release. We also have received several internal awards and have organized two workshops associated with our work.

Significance

The volume of textual data is increasing exponentially and analysis tools are critical to understanding the vast collection of human knowledge and current events. The capabilities developed in this project will provide intelligence analysts with the most efficient text processing capabilities available, significantly reducing turnaround time associated with data exploration, hypothesis testing, and collaborative analysis, speeding analysis and detection of national security threats.

Refereed Communications

P.J. Crossno, D.M. Dunlavy, and T.M. Shead, "LSAView: A Tool for Visual Exploration of Latent Semantic Modeling," *IEEE Proceedings of the Symposium on Visual Analytics Science and Technology*, October 2009.

Scaling I/O for High Performance Commodity Clusters

117789
Year 2 of 3
Principal Investigator: H. L. Ward

Project Purpose

While machine capabilities grow, file system advancement is falling far behind. Specialized distributed parallel file systems are developed outside of the Linux mainstream. Although the Linux mainstream distributed file system, NFS (network file system), is slowly being improved in functionality, the bulk of the effort is aimed at improving random input/output (I/O) for business applications rather than streaming I/O of high performance computing (HPC) applications. Recent benchmarking efforts show that less than 15% of the available bandwidth is utilized for streaming NFS writes, even though the same tests achieved 90% or more for reads.

We identify two strategies to optimize streaming writes on the client side. First, re-implement the Linux NFS client to be procedure-based, multithreaded and asynchronous. The NFS client can then perform network I/O simultaneously with the application data writing on multicore machines. Second, improve the behavior of the Linux virtual file system (VFS) and virtual machine manager (VMM) to increase overlapping of application and network I/O. We will collaborate and consult with the Linux NFS, kernel, and network researchers in designing, testing, and building community support for changes to the Linux NFS that will enable open-source systems to achieve high streaming write throughput required by HPC applications. We propose to study the new algorithms on HPC clusters not commonly available in the NFS and kernel developer communities, to demonstrate changes to the NFS implementation to remove the bottleneck in NFS writes, and to build community advocacy for having these HPC-favorable changes migrated into the Linux mainstream.

This is an LDRD project because the scope of the effort is longer than can be accommodated by short-term ASC milestones and more basic than the applied research constraints imposed by ASC funding sources.

Summary of Accomplishments

Past milestones all addressed the tasks of diagnosing bottlenecks, removing or mitigating those bottlenecks, propagating the required changes to the Linux kernel to the maintainers, and publishing our results. We are proud to report that all of these milestones have been accomplished.

To diagnose the issues preventing good utilization, we worked up a set of baseline measurements and then instrumented the Linux kernel to ascertain throughput at various key points. This work showed two key points of the issue. First, that the Linux NFS stack, with or without bypass-enabled transports such as NFS/RDMA (remote direct memory access) was only capable of 600 MB/s (out of a potential 1.2 GB/s). Second, that the NFS/RDMA transport was only preregistering small payloads for each remote direct memory access (DMA) operation.

We corrected the identified issues, resulting in an improvement from ~320 MB/s to 425 MB/s. To correct the issues we, first, modified the Linux kernel NFS/RDMA transport to attempt payloads twice as large as previously and, second, profiled the kernel which identified the memory copies between user-space and memory-space as the prime contributor in the inherent limitation identified in the diagnostic phase. The NFS/RDMA transport changes improved performance in all cases. Elimination of the memory copies required application changes and, so, only improved applications realized this benefit.

We propagated our changes by working with the maintainers of the affected source codes. We developed a “supermon” reader called “FTQ-IO.” The supermon changes have been made available to the maintainers at Hewlett-Packard and IBM has requested the FTQ-IO reader.

We have reported via submission of a paper titled “On Scaling I/O for Commodity Clusters” to Cluster ‘09, a peer reviewed conference.

Significance

This work is relevant to the goal of nuclear weapons stewardship, and supports the strategy of developing capabilities needed for long-term stewardship in the future. Many scientific applications perform periodic streaming writes for either check-pointing or storing intermediate results. These applications will benefit from the overall performance gain if we eliminate the NFS write bottlenecks on the client, yielding more timely simulation results as we scale to larger machines.

Surface Rheology and Interface Stability

117790
Year 2 of 3
Principal Investigator: L. A. Mondy

Project Purpose

We propose to experimentally investigate the surface rheological properties and stability of interfaces to extend our physical knowledge of multiphase flows and guide the development of constitutive models for the mechanical behavior of interfaces. Interfacial properties are distinct from bulk properties on either side of the boundary, are not well understood, and are difficult to predict. Although interfacial properties have been studied for some time, the complexities of interactions among surfactant molecules, adsorption characteristics, dependence on the geometry of the interface, and the inherent multiscale nature of the interfaces, means that much interfacial physics remains a mystery. The effects of colloidal particles, which tend to gather at an interface, are even less understood. We will establish unique laboratory capabilities by coupling information obtained using interfacial stress rheometers with that obtained through microrheology using particle optical trapping to provide cutting-edge experimental discovery necessary to extend current computational models. Gathering data with multiple techniques will allow separation of effects, leading to a much better understanding of phenomena than could be obtained with any one experimental method. The newly developed constitutive models will be incorporated into Sandia's multiphysics codes improving Sandia's core capability in modeling and simulation of fluid flow and complex coupled phenomena.

Summary of Accomplishments

To date we have modified and calibrated an interfacial stress rheometer (ISR), which measures viscoelastic properties of the interface from the amplitude and phase shift of the periodic needle displacement caused by a magnetic field. Modifications included construction of different diameter flow cells that alter the sensitivity of the measurements. Recently, we have also explored using other surface coatings on the needle to allow a wider variety of liquids to be tested.

This year we completed construction of a novel micro-interfacial rheometer. Using a micron-sized particle as a probe instead of a needle may improve the sensitivity to surface viscosity above that of the ISR. Forces as small as piconewtons that create a known displacement of the particle can be measured. This year we have demonstrated the ability to manipulate particles at an air-water interface and perform passive rheology.

With the ISR, it is possible to create surface flows that occur at constant surface area, which separates shear from dilatational deformations. To study the latter, we have developed a more reliable and robust surface dilatational rheometer (SDR) this year. A time-dependent surface area is generated by varying the volume of a drop and the resulting changes in surface tension are analyzed to measure an effective surface dilatational modulus. The dilatational viscosity of an interface can be directly related through theory to the dilatational viscosity of a foam material, important to Sandia's foam models and difficult to measure directly.

Finally, this year we have continued development of surface rheology modeling capabilities. In addition, numerical studies have continued to aid the interpretation of data, including determination of the deflection of the free surface in the ISR due to the presence of the needle and determination of the time for a bubble to reach an equilibrium shape in the SDR.

Significance

This work will contribute world-class science and improve our core capability in modeling and simulation of fluid flow and complex coupled phenomena, establishing Sandia as a leader in modeling interfacial rheology. Side-effects will include benefits to DOE's energy and environmental management programs from better de-foaming strategies in processing nuclear waste. Nuclear weapons stewardship will benefit from better foaming strategies for encapsulation in weapons manufacturing.

Refereed Communications

T.P. Koehler, C.M. Brotherton, and A.M. Grillet, "Comparison of Interparticle Force Measurement Techniques Using Optical Trapping," to be published in *Langmuir*.

"Equation-Free" Simulation Methods for Multiple Timescale Diffusion Processes in Solids

130732
Year 1 of 3
Principal Investigator: G. J. Wagner

Project Purpose

Many of the most important and hardest to solve problems related to the synthesis, performance, and aging of materials involve diffusion through the material or along surfaces and interfaces. Unfortunately, traditional molecular dynamics (MD) simulation is not tractable for most of these problems because of the long timescales involved. To make progress, we can note that the quantities most of interest to a modeler, such as concentrations and structural feature sizes, can be described at a much coarser level than the atomic scale. One method that takes advantage of this fact is the so-called "equation-free" approach, which uses microscale computations, like MD simulations, as a set of numerical experiments from which can be distilled macroscale information, such as time derivatives of coarse scale variables. We propose to use equation-free methods to extend the timescale in atomistic simulations to that necessary to accurately simulate and predict diffusion processes. However, an equation-free method that uses MD for its fine-scale simulations is likely to fail for problems driven by rare events, like atom hopping in diffusion, since MD cannot capture enough events in a short amount of time to be statistically relevant. The key innovation in our proposal is to use extended timescale methods, like kinetic Monte Carlo (KMC) and temperature accelerated dynamics (TAD), for the fine-scale computations that inform the continuum-level evolution in an equation-free approach; these methods by themselves have their own size and timescale limitations that can be overcome by our novel combination of approaches. This project, if successful, will fill an important gap in the Laboratories' ability to perform atomic scale simulation of material stability and nanoscale transport over long times, phenomena that are vital to modeling aging of the nuclear stockpile as well as to the synthesis and performance optimization of nanostructured materials.

Summary of Accomplishments

The first major goal of our project is to develop extended timescale methods for surface diffusion. We have implemented a simple model of surface diffusion, the solid-on-solid (SOS) model, in the Sandia kinetic Monte Carlo code SPParKS, and verified that it correctly mimics curvature-gradient driven continuum surface diffusion for limiting cases. Using this model, we have explored the effects of various interscale operators on system dynamics; these operators are key to extending simulation timescales using equation-free projective integration (EFPI). We have found that operators based on the 2-point correlation function of the surface profile allow accurate reconstruction of the surface and its dynamics, and we have begun developing an EFPI algorithm that makes use of this type of operator to achieve long timescales in 2D (and eventually, 3D) surface diffusion.

The second major goal of the project is to develop EFPI for interlayer diffusion of unlike metals. In FY 2009, we have begun studying the use of temperature accelerated dynamics (TAD) for simulations of interlayer diffusion. We have acquired a TAD research code in order to understand the method's implementation and determine its suitability for our problems of interest, and we have begun using TAD to simulate bulk diffusion of atomic vacancies. As a step toward full implementation of TAD in parallelized Sandia codes, we have nearly completed implementing a related method, parallel replica dynamics (PRD), in the molecular dynamics code LAMMPS. PRD uses some of the same basic algorithmic components as TAD and thus lays the groundwork for full implementation of both; it is also a useful method in its own right and may be used as a microscale simulator in our extended-timescale simulations. Finally, we have developed interscale operators describing vacancy concentration in a 3D bulk solid, a preliminary step toward operators suitable for the interlayer diffusion.

Significance

This project will fill an important gap in our ability to perform atomic scale simulation of material stability and nanoscale transport over long times, phenomena that are vital to modeling aging of the nuclear stockpile as well as to the synthesis and performance optimization of nanostructured materials. These materials have applications that span Sandia missions, including emerging energy technologies such as next-generation batteries, supercapacitors, thermoelectrics, and photovoltaics.

The first set of applications that will benefit from our work are problems in which surface diffusion is the main mode of material transport; this is the class of problem for which the fewest technical hurdles remain. Included in these applications are projects studying the synthesis and aging of nanoporous metals being developed for gas and electrical storage.

Bayesian Data Assimilation for Stochastic Multiscale Models of Transport in Porous Media

130734
Year 1 of 3
Principal Investigator: J. Ray

Project Purpose

We will develop new Bayesian inference methodologies that characterize coupling across multiple spatiotemporal scales and heterogeneous physical processes by conditioning on observational data. Our techniques are general, but will be demonstrated on problems in porous media.

Multiphase transport-chemistry interactions in porous media underpin applications of great importance to energy and the environment (e.g., fuel cells, subsurface nuclear waste storage, CO_2 sequestration). These physical processes are inherently multiscale, driven by pore-scale characteristics such as capillarity, relative permeability, and reactivity. A fundamental difficulty in multiscale modeling is indeterminacy in extrapolating from microscale simulations to macroscale characteristics, and conversely, the inability of a macroscale model to resolve all the inputs needed at the microscale. Traditional upscaling/homogenization techniques ignore or arbitrarily simplify these uncertainties, failing to reproduce measured processes at multiple scales. Crucial statistical information and opportunities to provide validated predictions, are therefore lost.

We address these shortcomings by developing statistical inversion algorithms that infer the correct interscale coupling by conditioning on observables. Our algorithms will provide macroscale properties with quantified uncertainties, using spectral representations of multiscale random fields. Novel reduced-order representations of state variables and joint uncertainties at multiple scales will preserve computational tractability. The data-driven methods developed here will enable rigorous updating and refinement of computational characterizations and forecasts in conjunction with experimental observations, thus opening new frontiers in the predictability of complex coupled physical processes.

Summary of Accomplishments

In FY 2009, we developed a Bayesian inversion technique that infers an unknown permeability field (in a porous medium) from sparse static (permeability) and dynamic (tracer flow) measurements. The unknown permeability field is modeled as a random field and is represented using Karhunen-Loeve bases. The coefficients of the bases are the object of inference. This decouples the dimensionality of the inference problem (between 30-45 coefficients) from the resolution of the mesh, allowing the inference of well-resolved permeability fields as well as those whose spatial variations indicate a small correlation length scale. The technique was applied to infer permeability fields in the 10th Society of Petroleum Engineers (SPE) comparison study.

A second thrust of our multiscale investigations has involved the construction of subgrid models for multiscale random field. In FY 2009, we have addressed binary media (e.g., concrete, human skin, etc.) where low permeability inclusions may be embedded in a high-permeability matrix. The binary medium is modeled using truncated Gaussians. The kernel width, the inclusion proportion, and the permeabilities of the two components form the inputs to the subgrid model, which then predicts the resultant permeability. This reduced-order model was used to infer a spatially variable inclusion-volume-fraction field from static and dynamic data. Karhunen-Loeve expansions were used to model the unknown field.

The results of our investigations were presented at the conference of the International Association of Mathematical Geosciences (Stanford; August 2009) and the Meeting of the American Geophysical Union (San Francisco, December 2009). The subgrid model is being extended to model anisotropic permeability fields.

Significance

Multiscale Bayesian data assimilation enables validated, predictive simulations critical to DOE's national security missions. Storage of nuclear waste, multiphysics weapon simulations, and contaminant identification and mitigation, are plagued by uncertainties at multiple scales; data is needed to improve and refine models in this context. Similarly, DOE's energy security mission involves subsurface carbon sequestration, which rests on long-time prediction and data-driven models enabled here.

Computational Mechanics for Geosystems Management to Support the Energy and Natural Resources Mission

130739
Year 1 of 3
Principal Investigator: C. M. Stone

Project Purpose

US energy needs include more-economical extraction of fossil fuels, increasing recoverable reserves, protection of water resources, reduction of the impact of fossil fuels on climate change, mining nuclear fuel sources with minimal environmental impact, and technologies for safe disposal of energy wastes. Long-term solutions to these needs will require the ability to simulate, model, and predict behavior of subsurface systems including complex, heterogeneous mineral and porous rock thermochemomechanical behavior as well as the interactions with multiphase pore fluids and microbial activity. Accordingly, we are proposing a research and development project enabling a coupled thermal, hydrological, mechanical, chemical (THMC) simulation capability for massively parallel applications. Key research issues to be addressed are related to phase appearance/disappearance, geologic heterogeneity, and other subgrid phenomena, robust solvers for fully coupled systems, and methods to deal with disparate time and length scales for the coupled multiphysics. To solve these complex issues, this proposal integrates research in numerical mathematics and algorithms for chemically reactive multiphase systems with computer science research in adaptive coupled solution control and framework architecture. The resulting coupled THMC code would be unmatched by any commercial or proprietary software. The new software would allow for multiphysics modeling on spatial/temporal scales not currently available. This development directly impacts Sandia's ability to respond to immediate national needs for energy security and solutions to global climate change.

Summary of Accomplishments

The research for FY 2009 is on schedule to meet the milestones as stated in the original FY 2009 proposal. We have successfully demonstrated the solution of several single phase coupled porous flow/geomechanics benchmark problems. We have developed the necessary models for two-phase flow capability in ARIA and the capability is undergoing testing in preparation for the milestone of a benchmarked coupled two-phase flow/geomechanics example. A number of geochemical packages were reviewed for capabilities, and also a number of Sandia geochemists were interviewed on software applicability and functionality. PHREEQC (US Geological Survey computer program for low-temperature aqueous geochemistry calculations) and EQ3/6 (originally developed to model geochemical processes of relevance to the Yucca Mountain Site Characterization Project, were two geochemistry packages that were selected based on their ability to solve for a variety of salinities and gas/fluid/mineral systems, availability of source code, and widespread use in the geochemical community at Sandia and globally. A third package, CANTERA, an open-source freeware distributed from the California Institute of Technology (Caltech) is being examined specifically for its employment of the Pitzer methodology for brine-gas solution thermodynamics. CANTERA is being brought into ARIA, and we could also make use of its equation-of-state capabilities, and solvers for kinetics problems. We have explored existing SIERRA capability to drive adaptive solution algorithms for porous flow/geomechanics and heat transfer/mechanics using code specific solution control and the Encore toolkit contained within SIERRA Mechanics. We have an initial adaptive implementation and we are now working to broaden both the algorithm variation as well as the problem data used by the adaptive algorithms.

Significance

The DOE strategic goals of energy, science and environment are relevant to this project, which addresses many of the issues associated with protecting our economic and national security by supporting the development of a diverse energy portfolio. This requires significant advancements in our understanding of multiphysics, multiscale processes associated with complex, heterogeneous mineral and porous rock behavior as well as the interactions with multiphase fluids and microbial activities.

Experimental Characterization of Energetic Material Dynamics for Multiphase Blast Simulation

130740
Year 1 of 3
Principal Investigator: S. J. Beresh

Project Purpose

Accurate simulation of energetic material detonation is crucial to a variety of national interests involving explosive devices, including vulnerability of weapons and structures to nearby explosions, blast mitigation, improvised explosive device (IED) protection, and enhanced blasts. Unfortunately, such predictive capability is limited by a lack of knowledge of the underlying phenomena of the earliest stages of the blast, where the particle dynamics of the fragmented materials within the gas expansion products are pivotal to understanding the continuing reaction. The complication is that, at the explosion's onset, the particles are densely packed within the expanding flow, whereas our knowledge of the process is restricted to dilute concentrations. We propose to fill this gap by constructing an unprecedented multiphase shock tube that can drive a shock front into a particle/gas mixture of a selected fill fraction, then measure the motion of the densely packed particles within the expanding gas. One of the great challenges of the problem is that the opacity of the flow prevents usage of common fluid dynamics diagnostics and instead will require the development of unconventional measurement approaches. We seek to exploit measurement concepts previously utilized for multiphase flows and high-energy physics and adapt them to the uncommon difficulties of the present problem. The most promising approaches concern the use of x-ray sources to penetrate the dense flow and provide measurement of the particle velocities, or potentially using strong sources of incoherent visible light in concert with specifically designed tracer particles. Finally, while velocity measurements are of the greatest value, the lack of knowledge of this flowfield is so profound that even delivery of simpler measurements such as shock speeds and pressure histories would represent a valuable contribution. By providing crucial new physical data, we can boost the level of fidelity in algorithms used to simulate blasts in national security applications.

Summary of Accomplishments

The principal activity of the first year of the project is devoted to the design, construction, and testing of the two-phase shock tube. This novel facility can be conceptually divided into two portions: the shock tube itself to initiate a planar shock wave traveling through a duct, and the particle-laden test section to study the interaction of the shock with the dense particle/air mixture. A conceptual design for the test facility has emerged in which a horizontal, square shock tube propels a shock wave into a curtain of falling particles created as they pass through a contoured gravity-fed column. Favorable results have been achieved with a benchtop test bed that has been shown to deliver particle volume fractions of 5%–30%, encompassing the range of interest to blast simulations, and possessing acceptable uniformity as well. Moreover, this benchtop test bed appears ideal for the development of the novel diagnostics needed to interrogate optically dense flows. In concert with the facility development, we are analyzing new diagnostic approaches for feasibility with the two-phase shock tube and particle curtain. Particle-shadow velocimetry shows promise to measure particle velocities and is compatible with the flow opacity, in which a particle curtain composed primarily of weakly attenuating particles is seeded with a small fraction of highly attenuating particles that function as tracers when backlit with x-rays or potentially with strong incoherent visible light. Two frames taken in rapid succession can track the motion of the shadow images using cross-correlation algorithms similar to those employed in particle image velocimetry. We have performed design calculations to size the required x-ray source and intensified detector, and we are exploring simpler and less expensive backlighting approaches using visible light. We presently are constructing diagnostic experiments in conjunction with the benchtop particle-curtain facility to investigate the effectiveness of these approaches.

Significance

Although explosives researchers have for many decades futilely sought gas dynamics data in densely packed shock-driven two-phase flows, more recent improvements in energetic materials and, most particularly, growth in nonintrusive measurement capabilities make this field currently ripe for further development. Even partial success in the current project would provide a unique capability within the broader national establishment and be of significant service to the explosives community. A consequential improvement to blast simulation is unlikely to occur without improving the physical understanding of the reaction regime immediately following detonation. Because of the almost complete lack of knowledge of such complex flow physics, both at Sandia and throughout the scientific community, the provision of even limited data would be a great boon to modeling and simulation efforts used to support both explosive design and vulnerability assessment. Such improvements would benefit core Sandia responsibilities regarding vulnerability of weapons and structures to nearby explosions, facilities protection, and blast mitigation. Furthermore, given that Sandia is involved in other research initiatives covering such explosive topics as enhanced blasts, structure-coupled blasts, IED protection, and thermobaric explosives, an infusion of new data is of direct and wide-ranging importance. Potential also exists to port newly developed diagnostics to related explosive tests and field-scale validation activities. Thus, this research effort is of great interest to Sandia's defense programs, and additionally to the broader national defense establishment.

Nanomanufacturing: Nanostructured Materials Made Layer-by-Layer

130741
Year 1 of 3
Principal Investigator: P. R. Schunk

Project Purpose

Large-scale, high-throughput production of nanostructured materials is crucial to national security and a strategic area in manufacturing, with markets projected to exceed $1T by 2015. Nanomanufacturing is still in its infancy; process/product developments are costly and only touch on potential opportunities enabled by growing nanoscience discoveries. This project expedites such exploration through enabling predictive simulation.

A promising way to build novel functional materials at high throughput is by layering nanoscale-patterned films. Many of these proposed nanostructured materials manufacturing processes involve liquid-phase imprinting, solid-phase embossing, solidification, and solid-phase release. Subsequent coating of imprinted features with assembled nanoparticles is often used to build selective functionality, like conductive pathways. These four unit operations of imprinting/embossing, solidification release, and dispersion coating serve as prototypes for this work because of broad applicability to a variety of integrated fabrication techniques for applications like photovoltaics and imprinted circuits. Underpinning research challenges, especially those arising at higher throughput, will be the focus. Physical models will be developed with experimental guidance to capture feature scale phenomena such as wettability, film rupture, adhesion, and atomistic friction. Scales for these models will bridge from atomistic (<1 nm) to feature (~10–100 nm) and will make clear the key defect mechanisms. These models will be up-scaled to machine levels (~1-10 cm) using additional coarse-graining techniques.

The outcome of this project will increase fundamental scientific understanding of defect mechanisms and enable Advanced Simulation and Computing (ASC)-class modeling and simulation (M/S) capabilities to be applied to nanomanufactured materials process design. Enabling technology for M/S will be in two major thrusts: validated multiscale models and novel algorithms.

Summary of Accomplishments

Progress towards creation and exploration of single and multiple feature imprinting and molding models at the nanoscale were the highlights of the first project year. Models were developed and tested for liquid-state and solid-state imprinting/embossing processes. Additional exploration and development were pursued in the up-scaling task to enable the connectivity of local defect rate (feature no-fill) and long-range order to machine-level parameters of the step and flash imprint lithography (SFIL) process. The first experimental prototype of imprinting on nanoparticle-laden liquids was also accomplished, which lays the groundwork for our printed circuit application. More specifically, we have accomplished the following:

1. Initial models of single-feature filling via pressure loading on the template were completed in ARIA.
2. Development and application of a lubrication element type complete with surface tension and free-and-moving boundary capability was completed to lay the groundwork for the machine-scale model. Additional research and development towards integration of this element type with structure shells for template flexure was also pursued.
3. Through in-situ x-ray scattering experiments, we have discovered, for the first time ordered nanocrystal mesophase transition from polycrystalline to single crystalline gold nanocrystal lattices induced by ultrahigh hydrostatic pressure. Such pressures are typical of a manufacturing imprint process.

4. Initial finite element analysis (FEA) and molecular dynamics (MD) work was focused on simulating the molding of a single, nanometer-scale feature. PRESTO finite element analyses have shown that adhesion and atomistic friction play an important role in the filling of features at this scale.
5. Initial MD simulations utilized single- and multiple- nanometer-scale feature(s) impressed into a liquid polymer melt in order to determine an effective parameter phase space.

Significance

This project increases DOE's return on investment in nanoscience. Control of nanostructure in high-throughput processes expands application space, particularly in energy: photovoltaic and thermoelectric devices are multilayered, nanostructured materials but current manufacturing is often cost-prohibitive. Beyond energy, impact is enormous in all missions, particularly in those requiring large-area films with certain physical/chemical/thermal attributes (e.g., electrical, optical, sensing, adhesion, separations).

Optimization of Large-Scale Heterogeneous System-of-Systems Models

130742
Year 1 of 3
Principal Investigator: W. E. Hart

Project Purpose

A major challenge for decision-makers is the analysis of national-scale manmade systems, which are composed of interacting subsystems. Effective integration of subsystem models is difficult, there are many discrete system parameters to analyze in these systems, and there are fundamental modeling uncertainties that complicate an analysis.

This project will develop methods to effectively analyze heterogeneous system of systems (HSoS) models, which have emerged as a promising approach for describing complex manmade systems. An HSoS model is a heterogeneous assembly of system models that can operate as a single integrated system whose behavior reflects the interactions of the constituent system models. HSoS models can leverage system domain expertise in a modular fashion, so diverse aspects of manmade systems can be integrated into an HSoS model (e.g., climate, human behavior, economics).

We will develop efficient optimization techniques that can address modeling uncertainties in the analysis of large-scale manmade systems. This project will deliver a differentiating capability in the form of peer-reviewed publications and software that can analyze large-scale HSoS models, including:

1. Multistage stochastic optimization with recourse to model human decision-making given uncertain information about the future.
2. Risk management to identify system parameters that are insensitive to data uncertainties.
3. Multicriteria optimization to assess tradeoffs between performance criteria.
4. Model analysis techniques to identify critical modeling uncertainties and quantify model confidence.

The simulation cost of large HSoS models makes black-box optimization prohibitively expensive. Thus, these optimization techniques will exploit mathematical structure to enable global analysis of mixed-continuous decision spaces.

Two prototypical HSoS applications will be used to motivate and evaluate these optimization techniques: analysis of future energy infrastructure and multiplatform intelligence collection systems. These systems will illustrate decision support capabilities to assess the impact of new technologies, identify system bottlenecks, evaluate policy choices, and design future systems.

Summary of Accomplishments

The COLIN optimization interface library for DAKOTA was extended to provide a more extensible framework for hybrid optimization. These extensions include support for automatic problem reformulation and evaluation of stochastic problems.

The PySP tool was developed, which provides stochastic programming extensions of the Pyomo (python optimization modeling objects) modeling software. PySP includes a generic implementation of progressive hedging (PH), which can optimize mixed-integer stochastic programs with recourse. This generic implementation is a unique capability that can be applied without application-specific customizations.

Cutting planes were developed that can linearize the quadratic equations used in PH, thereby enabling the application of mixed-integer programming (MIP) solvers to PH subproblems.

The Pyomo software was extended to include a plug-in framework that greatly enhances the extensibility of Pyomo. This framework supports and manages extensions developed by core-developers without risk of destabilizing core functionality, and it enables dynamically loaded plug-ins to automatically register optimization solvers.

The SUCASA software was created to automatically generate MIP solvers that can leverage algebraic problem structure. This tool generates a custom PICO (parallel integer and combinatorial optimization) MIP solver with algebraic structure that can be used tailor the MIP search process.

Model aggregation and simplification techniques have been explored in the context of a water security application. Sensitivity analysis has been used to study how aggregation and simplification impact data uncertainties.

The project members gave 15 presentations at international conferences, and they published one journal article.

Software releases were prepared for several packages that are related to these capabilities: Acro 2.0, UTILIB 4.0/4.1, PyUtilib 1.0/2.0.1/2.1, FAST 2.0/2.1 and Coopr 1.0/1.1. There have been several hundred downloads of these releases in FY 2009.

A variety of prototype applications have been explored, including planning for energy investment with water constraints, energy grid planning problem, forestry planning, and analysis of energy usage in buildings.

Significance

Many Sandia and DOE missions concern the analysis of complex manmade systems, and national infrastructure models are being used to inform government policy, assess risks, and evaluate system interdependencies. These optimization methods can analyze models for the Sandia Water-Energy Nexus, DOE Hydrogen Program, the National Energy Modeling System, and related problems for the Environmental Protection Agency (EPA), the Defense Threat Reduction Agency (DTRA), DOD and DHS.

Refereed Communications

J.P. Watson, R. Wets, and D. Woodruff, “Scalable Heuristics for Stochastic Programming with Scenario Selection,” to be published in *INFORMS Journal on Computing*.

W. Hart, “Pyomo: Python Optimization Modeling Objects,” INFORMS Computing Society Conference, January 2009.

System-Directed Resilience for Exascale Platforms

130743
Year 1 of 3
Principal Investigator: R. A. Oldfield

Project Purpose

Resilience on massively parallel processing (MPP) systems has traditionally been the responsibility of the application, with the primary tool being application-directed checkpoints. However, as systems continue to increase in size and complexity, the viability of application-directed checkpoint as a solution decreases. Recent studies performed at Sandia projected that as systems grow beyond 100,000 components, a combination of factors lead to checkpoint overheads in excess of 50%. In this project, we will investigate critical changes required in MPP systems software to support system-directed resilience. The goal is to provide efficient, application-transparent resilience through coordinated use of system resources. The primary research topics focus around the problem of continuous computing in the event of a component failure. A preliminary list of required new capabilities include:

- Application quiescence: the ability to suspend CPU, network, and storage services used by an individual application without interfering with the progress of other applications;
- State management: the ability to identify, extract, and manage application state in a transparent, efficient, and non-intrusive way; and
- Fault recovery: the ability to transparently replace a failed component without restarting the entire application.

Summary of Accomplishments

The goals of FY 2009 were to understand application requirements for resilience and explore the viability of alternative resilience approaches on capability-class systems. We completed an extensive set of memory characterizations studies, we developed tools to identify periods in an applications execution where quiescence has minimal impact, and we began to explore a hybrid approach to resilience that combines traditional checkpointing with redundant computation.

The memory characterization study satisfied our FY 2009 milestones to characterize application behavior and identify application-critical state. We developed an approach to identify all blocks of memory that change between two periods in time. The idea was to understand if incremental approaches were viable for the types of applications common to the Advanced Simulation and Computing (ASC) program. We ran characterizations on HPCCG (high performance computing conjugate gradient), CTH, Sage, and LAMMPS. Results will be published in a SAND report.

To satisfy our milestone to investigate options for quiescence, we are actively involved in discussions with Cray about their solution for quiescence of the XT series systems. Cray is particularly interested in how to suspend applications that have active connections to file systems and other shared services. We are trying to collect and correlate trace data for network and I/O activity that could identify “windows of opportunity” during an application’s execution where quiescence has little or no impact on external services.

We also completed development of a message passing interface (MPI)-based “partial-redundant” computation scheme that duplicates some application processes to reduce the probability of failure for the entire application. This approach, when combined with traditional checkpoint-based resilience, reduces the frequency of checkpoints allowing checkpoint-based approaches to scale to much larger application sizes. We believe this approach shows promise as a viable alternative to pure checkpoint-based methods.

Significance

This project has direct relevance to the scientific discovery and innovation mission; if successful, it will have a direct impact on capability-class applications in virtually all areas of advanced computing.

Computational Investigation of Thermal Gas Separation for CO_2 Capture

138718
Year 1 of 1
Principal Investigator: J. R. Torczynski

Project Purpose

The purpose of this project is to perform a computational investigation of thermal gas separation for CO_2 capture from air. Effective methods of capturing atmospheric CO_2 are essential for climate-change mitigation and carbon-neutral-cycle transportation-energy production. Thermal separation offers advantages over centrifuges and diffusion by employing no moving parts and no complicated materials. The basic principle is that a temperature gradient imposed on a gas mixture causes the lighter and heavier components to migrate to regions of higher and lower temperatures, respectively. Thermal gas separation is most effective for mixtures of species with widely differing molecular weights. Molecular-gas-dynamics simulations have demonstrated this effect for argon-helium mixtures, which have a molecular-weight ratio of 10. Molecular-gas-dynamics simulations will be performed to quantify the effectiveness of thermal separation for CO_2-air mixtures. Because their molecular-weight ratio is only 1.5, massively parallel simulations will be required to quantify the concentration gradient as a function of the CO_2 mole fraction and the nominal temperature.

Summary of Accomplishments

Thermal gas separation for a binary mixture of carbon dioxide and nitrogen was investigated using the direct simulation Monte Carlo (DSMC) method of molecular gas dynamics. Molecular models for nitrogen and carbon dioxide were developed, implemented, compared to theoretical results, and compared to several experimental thermophysical properties. The molecular models included three translational modes, two fully excited rotational modes, and vibrational modes, whose degree of excitation depends on the temperature. Nitrogen has one vibrational mode, and carbon dioxide has four vibrational modes (two of which are degenerate). These models were used to perform a parameter study for mixtures of carbon dioxide and nitrogen confined between parallel walls over realistic ranges of gas temperatures and nominal concentrations of carbon dioxide. The degree of thermal separation predicted by DSMC was slightly higher than experimental values and was found to be sensitive to the details of the molecular models.

Significance

Sandia's roadmaps for climate change and transportation energy specify the goals of "climate change mitigation" and a "carbon neutral cycle." By developing a novel technology to separate CO_2 from air, this project supports both goals and positions Sandia for a leadership role in this area. Furthermore, this technology offers the possibility of capturing other key greenhouse gases such as methane in the same way.

Feedback Dynamics of Climate Impacts

138735
Year 1 of 1
Principal Investigator: G. A. Backus

Project Purpose

Government climate-change policies could radically affect the interacting economic sectors of the United States. Existing analyses of climate impacts miss the economy-wide system effects of uncertainty when comparing intervention to nonintervention conditions. Essentially all of the current analysis approaches are implicitly or explicitly static rather than dynamic, and they thereby neglect delays, nonlinearities, and secondary consequences, Macroeconomic feedback dynamics, resource-usage chains, market interactions among economic sectors, the financial environment, and hydrological impacts can cause static, insular analyses to support policy recommendations that are inconsistent with regional and market realities. This effort would establish a risk-assessment analysis capability by combing and advancing uncertainty quantification (UQ), hydrological modeling, and socioeconomic modeling. We would extend the conventional engineering UQ to map climate uncertainty into assessment models that are also modified to quantify climate-change effects.

Our primary objective is to establish an analysis capability and demonstrate the usefulness of this capability by first applying it to the full risk spectrum of climate change in the absence of government policies. The primary output of the effort will be an integrated risk assessment framework for analyzing climate change impacts with full recognition of uncertainty. While the system would be fully functional with a high level of analytical validation, the scope of the project does not include a fully automated, self-contained application.

Summary of Accomplishments

We developed the methods to combine physical and socioeconomic simulation models for the self-consistent assessment of future risks. We developed uncertainty quantification methods that allow the use of highly uncertain data to determine impacts at multiple levels of spatial and temporal resolution. We produced the first climate change risk assessment with industry and state level detail for the US across the entire probability distribution of impacts. We analyzed the summary risk of climate change, in the absence of climate policy, between 2010 and 2050 for the United States. We expanded the Sandia capabilities in hydrology to convert climate impacts to physical impacts affecting the economy. We added the ability to Sandia hydrology models to address climate change on state-level agriculture.

Significance

Global warming will have a huge effect on the nation's economy and policies that do not consider uncertainty and feedback consequences could have severe counterproductive impacts. Having the predictive ability to quantify these effects will ensure Sandia can provide DOE and the nation with the required analytical capabilities.

Quantifying Uncertainty from Material Inhomogeneity

138738
Year 1 of 1
Principal Investigator: C. C. Battaile

Project Purpose

Sandia's materials science and technology roadmap recognizes the need to establish a capability and core competency in the quantification of margins and uncertainties in materials microstructures and properties. Most engineering materials are inherently inhomogeneous in several ways: in the conditions under which they are processed, in their internal structure, in their properties, and ultimately in their performance. These imhomogeneities manifest across multiple length and time scales, leading to variabilities, i.e. statistical distributions, that are necessary to accurately describe each stage in the process-structure-properties hierarchy, and ultimately to uncertainty in performance, which is usually ignored by describing material properties as averaged, scalar quantities. A robust and predictive assessment of materials performance must incorporate a meaningful treatment of the variability in materials properties at the microstructure scale. We have examined the connection between materials variability and performance, by exploring the plastic damage near defects in polycrystalline brass, as a function of the local microstructure of the material. The results clearly demonstrate the strong influence of local microstructure on materials behavior.

Summary of Accomplishments

Brass sheet was annealed under varying conditions to produce a range of grain sizes, and then machined into tensile specimens. Microstructure-scale holes were then drilled into each specimen using a femtosecond laser. Experiments and simulations of the uniaxial, tensile deformation of the specimens were performed to ascertain the role of microstructure on the deformation behavior near the hole. Electron backscatter diffraction and digital image correlation were both used to elucidate the impact of microstructure on local materials response. Finite element simulations were performed to estimate the plastic deformation near cylindrical holes in single, square crystals subjected to uniaxial tension. These calculations showed that the amount and diffusivity of plastic deformation was highly dependent on the crystal orientation. Finite element simulations of uniaxial tension were also performed on computer-generated microstructures containing both holes of varying sizes, and a rounded slot. In the former case, the distribution and magnitude of plastic deformation was found to be qualitatively consistent with experimental data. In the latter case, the maximum plastic strain was extracted from multiple simulations, and statistically analyzed to histogram. The standard deviation of the maximum plastic strain was found to be nearly 20 percent of the mean. These results demonstrate that in regimes where the characteristic length scale of a material's internal structure approaches that of the phenomena that are critical in determining the material's properties, the inherent variability in internal structure produces uncertainty in the properties. This is especially relevant to localized phenomena, like deformation near defects; and to components that are small relatively to the internal structure of the constituent material(s).

Significance

Modeling and simulation of system performance have matured into core competencies that apply to a large portion of the DOE mission space. Relatively recent attention has been paid to the inherent uncertainty in performance, but generally with little tie to its physical origins, which often lie in materials variability. Understanding the origins and effects of materials variability is key to a robust and predictive assessment of uncertainty in system performance. The results from this work assert that, in a wide range of engineering applications, the impact that the variability in a material's processing and structure can have on its properties and performance simply cannot be safely ignored. Sandia must foster a significant and viable effort to establish generalized knowledge, procedures, and protocols for the implementation of deterministic models in a statistical, nano- and microstructure-driven context that connects unavoidable variability in materials processing, to the inhomogeneity of its structure, to the statistics that describe the resultant properties, and finally to uncertainty in performance. As demonstrated by this project, this can certainly be true in "classical" engineering problems like defect mechanics. It is also of prime importance as we attempt to further miniaturize the components and systems that we design, manufacture, and deploy. By exercising Sandia's immense resources in high-performance, high-fidelity, deterministic, physical models, in a context that captures the inherent variability in both present and future engineering materials, we can establish a predictive, science-based capability that accurately captures not only the materials properties themselves, but also the statistics that underpin those properties. Only then can we hope to robustly address the sources of variability that produce uncertainty in the performance and reliability of the systems that are critical to Sandia's missions.

Measurement of Systemic Resilience Using an Optimal Control Framework

138739
Year 1 of 1
Principal Investigator: E. D. Vugrin

Project Purpose

A paradigm shift from critical infrastructure protection toward "all hazards" critical infrastructure resilience is becoming a priority of federal homeland security authorities. Though resilience has been discussed in homeland security, economics, and various other arenas, little work has been done to quantitatively measure resilience, and no effort has been made to develop a rigorous, mathematical framework for measuring resilience.

Within the context of infrastructure and economic systems analysis, resilience is defined as follows: given the occurrence of a particular, disruptive event (or set of events), the resilience of a system to that event (or events) is its ability to efficiently reduce both the magnitude and duration of the deviation from desired system performance levels. That is, resilience to a particular disruption encompasses both the system's capability to mitigate system output impacts and the ability to recover rapidly and "cheaply." This definition of resilience is amenable to objective functions typically used for reference tracking of system performance in optimal control theory, and, thus, resilience is well-suited to be formulated within an optimal control framework.

We propose to develop a mathematical framework for measuring and optimizing systemic resilience. To this end, investigations will be undertaken to determine control design methods (e.g., linear quadratic regulator [LQR], H-infinity, etc.) most appropriate and feasible for analyzing system resilience. These investigations will determine theoretical system resilience requirements necessary for application of optimal control methods. Resulting feedback control laws will be designed and applied to a basic prototype system. This prototype will be used not only to measure resilience but also as a model with which optimal recovery strategies can be explored.

Summary of Accomplishments

We investigated the development of quantitative resilience through application of control design methods. Specifically, we conducted a survey of infrastructure models to assess what types of control design might be applicable for critical infrastructure resilience assessment. As a result of this survey, we developed a decision process that directs the resilience analyst to the control method that is most likely applicable to the system under consideration. Furthermore, we developed optimal control strategies for two sets of representative infrastructure systems to demonstrate how control methods could be used to assess the resilience of the systems to catastrophic disruptions. In the first application, we evaluated the resilience of a set of supply-consumption systems. Through this example, we quantitatively verified qualitative observations about resilience enhancement strategies. In the second application, we considered a chemical supply chain prototype model. This system is modeled by a set of coupled partial differential equations. The number of states required to simulate this system is large and computationally intensive, a common challenge for modeling infrastructure systems. The purpose of this investigation was to demonstrate that reduced order modeling techniques, such as proper orthogonal decomposition (POD), can be used on high order systems and then combined with optimal control strategies to perform resilience analyses. We also developed recommendations for future work to continue the development of quantitative resilience analysis methods.

Significance

Increasing the resilience of national infrastructures will enhance national security by ensuring that the critical systems maintain functionality during disruption. A sound mathematical approach to resilience analysis will provide a consistent methodology for critical infrastructure resilience analysis. We provided a first step towards that goal.

Refereed Communications

E.D. Vugrin, D.E. Warren, M. A. Ehlen, and R.C. Camphouse, “A Framework for Assessing the Resilience of Infrastructure and Economic Systems,” to be published in *Sustainable Infrastructure Systems: Simulations, Imaging, and Intelligent Engineering,* New York, New York: Springer-Verlag,

Enhanced Molecular Dynamics for Simulating Porous Interphase Layers in Batteries

139074
Year 1 of 1
Principal Investigator: J. A. Templeton

Project Purpose

Understanding of solid/electrolyte interfaces, including the formation, dynamics, and degradation of the solid electrolyte interphase (SEI), is a key technological issue limiting battery development. Molecular dynamics (MD) is a promising tool to study the SEI due to its ability to explicitly represent the complex atomic structure of the interphase and the transport of ions. However, one of the most important physics missing from the simulation of the SEI with MD is the inclusion of electric field effects. We therefore propose to develop a method that includes an electric field and its effects on ion motion in solution by leveraging our previous efforts in electron/phonon two-temperature modeling for MD of solids.

Our approach will be formulated using an atomistic-to-continuum framework wherein the solvent, solute, solid, and interphase will be represented in MD while an electric potential is computed on an overlaid finite element (FE) mesh. Bidirectional coupling will ensure that the MD and FE each receive the appropriate information to accurately simulate the system, e.g. location of the ions and their effects on the electric field. To improve the utility of this work for the wider community, this project will deliver a documented method to simulate electrostatic effects on ionic fluids in porous media and its implementation in Sandia's molecular dynamics code LAMMPS.

Summary of Accomplishments

We developed the multiscale modeling approaches necessary to include anisotropic electric fields in molecular dynamics (MD) simulations by coupling them to external finite element (FE) models using atomistic-to-continuum (AtC) methods. The correctness of these techniques was demonstrated by implementing them in the Sandia MD code LAMMPS and performing a series of computations of systems similar to the solid-electrolyte interphase (SEI) layer. Bidirectional physics coupling is enabled by computing the electric potential on a FE mesh with source terms determined from MD. The resulting electric field is applied to the atoms to account for their long-range electrostatic interactions. Short-range corrections were also developed and implemented to make the method compatible with many interatomic electric potentials already in LAMMPS. Synthesis of all these components provides a model that can account for consistent long- and short-range interatomic electrical interactions without the need to use periodic boundary conditions, inappropriate for the SEI layer. Another important differentiating factor between this and other work is that the FE solution for the electric potential allows boundary conditions to be applied to the electric field, and hence the atoms. In addition to standard boundary conditions involving fixed potentials or electric fields, we designed and tested specialized boundary conditions to handle the charged surfaces found in batteries.

Quantitative comparisons were made between the models developed in this work and existing methods that account for long-range electrical interactions. Good agreement between them and the AtC model was obtained. Further simulations were performed of technologically relevant configurations, such as salt water flow in a nanochannel and ion transport through carbon nanotubes to a charged surface. The latter case serves as a surrogate for the SEI layer and demonstrates the ability of the model to capture the relevant physics of nanoscale flows through porous media in the presence of electric fields.

Significance

This project supports the DOE's mission to foster energy security for the United States since mitigating environmental impacts of energy usage will be forwarded by developing battery technology for large scale vehicle electrification. Our method will provide a competency for continuing work involving multiscale simulation of charge transport in porous media with the end goal being a comprehensive capability for rational materials design of battery/supercapacitor electrodes.

Approaches for Scalable Modeling and Emulation of Cyber Systems

139147
Year 1 of 1
Principal Investigator: J. Mayo

Project Purpose

The scale and sophistication of modern computer software, hardware, and deployed networked systems have significantly exceeded the computational research community's ability to understand, model, and predict current and future behaviors. This predictive understanding, however, is critical to the development of new approaches for proactively designing new systems or enhancing existing systems with robustness to current and future cyber attacks. Theoretical and modeling capabilities are needed that will allow us to answer questions such as: How would we reboot the Internet if it were taken down? Can we change network protocols to make them more secure without disrupting existing Internet connectivity and traffic flow? Can a quantifiable increase in Internet security be achieved by greater diversity in "ubiquitous" software and hardware implementations? We propose to begin to address these issues by developing new capabilities for understanding and modeling Internet systems at scale. Specifically, we will address the need for scalable network simulation by carrying out emulations of networks with large numbers of virtualized operating-system instances on high performance computing clusters, and study the interaction networks (physical or virtual) in real and emulated computer systems to understand their overall emergent behavior and identify system characteristics that lead to global robustness. The combination of complexity science-based analysis of heterogeneous cyber systems coupled with simulation/emulation tools that will be developed in this project will provide a foundation for future predictive tools for cybersecurity, and a game-changing capability for Sandia and its national security and research customers.

Summary of Accomplishments

We combined theoretical and computational approaches to better understand the potential emergent behaviors of large-scale cyber systems. We developed new capabilities for understanding and modeling Internet systems at scale. Specifically, we addressed the need for scalable network simulation by carrying out emulations of a network with 1 million virtualized operating system instances on a high-performance computing cluster — a "virtual Internet". We also explored mappings between previously studied emergent behaviors of complex systems and their potential cyber counterparts. Our results provide foundational capabilities for further research toward understanding the effects of complexity in cyber systems, to allow anticipating and thwarting hackers. In addition, the capability for large-scale emulation offers a new application for high-performance computing resources that complements traditional scientific computing.

Significance

Understanding of cyber threats is critical to better protecting our information technology infrastructure. The work done in this project will help address critical needs for scalable cyber network modeling, simulation, and emulation, and will enable development of predictive modeling capabilities for cybersecurity applications.

NANOSCIENCE TO MICROSYSTEMS INVESTMENT AREA

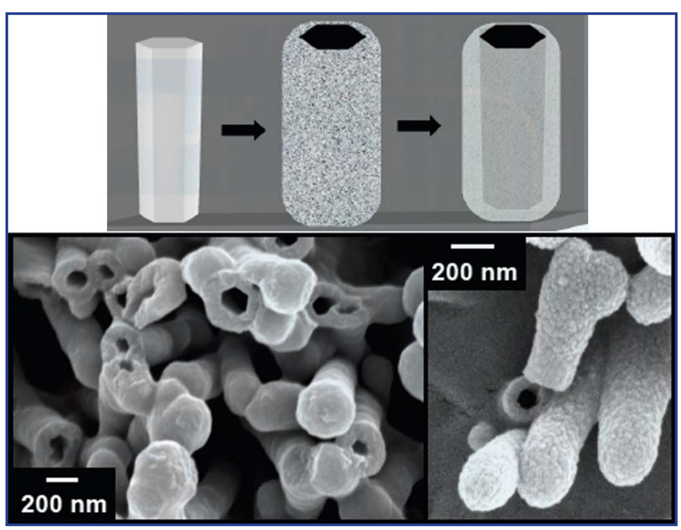
This investment area (IA) funds both fundamental and applied research into phenomena that arise from the distinctive properties of matter at the nanoscale (billionths of a meter), the scale of single atoms, small clusters of atoms, and small molecules, and of structures at the microscale (millionths of a meter). This includes both inorganic nanoparticle research and applications, for example, single atomic nanoparticle of metals such as gold, and also biological nanoparticles and nanomachines — and often, the combination of inorganic and biological, with bio-nanostructures sometimes providing models for developers to emulate.

Applications range from micromachines such as tiny heat engines and microelectromechnical systems (MEMs), to quantum cascade lasers to improved computer memories and new types of computing data structures (as in quantum computing), as well as nano- and microstructures showing novel optical and electromagnetic properties that tend not to be observed at larger scales. In addition to fundamental insights into the nature of materials and nanostructures, this IA, ultimately, offers solutions to problems in energy security, climate change, secure communications, cryptography, remote sensing and threat detection, and other arenas germane to national and global security.

Templated Synthesis of Nanomaterials for Ultracapacitors

Project 117832

A hybrid between batteries and capacitors, an ultracapacitor exhibits the best aspects of both energy-storage devices, enabling both the high energy density of batteries and the high power density of capacitors. This project is investigating the use of self-assembly processes to organize nanomaterials into nanoscale architectures, thus maximizing electrode-electrolyte contact area and the use of electrochemically active material in the device in order to optimize its performance. Several synthesis approaches, involving both organic and inorganic templates are being assessed, leading to nanoarchitectures that facilitates access to electrolyte solutions. Oxides of ruthenium and niobium have proved promising in this regard, and anodized alumina substrates have been utilized as templates for deposition of conductive organic polymers. Mathematical models are used to analyze the results of these electrochemical syntheses, and conversely, once performance parameters are established, the models can predict nanoarchitectures that maximize performance. This research has indicated that highly desirable energy storage parameters of ultracapacitors — their rapid storage and release of charge — can be achieved relatively inexpensively and by several alternative routes.

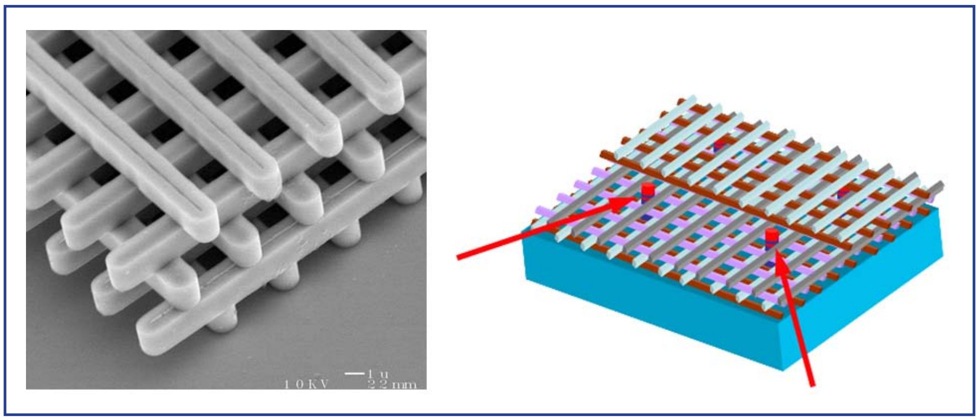


Hollow-rod nanostructures that are ideal for promoting electrolyte access to the electro-active materials previously deposited

Enhanced Spontaneous Emission Rates in Visible III-Nitride LEDs Using 3D Photonic Crystal Cavities

Project 105917

The propose of this project is to investigate interaction between semiconductor emitters and three-dimensional (3D) photonic crystal cavities in the visible spectrum. The goal is to use a dielectric structure to dramatically enhance the spontaneous emission rate for visible emitters. This will allow improvement of the overall efficiency of InGaN LEDs. A process has been developed using aerogel to incorporate quantum dots (QDs), such that emitters can be placed in suitable locations within the photonic crystal structure to see changes to the spontaneous emission. Samples with incorporated QDs showed luminescence enhancements as large as three fold, as well as suppression of emission by up to a factor of four. Time-resolved photoluminescence measurements were used to demonstrate that these changes are due to photonic crystal–related changes to the photonic density of states.



Scanning electron micrograph (left) of a logpile photonic crystal, with drawing (right) of such a crystal with implanted indium gallium nitride (InGaN) LEDs (light-emitting diodes [red arrows]).

NANOSCIENCE TO MICROSYSTEMS INVESTMENT AREA

Research on Microsized Acoustic Bandgap Structures

105873
Year 3 of 3
Principal Investigator: R. H. Olsson

Project Purpose

Precise control of phonon propagation/distribution can offer revolutionary capabilities to design and integrate devices which route/control high-frequency electromagnetic signals (radio-frequency [RF] and optical filters, phase modulators, couplers, resonators). This will dramatically impact applications such as RF communications, sensors, analog spectral processing, and acoustic imaging. Acoustic bandgap (ABG) structures are the acoustic wave equivalent of photonic bandgap (PBG) structures, where a range of acoustic frequencies are forbidden to exist in a structured material. At the outset of this project, most prior ABG work was either theoretical or was performed using large hand assembled structures in high acoustic loss liquids or epoxies operating in the 0.1–1 MHz frequency range. Utilizing microfabrication and finite difference time domain (FDTD) modeling we have demonstrated the first microelectromechanical system (MEMS) ABGs in solid, low-loss materials; first at 70 MHz, and more recently at 1 GHz. We have also demonstrated the first micro-ABG based devices, W1 and W3 waveguides formed by removing 1 and 3 rows of scattering inclusions from an acoustic crystal. ABG waveguides are useful for routing acoustic signals and forming miniature delay elements. Utilizing FDTD modeling, a high quality factor (Q=100,000) cavity has been designed based upon our experimentally verified ABG structures. ABG filters/resonators allow the cavity and electro-acoustic coupler design to be decoupled, awarding significant improvement in Q or insertion loss when compared to existing micro-technologies which necessarily trade one for the other.

Summary of Accomplishments

Our group was the first to demonstrate acoustic bandgap (ABG) devices at the microscale in solid-solid material systems, first at 70 MHz with a lattice constant of 90 microns and later at 1 GHz with a lattice constant of 2.5 microns. While polymer based microscale ABGs had been previously demonstrated, these devices had high acoustic losses and were characterized using expensive, $100 K, large, external optical measurement techniques. Our team not only scaled ABGs to low-loss solid material systems but also integrated piezoelectric electro-acoustic couplers with the ABGs for rapid and cheap characterization. These couplers are vitally important, as are low losses, for realizing ABG devices such as waveguides, focusing, and cavities that can be used in real systems. Scaling to an all solid material system required the development of new physical understanding and modeling tools. Our group was the first to report key findings in microscale ABGs such as the desire to have high acoustic impedance contrast but low velocity contrast between the materials forming the ABG. Previous understanding was to maximize both acoustic impedance and velocity mismatch. New modeling capabilities that take into account the finite thickness of the ABG were also developed under this project and were needed to accurately predict the response of the 1-GHz devices. Finally, low-loss acoustic waveguiding inside an acoustic crystal was demonstrated in both the very high frequency (VHF) and ultra (UHF) high frequency bands.

Significance

This research promises to revolutionize communications systems in the frequencies 100 MHz to 3 GHz and put Sandia at the forefront of a new branch of science of direct interest to our DOE and DOD customers. Phonon control research and devices such as acoustic signal processors and lenses are important to several of Sandia's national security missions including nuclear weapons security, weapons of mass destruction (WMD) nonproliferation, homeland security, and maintaining the technological superiority of the US military.

Refereed Communications

R.H. Olsson III and I. El-Kady, "Microfabricated Phononic Crystal Devices and Applications," *Measurement Science and Technology*, vol. 20, p. 012002 (1-13), January 2009.

Intelligent Front-End Sample Preparation Tool Using Acoustic Streaming

105874
Year 3 of 3
Principal Investigator: D. W. Branch

Project Purpose

The purpose of this project is to rapidly and efficiently extract nucleic acid from biological samples prior to detection. At present, biological samples must be manually prepared requiring additional time, effort, and equipment, often reducing the effectiveness of a microsystem solution. The lack of efficient front-end sample handling technology impacts a broad range of biosensor systems, ultimately limiting their portability, reducing sample throughput, and causing detection variability. Current field deployable systems such as the BioBriefcase and BioWatch lack any sort of front-end sample handling and instead rely on operator intervention and the use of reagents.

To address these problems, we are creating an intelligent front-end sample preparation tool for bioagent detectors using acoustic wave streaming. Acoustic wave streaming technology is known to be a highly efficacious method to exert controlled forces on fluids, cells, and particles. We have successfully demonstrated the ability to lyse cells flowing within microchannels and bound to surfaces. In addition, we have demonstrated rapid fluid mixing, particle trapping, and elective removal of nonspecifically bound particles and proteins, using only acoustic energy with no reagents. To enable complete sample-handling bioagent detection systems, we propose to build a front-end preparative cell lysis and particle manipulation tool for integration with our existing acoustic and optical microsensor technology for a complete on-chip solution. Our overall goal is to perform all sample handling and detection using an integrated device.

Summary of Accomplishments

We have successfully developed a nucleic acid extraction system based on a microacoustic lysis array coupled to an integrated nucleic acid extraction system, all on a single cartridge. The microacoustic lysing array is based on 36º Y-cut lithium niobate, which couples bulk acoustic waves (BAW) into the microchannels. The microchannels were fabricated using Mylar laminates and fused silica to form acoustic-fluidic interface cartridges. The transducer array consists of four active elements directed for cell lysis and one optional BAW element for mixing on the cartridge. The lysis system was modeled using 1D transmission line and 2D FEM models. From the computational models, a flow rate of 10 µL/min produced a temperature rise of 23.2 ºC and only 6.7 ºC when flowing at 60 µL/min. The measured temperature changes were 5 ºC less than the model. The computations were used to optimize the acoustic coupling to the microchannel region. Using *Escherichia coli*, we achieved a lysing efficacy of 49.9 ± 29.92% based on a cell viability assay with a 757.2% increase in ATP release within 20 seconds of acoustic exposure. A bench-top lysing system required 15–20 minutes operating up to 58 watts to achieve the same level of cell lysis. We demonstrated that active mixing on the cartridge was critical to maximize binding and release of nucleic acid to the magnetic beads. When using a sol-gel silica bead matrix filled microchannel, the extraction efficacy was 40%. The cartridge based magnetic bead system had an extraction efficiency of 19.2%. For an electric field based method that used Nafion films, a nucleic acid extraction efficiency of 66.3% was achieved at 6 volts DC. For the flow rates that we tested (10–50 µL/min), the nucleic acid extraction time was 5–10 minutes for a volume of 50 µL.

Significance

This project represents a critical step toward the development of a rapid, autonomous, and adaptable sample preparation tool for the lossless extraction of DNA from cells and spores without the need for reagents. Our proposed technology promises an innovative approach to provide much needed intelligent front-end sample handling to support future biodetection systems to detour the production of biological weapons that threaten the peace and security of America and its allies.

Refereed Communications

K.E. Achyuthan, J.L. McClain, Z. Zhou, D.G. Whitten, and D.W. Branch, "Spectroscopic Analysis of the Noncovalent Self-assembly of Cyanines Upon Various Nucleic Acid Scaffolds," *Analytical Science*, vol. 25, pp. 469-474, April 2009.

Development of a Multivariate Electrochemical Tool (MET)

105875
Year 3 of 3
Principal Investigator: C. L. Stork

Project Purpose

The heart of this project is the development of a multivariate electrochemical tool (MET) that will help understand a diverse set of electrochemical systems such as electrocatalyst development, fuel cell operation, corrosion and materials reliability, and sensing. There are three key features of this approach: (1) the ability to identify subtle controlling aspects of an electrochemical system leading to fundamental scientific understanding; (2) the ability to identify and isolate features of the electrochemical response that are relevant to a material of interest; and (3) identification of interdependencies in the system response for a subset of materials which lowers the barrier to understanding complex behavior. The function of the MET is to mathematically extract information regarding the underlying chemistry and physics of a system of interest using the wealth of information contained in the electrochemical response. The MET will give the researcher an ability to learn unique characteristics about materials not possible using traditional investigative techniques. Two challenges that must be overcome for this project to be successful are (1) developing the necessary understanding to bridge electrochemical science and multivariate data analysis (MVA), and (2) validating the MET approach by applying it to a critical issue in electrochemical materials science. Meeting the first challenge is an iterative process between electrochemical experimentation and development of the MVA techniques in such a fashion as to address physical influences (e.g., electrode size, ion concentration and speciation, fouling) and inherent complexities of electrochemical data (nonlinear response, peak shifting, etc.). To meet the second challenge the focus will be on a corrosion science problem since this corrosion is inherently difficult to treat using automated, quantitative data analysis techniques. MVA will be used to extract correlations between short-term electrochemical impedance spectroscopy (EIS) measurements and long-term exposure tests of coated metals.

Summary of Accomplishments

One key project accomplishment was the systematic analysis of cyclic voltammetry data from an electrode array, enabling the accurate prediction of the concentrations of the sugars, fructose, galactose, and glucose in complex, multicomponent systems. A unique feature of the developed electrode array relative to other published work is the wide diversity of electrode materials incorporated in the array, with 41 different metals and metal alloys represented. Employing a powerful data-visualization technique developed in this project, correlation plots identified potential regions and electrodes that scaled most linearly with sugar concentration, and the number of electrodes used in building predictive models was reduced to 15. Partial least squares regression models relating electrochemical response to sugar concentration were constructed using data from single electrodes and multiple electrodes within the array, and the predictive abilities of these models were rigorously compared using a nonparametric Wilcoxon test. While including data from multiple electrodes offered no benefit in predicting sugar concentration, use of the array afforded the versatility of selecting the best single electrode for each analyte. A second key accomplishment was the successful application of the MET approach to a complex corrosion problem, namely the assessment of coating performance in corrosive environments. Multivariate analysis (MVA) methods were used to extract chemically meaningful correlations between short-term (week 1) electrochemical impedance spectroscopy (EIS) measurements and long-term (weeks 6 and 8) exposure tests of coated metals. However, the extracted correlations were complex and not universally applicable to all samples. The entire frequency spectrum was utilized in the MVA of the short-term EIS data, allowing one to identify which portions of the EIS data were critical for predicting longer-term corrosion degradation of the coated metals. MVA models indicated that the mid-frequency range, from approximately 1 to

100 Hz, was most useful in assessing long-term coating performance, providing valuable information regarding potential coating breakdown mechanisms.

Significance

The MET will help solve electrochemical material science issues related to virtually every DOE goal from defense (stockpile stewardship through corrosion science, embedded surveillance), energy (H_2 economy through electrocatalysis, fuel cells), science (through fundamental scientific understanding of electrochemical materials), homeland security (sensing in water and process streams), and environment (through corrosion protection of nuclear waste containment systems such as Yucca Mountain).

Refereed Communications

W.A. Steen and C.L. Stork, "Using Multivariate Analyses to Compare Subsets of Electrodes and Potentials Within an Electrode Array for Predicting Sugar Concentrations in Mixed Solutions," *Journal of Electroanalytical Chemistry*, vol. 624, pp. 186-196, December 2008.

R. Polsky, C.L. Stork, D.R. Wheeler, W.A. Steen, J.C. Harper, C.M. Washburn, and S.M. Brozik, "Multivariate Analysis for the Electrochemical Discrimination and Quantitation of Nitroaromatic Explosives," *Electroanalysis*, vol. 21, pp. 550-556, February 2009.

RF/Microwave Properties of Nanotubes and Nanowires

105876
Year 3 of 3
Principal Investigator: M. Lee

Project Purpose

The purpose of this project was to execute new experimental and theoretical efforts to discover and understand electrodynamic properties of carbon nanotubes and semiconductor nanowires, emphasizing silicon and ZnO. While much research exists on DC electrical properties of nanowires, electrodynamic characteristics represent a major new frontier in nanotechnology. We generated world-leading insight into how low dimensionality and restricted geometry of nanowires yields unique microwave properties outside standard Drude model electron dynamics. The knowledge gained will be directly useful to application of nanowires in a new generation of high-frequency electronics.

We are among the first to open this frontier with a focused effort to measure and model the basic AC conductance of nanowires across frequencies relevant to high-speed communication, computation, radar, sensing, etc. (0.1 to 50 GHz). The research effort spanned the following: 1) synthesis of silicon and ZnO nanowires with varied dimensions, carrier concentrations, and surface states; 2) integration of carbon nanotubes and nanowires into very broad frequency range compatible test platforms; 3) measurement of electromagnetic field scattering by nanowires as a function of frequency and temperature; and 4) theoretical calculations to predict high-frequency characteristics of existing and possibly new physics. We successfully refined our techniques to measure as few as 10 nanowires.

Summary of Accomplishments

The primary goal of this project was to discover the currently unknown science underlying the basic linear and nonlinear electrodynamic response of nanotubes and nanowires in a manner that will support future efforts aimed at converting forefront nanoscience into innovative new high-frequency nanodevices. The project involved experimental and theoretical efforts to discover and understand high-frequency (MHz through tens of GHz) electrodynamic response properties of nanomaterials, emphasizing nanowires of silicon, zinc oxide, and carbon nanotubes. While there is much research on DC electrical properties of nanowires, electrodynamic characteristics still represent a major new frontier in nanotechnology. We generated world-leading insight into how the low dimensionality of these nanomaterials yields sometimes desirable and sometimes problematic high-frequency properties that are outside standard model electron dynamics. In the cases of silicon nanowires and carbon nanotubes, evidence of strong disorder or glass-like charge dynamics was measured, indicating that these materials still suffer from serious inhomogeneities that limit their high-frequency performance. Zinc oxide nanowires were found to obey conventional Drude dynamics. In all cases, a significant practical problem involving large impedance mismatch between the high intrinsic impedance of all nanowires and nanotubes and high-frequency test equipment had to be overcome. In addition, a theoretical study of high-frequency response in one-dimensional carbon nanotubes led to the prediction that the AC response in nanotubes can include collective plasmon oscillations, and that such oscillations can be turned on and off via an applied gate bias. This theoretical result may have significant implications for high-speed carbon nanotube based transistors in the future.

Significance

This effort has the potential to create a new field of nanomaterial electrodynamics, including discovery of new science in the quest to understand nanowire transport beyond DC. This will also serve as the foundational knowledge necessary to exploit properties of nanomaterials to create a new paradigm in innovative high-frequency electronics that can have impact in the following mission areas.

- DOE Defense: Discover foundational knowledge for new class of high-speed nanoelectronics for communication and radar with superior capabilities.
- DOE Science: Discover unconventional new physics on fundamental electrodynamic properties of new nanomaterials.
- DOE Environment: Discover foundational knowledge for new class of high-sensitivity atmospheric environmental sensors.
- DHS: Discover foundational knowledge for new class of high-sensitivity, highly selective toxic and hazardous gas sensors

Refereed Communications

D. Kienle and F. Léonard, “Terahertz Response of Carbon Nanotube Transistors,” *Physical Review Letters*, vol. 103, p. 026601, July 2009.

Novel Diagnostic for Advanced Measurements of Semiconductor Devices Exposed to Adverse Environments

105877
Year 3 of 3
Principal Investigator: M. L. Anderson

Project Purpose

Along with the continuous decrease in the feature size of semiconductor device structures comes a growing need for inspection tools with high spatial resolution and high sample throughput. Ideally, such tools should be able to characterize both the surface morphology and local conductivity associated with the structures. The purpose of this project was to explore and create a technique that may provide a solution to this problem. In particular, this project utilized the low-energy electron microscope (LEEM) to create an analytical technique to efficiently identify differences in dopant type and concentration. The goal was to gain a fundamental understanding of doped semiconductor imaging in order to apply the knowledge to engineering and science applications.

Summary of Accomplishments

In this project, we assessed the LEEM's potential as a semiconductor device imaging tool. Using the Microsystems and Engineering Sciences Applications (MESA) facility, we fabricated a variety of doped silicon test structures to extract the contrast mechanisms and to determine if it is possible to extract quantitative dopant concentration information from the measurements. We showed that the LEEM technique is able to provide reasonably high contrast images across lateral p/n, n/n+, and p/p+ junctions. The observed contrast is attributed to work function differences between the doped regions. In particular, we investigated doped n- and p-type regions buried under a thermal oxide and found that e-beam charging during imaging can lead to enhancement of the n/p contrast. In addition, we completed a LEEM investigation of another series of similar test structures in which the thermal oxide was removed by a chemical etch. With the oxide removed, we are able to obtain intensity-versus-voltage (I-V) curves through the transition from mirror to LEEM mode and determine the relative positions of the vacuum cutoffs for the differently doped regions. The relative positions in voltage of the vacuum cutoffs are a direct measure of the work function difference between the p- and n-doped regions.

Significance

The key achievement of this project has been to build a foundation for application-based LEEM work. With a fundamental understanding of contrast mechanisms for doped silicon (with and without an oxide) we will be able to leverage this knowledge for internal and external use. The results will be relevant to a number of DOE missions and Sandia programs including photovoltaic systems, solid state lighting, nanowire studies, and failure analysis.

Irradiation for the Novel Radiolytic Formation of Superalloy Nanoparticles

105878
Year 3 of 3
Principal Investigator: T. M. Nenoff

Project Purpose

We propose a fundamental science study into the radiolytic synthesis of nanoparticles that is more flexible and versatile than existing electrochemical, surfactant, and pyrolytic methods. Radiolysis presents an entirely new area of basic research into alloy and superalloy nanoparticle synthesis that holds the promise for a universal method of nanoparticle formation. Our main focus of the project is to develop a fundamental understanding of the materials science behind these nanoparticle formations and expand it to the field of Ni-based superalloys.

The project focuses on the basic research associated with both the nanoparticle formation (through the chemistry of the radiolysis of water and its effect on metal solution salts) and nanoparticle size retention (through interfacial chemistry of metal/alloys and organic capping agents). We propose an entirely new approach for the novel synthesis of superalloy nanoparticles, using gamma-irradiation for the radiolysis of solvating water from Sandia's uniform cobalt-60 source and pulsed proton irradiation using the directional external beam end-station of Sandia's tandem Van de Graff accelerator.

Our team will focus on the structure/property relationship between nanoscale materials and bulk scale effects; we will include density functional theory (DFT) modeling, inorganic synthesis, radiation testing, and characterization to develop a fundamental understanding of "how" and "why" nanoparticles form by radiolysis and maintain their size and integrity. For alloys, we will study the chemistry needed for the radiolysis of solutions containing several types of reducible metal ions. We will also focus on the materials science behind (1) alloy composition variation, (2) anisotropic nanoparticle formation, and (3) preservation of nanodimensioned particles. We will also study the interfacial science of interactions between nanoparticles and organic ligands (i.e., functional groups, concentrations). In particular, we will study the effects of different ligands on nanoparticle size stabilization.

Summary of Accomplishments

We used room temperature radiolysis, density functional theory, and various nanoscale characterization methods were used to synthesize and fully describe Ni-based alloy nanoparticles (NPs) synthesized at room temperature. These complementary methods provide a strong basis in understanding metastable phase regimes of alloy NPs whose reaction formation is determined by kinetic rather than thermodynamic reaction processes. Four series of NPs, (Ag-Ni, Pd-Ni, Co-Ni, and W-Ni) were analyzed and characterized by a variety of methods, including ultraviolet-visible (UV-vis) spectroscopy, transmission electron microscopy, high-resolution transmission electron microscopy (HRTEM), high-angle annular dark field scanning transmission electron microscopy (HAADF-STEM) and energy-filtered transmission electron microscopy (EFTEM) mapping.

In the first focus of research, AgNi and PdNi were studied. Different ratios of Ag_x- Ni_{1-x} alloy NPs and $Pd_{0.5}$-$Ni_{0.5}$ alloy NP were prepared using a high dose rate from gamma irradiation. Images from HAADF show that the Ag-Ni NPs are not core-shell structure but are homogeneous alloys in composition. EFTEM maps show the homogeneity of the metals in each alloy NP. Of particular interest are the normally immiscible Ag-Ni NPs which usually form core-shell structures in thermodynamically driven reactions. All evidence confirmed that homogeneous Ag-Ni and Pd-Ni alloy NPs were successfully synthesized by high dose rate radiolytic methodology. A mechanism was proposed to explain the homogeneous formation of the alloy NPs.

In the second set of work, CoNi and WNi superalloy NPs were attempted at 50/50 concentration ratios using high dose rates from gamma irradiation. Preliminary results on synthesis and characterization have been completed and are presented. As with the earlier alloy NPs, no evidence of core-shell NP formation occurs. Microscopy results seem to indicate alloying occurred with the CoNi alloys. However, there incomplete reduction of the Na_2WO_4 to form the W^{2+} ion in solution; the predominance of WO^+ appears to have resulted in a W-O-Ni complex that has not yet been fully characterized.

Significance

This project builds a foundation in materials research that will benefit DOE and Sandia national security missions and strategic goals. In particular: scientific discovery and innovation, energy security, and nuclear security for applications require lightweight, corrosion resistant, sintered refractory materials (e.g., weapons casings and connects, aircraft, satellites, power plants, gas turbine engines and burners).

Refereed Communications

Z. Zhang, J. Huang, D.T. Berry, P.P. Provencio, T.M. Nenoff, “Room Temperature Synthesis of Thermally Immiscible Ag-Ni Nanoalloys,” *Journal of Physical Chemistry C*, vol. 113, pp. 1155-1159, January 2009.

Microkelvin Molecule Production

105879
Year 3 of 3
Principal Investigator: D. W. Chandler

Project Purpose

Measurable amounts of molecules with a temperature on the tens of millikelvin range using a unique molecular beam scattering technique are produced. These experiments led us to propose a collision based technique, this project, for cooling molecules to the microkelvin temperature range. The new idea is to collide a molecule with a microkelvin atom of the same mass. Because the atom and molecule have the same mass there is a finite probability that the collision will result in the transfer of nearly all of the momentum of the molecule to the atom (much the same as when playing billiards and a shot results in the cue ball being stationary). The technology for producing stationary atoms is well established in the atomic physics community. We plan on utilizing this capability to produce a sample of ultracold atoms (^{87}Rb, initially). Initial experiments will center on collisionally stopping ^{85}Rb in the MOT (magneto-optical trap) of ^{87}Rb in order to demonstrate the viability of this technique for stopping a particle of nearly equal mass. After this first proof-of-principle experiment is performed we will move to the task of slowing and trapping of molecules. The ^{87}Rb sample will be exposed to gas of molecules of approximately the same mass (HBr molecules). A small fraction of these molecules will have collisions with the atoms that transfer sufficient momentum that they will then be slowed to a speed at which they can be captured by an external field (electric, magnetic or off-resonant laser field). These slow molecules will then undergo collision with the surrounding microkelvin temperature atoms and become thermalized at the microkelvin temperature. This project has the purpose of developing the technology and techniques required to produce and manipulate useful densities of microkelvin temperature molecules.

Summary of Accomplishments

The project's primary objective was to develop a new experimental technique for producing microkelvin temperature molecules via collisions with laser cooled samples of trapped atoms. The key scientific accomplishments are the following:

We have extensively developed the theory and underlying mathematics to formulate a novel technique for producing microkelvin cold molecular samples from room temperature and supersonic molecular beams. We have designed, built, and tested an experimental apparatus consisting of an ultrahigh vacuum chamber and four frequency stabilized diode laser systems, capable of producing microkelvin temperature atomic samples using the technique of laser cooling. Kinematic cooling between hot thermal molecules and these cold atomic samples is the fundamental tenet behind the microkelvin cold molecule technique. Finally, we have conducted several experiments which test the ability for elastic collisions to kinetically cool particles from supersonic beams down to near zero velocity in the laboratory frame. We have published an invited peer-reviewed article, and a book chapter detailing this research. A further paper is in preparation, which details the experimental results from our initial elastic scatting experiments.

Significance

The novelty of this technique is that it is a unique, general, broadly applicable, low-cost method for producing samples of cold molecules and cold atoms that cannot be laser cooled. These cold samples of molecules provide for a fundamentally new approach in chemical dynamics, in that we can now control and manipulate chemical systems on the quantum level. This research addresses an expressed desire from the DOE Office of Science to move fundamental research beyond observational science to directly controlling and manipulating atoms, molecules, and corresponding phenomena. The DOE Basic Energy Sciences Program is focused on describing molecular and atomic interactions at the most fundamental level, that of the potential energy surface between them. Cold molecule interactions are extremely sensitive to the shape of intermolecular potentials. Ultracold samples will allow for new quantum computers, ultrahigh-resolution spectroscopy that forms the basis for gravity gradient detectors, atomic clocks, and the measurement of fundamental constants of nature.

Refereed Communications

K. Takase, L.A. Rahn, D.W. Chandler, and K.E. Strecker, "The Kinematic Cooling of Molecules with Laser-cooled Atoms," *New Journal of Physics*, vol. 11, p. 055033, May 2009.

Compositional Ordering and Stability in Nanostructured, Bulk Thermoelectric Alloys

105893
Year 3 of 3
Principal Investigator: D. L. Medlin

Project Purpose

Thermoelectric materials have many applications in the conversion of thermal energy to electrical power and in solid-state cooling. The central materials research challenge is to improve the intrinsic energy conversion efficiency of the thermoelectric material. In general, materials development schemes to improve this efficiency are driven by the need to maximize the Seebeck coefficient, and to balance the competing requirements of high electrical conductivity, and low thermal conductivity. A useful parameter that characterizes the energy conversion efficiency of a material is the so-called thermoelectric figure-of-merit, ZT. Advances over the past decade show that it is possible to enhance ZT in nanoscale systems by taking advantage of quantum confinement and carrier scattering effects to enhance the Seebeck coefficient, and phonon scattering at interfaces to reduce the lattice contribution to thermal conductivity. Because many existing and envisioned thermoelectric applications will require a material that is itself of macroscopic dimension, recent reports of property enhancement in bulk alloys possessing nanometer-scale compositional modulations have generated much excitement. However, developing and applying such nanostructured, bulk thermoelectric alloys will require a greatly improved fundamental understanding of how these alloys form and the mechanisms by which their thermoelectric properties are enhanced. These issues motivate the questions posed in our project: namely, (1) What controls the formation of property-enhancing nanostructures in bulk thermoelectric alloys? and (2) How does this nanostructure relate quantitatively to the measured thermoelectric properties?

Summary of Accomplishments

Over the course of this project we investigated and analyzed key issues governing the mechanisms of interface formation in nanostructured bulk thermoelectric materials and how these nanostructures are quantitatively related to the measures of the thermoelectric performance, namely the Seebeck coefficient, thermal conductivity, and electronic conductivity. Accomplishments include, discoveries of the mechanisms of nanoscale precipitate formation in rocksalt structured tellurides, measurements of the connection between nanostructuring and thermoelectric performance in lamellar thermoelectric nanocomposites; and development of a theory and mechanism explaining how metallic inclusions in semiconductors can enhance thermoelectric performance via energy filtering and reduction of thermal conductivity.

Significance

Thermoelectric materials have diverse energy conversion and cooling applications that cut across much of our mission space in energy and nuclear security. Existing and potential future applications include long-term high-reliability power sources, localized cooling devices, low-temperature power scavenging, and high-temperature waste heat recovery. The fundamental discoveries derived from this research will provide predictive guidance for developing new thermoelectric materials with improved performance.

Refereed Communications

J.D. Sugar and D.L. Medlin, “Precipitation of Ag_2Te in the Thermoelectric Material $AgSbTe_2$,” *Journal of Alloys and Compounds*, vol. 478, pp. 75-82, June 2009.

D.L. Medlin and G.J. Snyder, “Interfaces in Bulk Thermoelectric Materials,” *Current Opinion in Colloid and Interface Science*, vol. 14, pp. 226-235, August 2009.

Phonon Engineering for Nanostructures

105906
Year 3 of 3
Principal Investigator: S. L. Shinde

Project Purpose

As advances in lithographic techniques have extended the limits of miniaturization, the role of phonons in modulating device performance has increased substantially. Consequently, future device design approaches will have to be based on a detailed understanding of the physics of phonon propagation and their interactions in structures. Currently, gaps exist in our knowledge of phonon behavior in solids. These gaps include phonon transport across arbitrary interfaces, the scattering of phonons from crystal defects, phonon interactions with delocalized electrons/collective electronic excitations, and solid acoustic vibrations when these occur in structures with small physical dimensions. Closing these gaps will enable the design of structures that provide novel thermal solutions, such as a phonon waveguide, and enhance our scientific knowledge of nanoscale electronics and nanomechanics, including electron transport from nanoclusters to surfaces and internal dissipation in mechanical resonators. Our strategy will be to develop experimental test structures that will reduce the complexity of phonon scattering phenomena and to use these structures to develop and test models of phonon transport. For example, test specimens will be produced using controlled stacked low-angle twist boundaries in Si to evaluate the role of phonon scattering at well-defined internal boundaries. Also, phonon channeling and confinement will be assessed in nanolithographically defined test structures in Si and diamond where good-quality phonon scattering measurements can be made and used for model comparison and assessment. Standard thermal conduction measurements, as well as surface probing with ultrafast laser pulses is being employed to study the phonon propagation. Practical benefits of the proposed physics-based, bottom-up approach to heat transfer include new thermal management solutions for high-power terrestrial and space-based electronics and robust phonon transport physics models for developing nanoelectronic/mechanical systems for sensing, energy harvesting, and optoelectronics.

Summary of Accomplishments

We analyzed the phonon transport across and along interfaces at nanoscale. To study the phonon transport across interfaces with known atomic structures, we created twist boundaries from Si single crystals and established the structure of the boundary using cross-sectional transmission electron microscopy (TEM), and chemical analysis at 2-nm scale at the interface. This processing itself established a new capability to produce bi-crystal structures with predetermined orientations to create interfaces with known atomic structures. The picosecond laser measurement technique developed at the Idaho National Laboratory (INL) for this project demonstrated the capability of measuring the Kapitza resistance of these interfaces, and concurrently optimized molecular dynamics simulations carried out at Stanford University established the capability to model such interfaces. This work has been reported in three published manuscripts and has generated follow-on funding.

The work on differential nanostructures is a completely new concept. It involved a very strong coupling between simulation and design to optimize a design that would produce experimentally discernable results. The work also involved extensive development of lithography techniques to actually produce these structures. This involved, after substantial initial lithography techniques explorations, three different lithography steps with optical, electron (e)-beam, and finally focused ion beam patterning to produce the final differential structures. The innovative nature of this work has resulted in it being offered as a part of the Center for Integrated Nanotechnologies (CINT) Platform in 2009.

In addition to the three published or submitted manuscripts, there are four other manuscripts being written for submission. The project results led to a full single-investigator and small-group research (SISGR) DOE Basic Energy Sciences proposal, two submitted invention disclosures, and three presented talks. This pioneering project has established key collaborations with Stanford, INL, and Rennselaer Polytechnic Institute, and the team is definitely planning to continue this activity in the years to come.

Significance

Understanding phonon transport opens applications in many areas: thermal management to allow co-location of high and low power devices, efficient operation of surface acoustic wave (SAW) devices by controlling phonon reflections, schemes for phonon channeling for acoustics, energy harvesting and phonon engineered devices. It is highly relevant to Sandia's efforts in thermoelectrics for energy harvesting and in electronics and optoelectronics, which will benefit efforts in energy efficiency and new Energy Frontier Research Centers (EFRC) by DOE.

Refereed Communications

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The Many Mechanisms for Strain Relaxation in III-Nitride Heterostructures: How, When and Why?

105914
Year 3 of 3
Principal Investigator: S. R. Lee

Project Purpose

III-nitride semiconductor alloys have been established as the materials of choice for bright, efficient emission of green, blue, or ultraviolet light. These materials will have broad impact in solid-state lighting, detection of chemical and biological weapons agents, non-line-of-sight communications, and high-frequency electronics. However, these important applications are limited by a host of scientific issues related to the high density of structural defects associated with nitride growth and lattice mismatch. While these issues bear similarity to those encountered in SiGe- and GaAs-based cubic-semiconductor systems, major complications arise from fundamental differences associated with the III-nitrides, including the hexagonal, highly polar crystal structure, the large lattice-mismatch strains, and the lack of readily available bulk-GaN substrates.

Epitaxial heterostructures with different compositions of InAlGaN lie at the heart of all applications for this system. The lattice-mismatch strains associated with these compositional differences are severe, and the corresponding mismatch stresses can be enormous, on the order of 1-10 GPa. A source of frustration, but also scientific opportunity, is that the III-nitrides exhibit a bewildering variety of mechanisms to relax the mismatch stress, including fracture, misfit dislocations, modified stoichiometry, v-defect formation, surface roughening, stacking-fault or inversion-domain generation, and inclination of pre-existing threading dislocations. These mechanisms are not fully understood, and it remains difficult to predict the primary relaxation pathway for growth of an arbitrary heterostructure.

In this project, we have conducted an in-depth investigation of selected relaxation processes in III-nitride heterostructures, with the primary goal being to understand particular mechanisms in detail, by making use of Sandia's world-class metal-organic chemical-vapor-deposition (MOCVD) facilities, combined with *in-situ* and *ex-situ* analysis of strain, structure, and composition. The knowledge we have obtained from these studies will help provide a rational basis for developing engineering solutions that enable better devices.

Summary of Accomplishments

In FY 2007, we investigated three main topics: The first topic involved experiments on inclined threading dislocations in AlGaN/AlN, where we focused on the effects of alloy composition and surface morphology on the inclination angle of threading dislocations. The second topic involved experiments on misfit dislocations in InGaN/GaN, where we focused on the use of low-threading-dislocation-density substrates and the use of nanoscale AlN interlayers to influence misfit-dislocation formation and glide. The third topic entailed use of a newly available FEI dual-beam ion mill to investigate the use of low-energy focused-ion beams to more efficiently micromachine higher-quality transmission electron microscopy (TEM) specimens needed for this project.

In FY 2008, we focused on four topics: The first was evaluation and optimization of cathodoluminescence and other alternative methods for imaging dislocations in the III-nitrides. The second topic was further research on strain-relaxation mechanisms operating in InGaN heterostructures, where growth of an extensive matrix of samples allowed us to determine that the intrinsic relaxation mode in strained InGaN proceeds via a stress-induced surface-roughening instability followed by introduction of localized misfit-dislocation loops. The third topic was further analysis of inclined-threading-dislocation behavior in specially designed trilayer-AlGaN heterostructures. Here, TEM and x-ray diffraction (XRD) examined the response of inclined dislocations to compositional-mismatch stress. The fourth topic was implementation of a new laser deflectometer on our MOCVD reactor.

In FY 2009, we studied three topics: The first topic examined the accuracy and reproducibility of the previously implemented in-situ wafer-curvature measurement apparatus. The second topic used the wafer-curvature system to analyze the time-dependent dynamics of strain relaxation in AlGaN/AlN heterostructures during growth. Here, we found that Si-doping during growth strongly increases dislocation inclination while in contrast, varying the III/V precursor ratio during growth has minimal effect on inclination. The last area of study involved detailed TEM of dislocations in higher-mismatch-strain AlGaN.

Significance

Technology solutions that address improved energy efficiency and homeland security are central to the DOE research portfolio. III-nitrides are important in the energy arena, through solid-state lighting, with the potential to save 125 billion dollars of US electricity over the next two decades. III-nitrides are also crucial for homeland security as optimal materials for deep-UV lasers and light-emitting diodes (LEDs) that will form the basis of sensitive detectors for surreptitious chemical and biological agents. The knowledge base produced by this project supports and underpins the ongoing development of these national security related technologies.

Refereed Communications

D.M. Follstaedt, S.R. Lee, A.A. Allerman, and J.A. Floro, “Strain Relaxation in AlGaN Multilayer Structures by Inclined Dislocation,” *Journal of Applied Physics*, vol. 105, p. 083507-1 to 13, April 2009.

Enhanced Spontaneous Emission Rates in Visible III-Nitride LEDs Using 3D Photonic Crystal Cavities

105917
Year 3 of 3
Principal Investigator: A. J. Fischer

Project Purpose

The fundamental spontaneous emission rate for a photon source can be modified by placing the emitter inside a periodic dielectric structure allowing the emission to be dramatically enhanced or suppressed depending on the intended application. The propose of this project is to investigate an unexplored realm of interaction between semiconductor emitters and three-dimensional photonic crystal cavities in the visible spectrum. Although this interaction has been investigated at longer wavelengths, very little work has been done in the visible spectrum. This is due in part to the difficulty of fabricating the small feature sizes required, but also to the difficulty of finding suitable dielectric materials. GaN is an attractive dielectric material due to its relatively high refractive index and transparency across the entire visible spectrum. Since GaN-based light emitting diodes (LEDs) have also shown emission across the visible spectrum, the merging of GaN-based emitters with three dimensional photonic crystal cavities is a natural choice for investigation of spontaneous emission enhancement. We will investigate three-dimensional photonic bandgap structures in the visible with embedded GaN-based optoelectronic emitters. An enhancement of the fundamental spontaneous emission rate is expected due to an increased photonic density of states (DOS) at the edge of the photonic gap. The goal will be to use a dielectric structure to dramatically enhance the spontaneous emission rate for visible emitters. This will allow us to improve the overall efficiency of InGaN LEDs which will be particularly useful in the green spectral region where current devices are dominated by nonradiative recombination. During the course of this project, we will demonstrate the shortest wavelength three dimensional photonic band gap structures ever made and utilize these structures to improve the efficiency of InGaN LEDs.

Summary of Accomplishments

During the course of this three-year project, spontaneous emission control was investigated at visible wavelengths using 3D photonic crystal structures. We have expanded our ability to fabricate 3D logpile photonic crystal structures such that structures for use at wavelengths as short as 400 nm with features sizes as small as 70 nm are now possible. New processing procedures were developed so that we could fabricate 3D photonic crystals from TiO_2 which was selected and utilized as the most suitable material for structures in the visible. One-dimensional dielectric distributed Bragg reflector (DBR) cavities were also fabricated with GaN emitters inside as a test case to show modifications to the spontaneous emission rate. This work in 1D has led to interesting fundamental physics studies including research on cavity polariton and strong coupling in wide bandgap semiconductors. In order to study changes to spontaneous emission, emitters were incorporated into a variety of different photonic crystal structures. For DBR cavities in 1D, the cavity was built around GaN emitters with an emission wavelength of 365 nm. Changes to the total photoluminescent (PL) intensity as well as to the luminescence decay time were measured for these samples. For 3D samples, we incorporated quantum dot (QD) emitters as well as fabricating whole structures from GaN. A process was developed using aerogel to incorporate QDs such that emitters would be placed in suitable locations within the structure to see changes to the spontaneous emission. Samples with incorporated QDs showed luminescence enhancements as large as three fold, as well as suppression of emission by up to a factor of four. Time-resolved photoluminescence measurements were used to demonstrate that these changes are due to photonic crystal related changes to the photonic density of states.

Significance

This project has advanced our understanding of spontaneous emission control using photonic crystals and will enable future photonic microsystems where the control and manipulation of light is crucial. Highly efficient InGaN LEDs for general illumination will reduce electricity consumption, reduce our dependence on foreign energy, and minimize our impact on the environment. This work has also led to follow-on funding from DOE Office of Basic Energy Sciences to investigate strong coupling for wide bandgap semiconductors.

Refereed Communications

G. Subramania, Y.J. Lee, A.J. Fischer, T.S. Luk, D. Dunphy, and C.J. Brinker, "Emission Modification of CdSe Quantum Dots by Titanium Dioxide Visible Logpile Photonic Crystal," to be published in *Applied Physics Letters*.

G. Subramania, Y.J. Lee, A.J. Fischer, and D.D. Koleske, "Optical Properties of TiO_2 Logpile Visible Photonic Crystals Nanocavities in the Near-UV and Visible Regime," to be published in *Advanced Materials*.

Advanced Optical Measurements and Novel Microsystems for Characterizing Photophysical Properties of Single Nanoparticles

105922
Year 3 of 3
Principal Investigator: S. M. Brozik

Project Purpose

Conductive and semiconductive nanoparticles having unique electronic, catalytic, or photophysical properties are considered to be promising tools applicable to nanotechnology. Even though the controlled manipulation and organization of these materials is of critical importance, there are currently few methods for generating functional and stable assemblies of bioconjugated nanomaterials. Numerous researchers have proposed different solutions to this challenge in order to generate structures that are both of inherent technological interest and provide a means to better understand the fundamental photophysical, chemical, and electronic properties of nanoparticles. Our approach to these ends focused on combining unique analytical methods, which probe interactions at the single particle level, with molecular self-assembly and recognition-based biochemical synthesis.

A second goal of this project was to demonstrate the use of chaperonins as templates for formation of ordered nanoparticle arrays. Chaperonins would serve as nanoreactors for synthesis and assembly of functionalized nanoparticles and allow release of one particle at a time for controlled assembly into pairs and then into larger multidimensional structures using DNA conjugates

Three primary single molecule optical methods, including hyperspectral fluorescence imaging (HSI), correlation spectroscopy (fluorescence correlation spectroscopy [FCS], dynamic light scattering [DLS]), and surface-enhanced Raman spectroscopy were employed in this work. Together these methods enabled detection and characterization of the resulting nanoassemblies, and pave the way for next generation sensor technologies based on nanoparticle interactions with biomolecules of interest.

Summary of Accomplishments

Formation of complex nanomaterials would ideally involve single-pot reaction conditions with one reactive site per nanoparticle, resulting in a high yield of incrementally modified or oriented structures. Many studies in nanoparticle functionalization have sought to generate highly uniform nanoparticles with tailorable surface chemistry necessary to produce such conjugates, with limited success. In order to overcome these limitations, we have modified commercially available nanoparticles with multiple potential reaction sites for conjugation with single stranded DNA molecules (ssDNAs), proteins, and small unilamellar vesicles. These approaches combined heterobifunctional and biochemical template chemistries with single molecule optical methods for improved control of nanomaterial functionalization.

Several interesting analytical results have been achieved by leveraging techniques unique to Sandia, and they provide multiple paths for future improvements for multiplex nanoparticle synthesis and characterization. Hyperspectral imaging has proven especially useful for assaying substrate immobilized fluorescent particles. In dynamic environments, temporal correlation spectroscopies have been employed for tracking changes in diffusion/hydrodynamic radii, particle size distributions, and identifying mobile versus immobile sample fractions at unbounded dilution. Finally, Raman fingerprinting of biological conjugates has been enabled by resonant signal enhancement provided by intimate interactions with nanoparticles and composite nanoshells.

One of the strategies to immobilize a functional GroEL was to genetically modify the GroEL protein to facilitate immobilization. Following published protocol Asp490, which is located on the outer surface of the equatorial domain, was substituted with cysteine for direct labeling with biotin maleimide.

Significance

This project represents new discoveries in nanoparticle properties and unique behavior of bionanoparticle assemblies which can be applied toward development of future device concepts and enabling advances in electronics, photonics, and sensor technologies. Success in the development of this novel nanoreactor technology based on chaperonin templated assembly of nanoparticles will impact several national security needs in energy, nonproliferation and defense systems.

Science at the Interface: Grain Boundaries in Nanocrystalline Metals

105931
Year 3 of 3
Principal Investigator: S. M. Foiles

Project Purpose

Interfaces are a critical determinant of the full range of materials properties, especially at the nanoscale. Recent advances at Sandia in the prediction of the properties of internal interfaces using atomistic simulations and advanced experimental methods place us in a unique position to advance the understanding of interfaces in nanograined materials. We will extend these computational and experimental methods to develop the first comprehensive model of nanograin evolution based on a fundamental understanding of internal interfaces in a novel material, nanocrystalline nickel. Metals with nanoscale grain structure are known to exhibit dramatically improved strength, but these materials tend to be brittle. It has recently been shown that nanocrystals with a bimodal grain-size distribution possess a unique combination of high-strength, ductility and wear-resistance. However, the practical application of the materials requires a detailed understanding of the microstructural evolution to tailor the structure and ensure its stability. We propose a combined experimental and theoretical investigation of the structure and motion of internal interfaces in nanograined metal. Our novel atomic-scale simulations will be extended and applied to the structure, energetics and mobility of nickel grain boundaries for multiple boundaries and temperatures with an emphasis on the differences between nanograined and micrograin boundaries. Experimentally, pulse-laser deposited nanocrystalline nickel films will be fabricated, annealed and characterized to provide discovery of critical mechanisms and to guide and validate the computational results. We will utilize the atomic-scale results in simulations of structural evolution and stability that incorporate realistic boundary driving force and motion in a crystallographically and geometrically realistic nanocrystalline film structure. The goal is to develop the first understanding of the formation of bimodal grain structures in these materials and the critical interfacial properties that control the structural evolution.

Summary of Accomplishments

Understanding the evolution of grains in nanograined metals combines the challenge of resolving decades-old problems in the field of materials science with that of understanding changes in materials properties due to features on the nanoscale. This project combined both experiment and computation. Experimental annealing and characterization of nanograin nickel grown via pulsed laser deposition highlighted the unique features at the nanoscale. In conventional materials, recrystallization and abnormal grain growth produce largely defect-free grains while this work showed that these growing grains have a high density of stacking-fault tetrahedra (vacancy related defects) and twin boundaries. More surprising is the observation that under certain annealing conditions, grains with a hexagonal-close-packed structure (hcp) undergo abnormal grain growth despite being the thermodynamically unfavorable phase. Computational studies in this project of grain boundary energy and mobility greatly expanded the database of such information. A new theoretical approach in the area of grain boundary crystallography enables the interpolation of grain boundary properties in such a database. The computational studies shed light on a long-standing question in grain growth: why does grain growth stagnate even in high purity samples? Extensive calculations of the mobility of grain boundaries using a novel Sandia developed method reveal the presence of both high- and low-mobility boundaries with relative populations that are temperature dependent. A mesoscale model incorporating this was developed and shows that it leads to growth stagnation. Direct molecular dynamics simulations of grain growth confirmed this picture.

Significance

Nanostructure and microstructure evolution models based on a fundamental understanding of interfaces will enable material design for enhanced strength, wear-resistance, corrosion resistance, reliability and fatigue life in traditional metals and especially in nanograined metals. Such materials will be of broad benefit to DOE and DHS.

Refereed Communications

D.L. Olmsted, “A New Class of Metrics for the Macroscopic Crystallographic Space of Grain Boundaries,” *Acta Materialia*, vol. 57, pp. 2793-2799, April 2009.

D.L. Olmsted, S.M. Foiles, and E.A. Holm, “Survey of Computed Grain Boundary Properties in Face-centered Cubic Metals: I. Grain Boundary Energy,” *Acta Materialia*, vol. 57, pp. 3694-3703, May 2009.

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Pumping Up CO_2 and Its Conversion into Synthetic Fuels and Other Useful Molecules

105932
Year 3 of 3
Principal Investigator: R. A. Kemp

Project Purpose

There may be no bigger issue facing the world's population over the next several decades than CO_2 production and its effect on global warming. As the end of the era of conveniently obtained oil approaches, questions regarding transportation also arise. The negative effects of CO_2 could be mitigated by conversion of CO_2 into useful molecules, or by providing new chemical routes to the recycling of CO_2, especially with the possible availability of hydrogen via nuclear and solar means. This is an area of critical national interest that has attracted attention across divisions at Sandia and other national laboratories. We are examining a span of chemical transformations of CO_2, from highly exploratory, unprecedented routes involving the concept of transition-metal stabilization of reactive fragments and trimerization/oligomerization reactions of CO_2, to the invention of new metal-based catalysts for the conversion of CO_2 into large volume products as valuable intermediates or end products. These would be useful for the fuels and chemical markets. An example would be new molecular-scale catalytic routes to dialkylcarbonates such as dimethylcarbonate (DMC), a gasoline additive and chemical building block, from CO_2 and methanol or ethanol. With the mixture of skilled staff available at Sandia to aid in this research (in computational chemistry, synthetic chemistry, catalyst characterization and testing skills, and overall conceptual process design), we are uniquely qualified to attack this problem. What is to be gained is a notable reduction of CO_2 going directly to the atmosphere, thus allowing CO_2 to be reused and recycled, resulting in a lowering of the levels of CO_2 in the atmosphere. Conversion of a "useless" molecule (CO_2) into valuable chemicals and possibly transportation fuels through homogeneous and nanoscale complexes designed to activate and insert CO_2 is the unifying theme of our work.

Summary of Accomplishments

Our results have yielded many discoveries. We have demonstrated that modifications to the Sn(II) structure of $R_2Sn(OMe)_2$ catalysts can affect the formation of DMC using either CO_2 or urea, and improvements can be made. In a key fundamental finding, we have studied by x-ray crystallography a key intermediate that demonstrates how the carbonate (CO_3^{2-}) moiety is formed using Sn(II) alkoxides as catalysts. We have investigated a novel system based on Zn^{2+} salts containing tetradentate, nitrogen-containing cyclen/cyclam ligands, preparing a number of new ligand/Zn combinations. We have demonstrated the preparation of methylated carbonates using this system; however, the preparation of DMC is hampered by the lack of reactivity of the methylated complex with methanol. The use of hemi-labile arms attached to the nitrogen ligands can potentially solve this issue. In our attempts to prepare organic isocyanates, we have synthesized exceedingly active main group metal amides that react with CO_2 in solution to stoichiometrically yield isocyanates and carbodiimides. Through judicious choice of metal/ligand combinations we have been able to control which isocyanate is formed, and can also make either isocyanates or carbodiimides with 100% selectivities in quantitative yields. In dealing with chemical sequestration of CO_2, we have examined the oligomerization of CO_2 using density functional theory (DFT), and we have allowed DFT to help guide our experimental efforts. We have now demonstrated this concept by preparing novel complexes based on Ca_6 or Sr_6 backbones that absorb and "fix" 12 moles of CO_2 into two new ligands – a phosphino-substituted carbamate as well as the completely unknown $[N(CO_2)_3]^{3-}$ ligand under extremely mild conditions. This ligand has "glued" together three moles of CO_2 with one N atom. This result is important as it demonstrates our concept of using metal ions for stabilization is feasible.

Significance

While all of our proposed project elements were highly speculative, the progress we made on the majority of our goals is of interest to many in the chemistry community. Our concept of "oligomerizing" CO_2 indirectly, rather than forming species such as $(CO_2)_x$ directly, is an intriguing one that we believe others will pursue. It may be possible to do "carbon capture" of CO_2 by further oligomerizing or polymerizing our "glued together" CO_2-containing complexes. The new work in DMC-formation catalysts will also be of interest to industry and DOE. We have captured and crystallographically characterized a key intermediate in the Sn(II) alkoxide catalyzed route to DMC that demonstrates how the carbonate (CO_3^{2-}) moiety is formed, a fundamental study with implications for commercially used systems. The novel Zn-based complexes that we have prepared can yield methylated carbonates stoichiometrically, and we anticipate future work in this area using more effective hemi-labile ligands may allow DMC to be formed catalytically. Significantly, these materials are inexpensive due to the low cost of zinc. In another project element, we have been able to show 100% selective formation of organic isocyanates using either Zn- or Cd-based complexes. If this process can be made catalytic by the use of heteroleptic alkoxy/amido metal species, it will then be of high interest to industrial companies, allowing isocyanates to be produced using waste CO_2. In another project area, DFT calculations indicate that oligomers or polymers of CO_2 $[(CO_2)_x]$ should be energetically favored, albeit barely. However, low energy barriers also indicate that these oligomers or polymers will be easily "unzipped" to re-form CO_2. This ease of decomposing $(CO_2)_x$ indicates that the best opportunities to prepare a thermally stable route to chemically sequestered CO_2 will lie in the oligomerization of the novel "glued together" ligands we prepared earlier.

Refereed Communications

D.A. Dickie, M.V. Parkes, and R.A. Kemp, "Insertion of Carbon Dioxide into Main-Group Complexes: Formation of the $[N(CO_2)_3]^{3-}$ Ligand," *Angewandte Chemie International Edition*, vol. 47, pp. 9955-9957, October 2008.

Nanoengineering of Active Interfaces for Organic-Inorganic Optoelectronics

105933
Year 3 of 3
Principal Investigator: D. R. Wheeler

Project Purpose

To develop the methodologies to truly nanoengineer active organic-inorganic interfaces, new fundamental knowledge is required. Current approaches generally focus on the assembly aspects of bringing together required components at the nanoscale and hoping that interface properties will be sufficient to produce the desired composite response to stimuli. While demonstrating that functional optoelectronic devices such as bulk heterojunction solar cells can be fabricated, these methods produce structures with far less than optimum performance. For example, when two materials are brought into contact the valence and conduction bands bend to maintain a continuous Fermi level. On the nanoscale, these "interfacial" interactions are in fact bulk effects in the nanoregime. We are undertaking a multipronged approach to manipulating the electronic structure of interfaces using bias-driven assembly techniques as well as using newly acquired understandings of interfacial organic polymer structure property relationships.

We have focused on the development of active interfaces and assembly processes that will enhance organic-inorganic hybrid photovoltaics. We will use chemistry to engineer the numerous interfaces that exist in organic photovoltaic devices. These include those between the conducting polymer and the electrodes. Surfaces will be controlled with a combination of onium-assembled monolayers as well as by other assembly techniques such as liquid crystal interactions between polymer chains and thiol and catachol coordination chemistry. Work this year has shown that more than just diazonium and iodonium chemistry is needed to truly engineer interfaces.

The fundamental understandings gained from organic-inorganic interfacial electronic structure research will impact graphene research and organic electronic devices such as organic field-effect transistors FETs and organic sensor platforms.

Summary of Accomplishments

Attempts were made to expand our existing diazonium chemistry to a variety of different oxides and nitrides. Electrochemical assembly of the molecules on a variety of different oxides and nitrides was examined. Poor assembly was realized. Attempts to understand this result were undertaken using x-ray photoelectron spectrometry (XPS) and time of flight secondary ion mass spectroscopy. Unfortunately, the results were inconclusive. Consequently, we expanded the scope of our work to include other chemistries, especially those related to important conductors such as zinc oxide.

We examined thiols on zinc oxide as a method to control the interaction between zinc oxide and poly(3-hexylthiophene) (P3HT). We have developed a new method to assemble different porphyrins and phthalocyanines on titanium oxide nanoparticles and gold nanoparticles using simple chemistry. This self-assembly approach allowed for the fabrication of complex, light-harvesting porphyrin arrays on nanoparticle surfaces, and we are currently exploring the fabrication of these arrays and the photophysical characterization of the resulting devices.

We have also measured the photovoltaic properties of a series of liquid crystalline polymers. This series included both known and unknown polymers that self-organize at interfaces. This interfacial self-organization was hypothesized to improve interfacial electron transfer. Improved photovoltaic response relative to P3HT/ZnO photovoltaics was realized. A study of electrochemical polymerizations of similarly fused thiophenes was undertaken.

Finally, we examined the diazonium assembly process with the goal of generating stacked layered structures containing different functional elements. Gradient structures such as these could be expected to have interesting electrical properties.

Our results are being applied to other applications such as ultracapacitors and battery electrodes. Our self-assembly techniques have dramatically improved our ability to generate electrochemically active surfaces for sensor applications.

Significance

Interfaces dominate photovolatic performance. Better photovoltaic technology could revolutionize energy options in the US. Calculations suggest organic composite photovoltaic devices could have efficiencies as high as 20% and be very inexpensive. Currently, the best devices have only achieved a fraction of this potential. Interfacial electronic control could impact sensors and organic electronics.

Refereed Communications

T.C. Monson, M.T. Lloyd, D.C. Olson, Y. Lee, and J.W.P. Hsu, "Photocurrent Enhancement in Polythiophene- and Alkanethiol-Modified ZnO Solar Cells," *Advanced Materials*, vol. 20, pp. 4755–4759, December 2008.

M.T. Lloyd, R. Prasankumar, M.B. Sinclair, A.C. Mayer, D.C. Olson, J.W.P. Hsu, "Impact of Interfacial Polymer Morphology on Photoexcitation Dynamics and Device Performance in P3HT/ZnO Heterojunctions," *Journal of Material Chemistry*, vol. 19, pp. 4609-4614, July 2009.

M.T. Brumbach, A.K. Boal, and D.R. Wheeler, "Metalloporphyrin Assemblies on Pyridine-Functionalized Titanium Dioxide," to be published in *Langmuir* .

J.C. Harper, R. Polsky, D.R. Wheeler, D.M. Lopez, D.C. Arango, and S.M. Brozik, "A Multifunctional Thin Film Au Electrode Surface Formed by Consecutive Electrochemical Reduction of Aryl Diazonium Salts," *Langmuir*, vol. 25, pp. 3282-3288, March 2009.

The Physics of 1D and 2D Electron Gases in III-Nitride Heterostructure Nanowires

105935
Year 3 of 3
Principal Investigator: G. T. Wang

Project Purpose

We propose using novel free standing III-nitride core-shell nanowires to examine the physics of one-dimensional and two-dimensional electron gases (1DEG/2DEG) formed at the interface in heterostructure nanowires. Specifically, we will focus on AlGaN/GaN core-shell nanowires synthesized by metal organic chemical vapor deposition (MOCVD). These heterostructure nanowires will also allow us to investigate the effects of band-gap engineering and interface manipulation on the transport and optical properties of semiconductor nanowires, an understanding of which may enable ultrafast and ultraefficient nanowire-based electronic and photonic devices. The experimental studies will be complemented by theoretical modeling to understand and predict the electronic and transport properties.

Summary of Accomplishments

III-nitride core-shell heterostructure nanowires were investigated as model systems for studying the formation and physics of 1DEGs and 2DEGs in semiconductor nanostructures, as well as for understanding how surface and interface issues affect the electrical transport and optical properties of GaN nanowires. GaN nanowires as well as AlGaN/GaN and AlN/GaN core-shell nanowires were synthesized and comprehensively studied using a battery of experimental techniques, including cross-section scanning transmission electron microscopy (STEM), energy-dispersive x-ray spectroscopy (EDS), 3D STEM tomography, deep-level optical spectroscopy (DLOS), ultrafast pump-probe measurements, electrical transport (current-voltage [I-V] and field-effect transistor[FET[) measurements, micro photoluminescence (μ-PL), and spatially-resolved cathodoluminescence (CL) measurements. We note that studying the properties of these nanostructures is not trivial, and often times not amenable to standard techniques to study planar III-nitride structures, and that many of our results represent the first successful application of these characterization techniques to III-nitride nanowires or even core-shell nanowires of any materials system. The experimental results show that the growth of AlN or AlGaN shell layers on GaN nanowires has beneficial effects on electrical transport and optical properties, and suggest that the shell-layers passivate detrimental surface states.

Theoretical modeling was also performed in order to calculate the structure of electron gases formed in these novel nanowires. Despite relatively large nanowire diameters, size quantization effects were observed with the formation of 1D electron gases in the AlGaN/GaN nanowires. Spontaneous and piezoelectric polarization effects relevant to the III-nitrides were incorporated into our models. Calculations on nanowires with either a Ga-face (0001) or N-face (000-1) revealed 1DEG formation in both cases for n-type nanowires, although the position of the 1DEG was located at the vertex opposite the (000-1) AlGaN/GaN interface for the N-face case.

Significance

The exceptional properties of nanowires, including ballistic transport, efficient light emission, high sensitivity, and lasing, make nanowires excellent candidates for ultraefficient photonic, sensing, and communications applications critical to Sandia missions in nuclear security and energy security. We demonstrated novel, freestanding III-nitride core-shell nanowires and investigated the role of surfaces and heterointerfaces on the transport and optical properties of nanowires, using a combined experimental and theoretical approach. Our improved understanding of their properties and manipulation of their interface states represents a critical step towards development of novel, ultrafast and ultraefficient nanowire-based electronic and photonic devices.

Refereed Communications

Y. Lin, Q. Li, A. Armstrong, and G.T. Wang, “In Situ Scanning Electron Microscope Electrical Characterization of GaN Nanowire Nanodiodes Using Tungsten and Tungsten/Gallium Nanoprobes,” *Solid State Communications*, vol. 149, pp. 1608-1610, October 2009.

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Injection-Locked Composite Lasers for mm-Wave Modulation

117819
Year 2 of 3
Principal Investigator: G. A. Vawter

Project Purpose

Since its invention, the diode laser has been hampered by limited frequency-modulation response resulting from nonlinear coupling of injected carriers with photons in the laser. This coupling has a relaxation resonance at 15-25 GHz, which limits the frequency response of laser modulation. Very recently, injection locking of small diode lasers has been observed to enhance the resonance frequency by a factor of two or more. However, the fundamental understanding of this frequency enhancement is not well developed. An opportunity and a need exist to more fully develop the theoretical basis of injection locking of strongly coupled laser cavities so as to enable development of high-performance microsystems which exploit injection locking. We will develop a new theoretical and practical understanding of strongly coupled laser microsystems using combined theoretical work and a novel "photonic lab bench on a chip." This synergistic use of our leading edge theoretical capability and a photonic microsystem purpose-built to create highly controlled laser cavity characteristics and intracavity coupling will lead to new science of coupled laser cavities and dramatic improvement of the modulation frequency. Shrinking the lab bench onto a photonic integrated circuit (PIC) requires that two primary obstacles be addressed, removal of the optical isolator and reduction of the timescale of interactions to only a few picoseconds. Accordingly, we will develop new theories for frequency- and time-dependent coupled laser systems on the scale of a photonic integrated circuit. We will further verify and extend this theory by building a photonic-lab-bench-on-a-chip which microscopically reproduces the laser characteristics and laser-to-laser coupling in order to observe regimes of stable, chaotic, and frequency-enhanced resonant oscillations. At the conclusion of this project, we expect to demonstrate world-record modulation frequencies for monolithic diode laser systems.

Summary of Accomplishments

In FY 2009, we improved the model and explored a number of injection locking configurations seeking an optimal frequency response enhancement without the mid-frequency drop-outs commonly seen in experimental work to date. We have demonstrated, theoretically, resonance enhancement without mid-frequency dropout for cavity detuning of 15 GHz.

Development of the experimental platform has progressed to realize the proposed PIC. The design allows great flexibility of use while retaining efficient, precisely designed, and reproducible optical coupling. Cavity Q of the lasers will be set by the reflectance of the DBR (distributed Bragg reflector) lasers, and mutual detuning of the cavity resonances can be set electrically with bias currents on the gratings and an internal optical phase section.

Our first PICs were completed in August of 2008. Unfortunately, tests showed the electrical contacts had been destroyed at some point late in the process sequence. Analysis established that these PICs experienced a destructive chemical attack by standard photoresist developer, removing the p-type electrical contact layer. To prevent this from happening again, we have new design rules for waveguide doping and tightened control of doping in the epitaxial growth reactors.

A second-generation injection-locked PIC mask set was created, taking into account recent output from the injection locking theory specifying particular mirror reflectivities of master and slave lasers. The effect is that this new PIC design will be much more flexible in definition of "master" and "slave" by allowing any or all lasers to be DC or RF modulated. We also have passive cavity pairs allowing for measurement of coupled cavity resonances and detuning in the absence of gain. These PICs are currently in fabrication.

Significance

Improved science of coupled laser PICs will impact Sandia's mission. Relaxation oscillation frequency improvements enable compact systems with ultrafast RF and millimeter-wave photonic data links, including highly efficient RF optical systems in the 30 to 60 GHz range, and direct digital modulation at 50 to 60 Gb/s. Inherently stable designs could be used as optical frequency sources and clocks. Quantum computing, optical logic and optical cryptography could use novel designs enabled by this work.

Refereed Communications

W.W. Chow, Z.S Yang, G.A. Vawter, and E.J. Skogen, "Modulation Response Improvement with Isolator-Free Injection-Locking," *IEEE Photonics Technology Letters*, vol. 21, pp. 839-841, July 2009.

Nanopatterned Ferroelectrics for Ultrahigh Density Rad-Hard Nonvolatile Memories

117820
Year 2 of 3
Principal Investigator: G. L. Brennecka

Project Purpose

The two goals of this project are to develop a general approach to bilevel patterning for the fabrication of controlled and ordered nanofeatures of a wide variety of materials upon essentially any desired substrate and to study the fundamental size effects of nanoscale ferroelectrics, ideally using the nanopatterning fabrication approach in development. The fundamental science of size, aspect ratio, and interface effects in integrated ferroelectric systems is of critical importance to a number of current and future applications; this project will focus primarily on the potential for using nanopatterned ferroelectrics for ultrahigh density rad-hard nonvolatile random access memories. Beyond employing this controlled nanopatterning approach for basic scientific studies of ferroelectrics, we will also endeavor to demonstrate the utility of such an approach to a variety of other integrated applications of interest for potential follow-on opportunities.

In addition to the two overall goals of the project, neither of which has been previously demonstrated, several of the other milestones of the projects represent world-firsts. For example, this project has been the first to demonstrate the MgO-mediated patterning of arbitrary micropatterns into ferroelectric $Pb(Zr,Ti)O_3$ and the first self-assembly of a copolymer mask directly on a ferroelectric (as well as other materials such as ZrB_2, MgO, and Pt). This project is also at the leading edge of nanomaterials characterization, as evidenced by the development of a scanning transmission electron microscope energy dispersive spectroscopy (TEM-EDS) based quantitative mapping technique with unprecedented spatial resolution.

Summary of Accomplishments

Throughout much of FY 2009, we were plagued by difficulties etching nanofeatures in appropriate pattern transfer materials such as MgO, but we believe that our recent advances have led to the development of routes for achieving the goals of the project despite these difficulties. Namely, the ability to assembly the diblock copolymer mask layer directly on materials such as Pt and $Pb(Zr,Ti)O_3$ themselves opens up a variety of new process possibilities. In addition to the direct-patterning breakthrough, we have also developed the capability to deposit alternative oxide electrodes ($LaNiO_3$ and $SrRuO_3$) that may result in cleaner (i.e., less atomic disorder) interfaces with integrated ferroelectrics such as $Pb(Zr,Ti)O_3$. We have assembled and tested our own piezoelectric force microscope for quantitative topography and property measurements of free-standing ferroelectric features. Our collaborations with the University of Florida on this project have resulted in the highest-known-resolution in-situ measurements of the phase development of integrated $Pb(Zr,Ti)O_3$ films during thermal processing. We furthered development of our world-leading cation mapping capabilities, began investigation of alternate electrode adhesion layer stacks for improved reliability and robustness during sequential processing, and carried out preliminary analysis of the interplay among interfaces, domain state distributions, and ferroelectric domain dynamics.

Significance

We are developing leading-edge techniques for complex oxide and electrode metal nanomaterials synthesis, nanoscale interface design and characterization. Our pioneering developments are of great interest to DOE defense and energy programs and to industry as well. The broad interest within Sandia for the general nanopatterning approach that we are continuing to develop under this project is evidenced by the additional

National Institute for NanoEngineering (NINE) and LDRD projects that it has spawned. These include an LDRD nanosensors project and a scanning transmission electron nanopatterned LDRD project beginning in FY 2010.

Our nanomaterials synthesis, nanoscale patterning and associated characterization tools have tremendous potential for other electronic applications. The ability to pattern both electrode and active ferroelectric structures at dimensions of 20 nm and less using economically viable techniques is essential to future Sandia rad-hard memory and next-generation piezoelectric nanosensor developments. Further, our fundamental science investigations of ferroelectric materials and associated electrode–complex oxide interfaces at the nanoscale investigations will impact many other nanomaterial applications. Examples of these applications include next-generation photonic device structures, metamaterials with nanoscale periodicity and THz applications.

Our accomplishments in FY 2009 will open up a new degree of freedom for the fundamental study of size effects in ferroelectric materials and will represent a novel, simple, and effective approach for the manipulation of a wide variety of materials on the nanoscale. Our approach can become a flexible method for the development of nanoscale structures specifically tailored for a wide variety of applications, such as metamaterials with nanoscale periodicity. Our target complex oxide electrode nanostructures will enable dramatic advances in the size and performance of a wide range of nano- and micro-devices. Our material-independent fabrication and pattern control approach could have even farther-reaching impact as a powerful platform for future devices.

Refereed Communications

C.M. Parish and L.N. Brewer, "Multivariate Statistics Applications in Phase Analysis of STEM-EDS Spectrum Images," to be published in *Ultramicroscopy*.

C.M. Parish and L.N. Brewer, "Key Parameters Affecting Quantitative Analysis of STEM-EDS Spectrum Images," to be published in *Microscopy and Microanalysis*.

C.M. Parish, G.L. Brennecka, B.A. Tuttle, and L.N. Brewer, "Quantitative X-Ray Spectrum Imaging of Lead Lanthanum Zirconate Titanate PLZT Thin Films," *Journal of the American Ceramic Society*, vol. 91, pp. 3690-3697, November 2008.

C.M. Parish, G.L. Brennecka, B.A. Tuttle, and L.N. Brewer, "Quantitative Chemical Analysis of Fluorite-to-Perovskite Transformations in $(Pb,La)(Zr,Ti)O_3$," *Journal of Materials Research*, vol. 23, pp. 2944-2953, November 2008.

Integrated Optical Phase Locked Loop (IO-PLL) for Attosecond Timing in Microwave Oscillators

117822
Year 2 of 3
Principal Investigator: M. Watts

Project Purpose

Phase noise in traditional microwave oscillators limits or compromises their use in applications that require high-precision clocking and/or fine phase resolution. To overcome the limitations of traditional microwave oscillators, we are locking a microwave oscillator to an integrated optical phase locked loop (IO-PLL). An optically referenced microwave oscillator represents a paradigm shift with the potential to move the clocking precision of a microwave oscillator from the femtosecond to the attosecond regime. This project is a collaboration between Sandia and the Massachusetts Institute of Technology (MIT) with MIT performing benchtop experiments and Sandia focusing on developing an integrated chip-level solution. Ultimately, our goal is to take the lab results generated by our Sandia-MIT team, and use the capabilities of the Microsystems and Engineering Sciences Applications (MESA) and the Center for Integrated Nanotechnologies (CINT) to integrate the required optical components onto an optoelectronic chip. Importantly, this work is not integration for miniaturization alone. Chip-scale integration will enable fundamental limits of phase noise to be reached by removing 1/f and other noise sources inherent to bulk optic setups. Thus, via integration, we aim to achieve sub-femtosecond timing resolution on a chip-scale device, a feat that has not been performed ever, in any form, large or small. So far, Sandia has demonstrated a key component required for integration, a silicon microphotonic modulator. Sandia's resonant silicon microphotonic modulator is not only the smallest, highest-speed, and lowest power resonant silicon modulator, but is also the only one demonstrated to date that can be driven by complementary metal-oxide semiconductor (CMOS) drive voltages. And MIT has demonstrated a record relative timing stability of < 6.8 fs over 10 hours or 1.9×10^{-19} between a pair of 10-GHz microwave oscillators locked to a femtosecond laser source. In short, we are well positioned to demonstrate our first IO-PLL..

Summary of Accomplishments

Accomplishment 1: We have demonstrated the smallest, highest-speed (10 Gb/s) and lowest-power resonant silicon amplitude modulators in the world.

Accomplishment 2: Our first silicon phase modulators have been designed and fabricated. Testing has started, and it appears the modulators are providing phase modulation.

Accomplishment 3: Our first IO-PLL has been designed and fabricated. Testing has begun.

Accomplishment 4: Our first germanium detectors have demonstrated low dark current.

Accomplishment 5: We have developed a V-groove process for fiber-attach to our waveguides. Initial results demonstrate 3 dB fiber-to-chip coupling losses.

Accomplishment 6: Our collaborators at MIT have performed a complete system characterization and analysis of fundamental timing errors in a voltage-controlled oscillator (VCO) locked to a femtosecond pulse stream / optical phase detector, and completed a report detailing the fundamental timing errors. Further, MIT demonstrated a phase noise of –130 dB 10 Hz from the carrier leading to 6.8 fs relative timing stability over 10 hrs (10^{-19}) between a pair of 10 GHz microwave oscillators using their bench top OPLL. This represents a new record for RF extraction of timing stability from a mode-locked laser.

Accomplishment 7: Gave an invited talk on our IO-PLL work at the Precise Time and Time Interval Meeting 2008

Accomplishment 8: Won an R&D100 Award for work that included technology developed as part of this project.

Significance

Given the universal need (e.g. RADAR, global positioning systems [GPS], and communications) of compact, low-power, and high-performance oscillators, the national security impact of this project will be substantial. This project will enable Sandia to solidify its silicon photonics platform for DOE/NNSA and DOD/Defense Advanced Research Projects Agency (DARPA)–related applications such as advanced computing, secure communications, etc. The project also includes university collaborations, a goal of DOE.

Refereed Communications

M.R. Watts, W.A. Zortman, D.C. Trotter, R.W. Young, and A.L. Lentine, "Low Voltage, Compact, Depletion-mode, Silicon Mach-Zehnder Modulator," to be published in the *Journal of Selected Topics in Quantum Electronics*.

Four-Wave Mixing for Phase-Matching-Free Nonlinear Optics in Quantum Cascade Structures

117825
Year 2 of 3
Principal Investigator: W. W. Chow

Project Purpose

Problem: While nonlinear optics has the potential for efficient, high-temperature generation of coherent THz radiation, considerable effort has to be spent satisfying phase matching conditions. At best, the need to phase match limits the interaction length, and therefore, the photon conversion efficiency.

Idea: We propose an optically pumped, electrically biased quantum cascade (QC) scheme (patent pending), where the four-wave mixing (a nonlinear optical process) is automatically phase matched. The scheme also provides drive photon recycling, resulting in conversion efficiencies that exceed the fundamental limit for pure optical pumping (the Manley-Rowe limit). With further development, the scheme can lead to efficient, high-temperature THz lasers.

Science, technology and engineering (ST&E) obstacles include the following: Four-wave mixing is being used successfully for new frequency generation in atomic and solid state systems. Replicating the results in a semiconductor system may be challenging because of intrinsic and extrinsic inhomogeneous broadening, as well as many-body effects.

Objectives: This project will demonstrate coherent THz radiation generation at elevated temperatures and with automatic phase matching. Modeling will be performed to guide proof-of-principle experiments and device optimization. There will also be experimental and theoretical explorations besides THz generation, e.g., nonlinear spectroscopy for chemical agent detection, entangled or correlated photon production for quantum computing, slow light for optical buffers in optical communications, and phase conjugation for wavefront correction.

Summary of Accomplishments

Work is progressing on evaluation of photon recycling and demonstration of four-wave mixing gain. Theoretical and experiment work has led to four invention disclosures in the areas of switches, detectors, high-brightness radiation sources and solar-powered lasers. We discovered the possibility of coherence collapse in our laser experiments that can have important impact on quantum cascade lasers (QCL) in spectroscopic applications. Work is continuing on the development of a fully quantized (i.e., quantized active medium and quantized radiation field) theory capable of treating the strong-coupling (polariton) limit.

Significance

The research advances semiconductor quantum optics and QCL device engineering. Success will give Sandia the state-of-the-art technology for high-temperature THz quantum cascade lasers and impact the field of quantum computing, optical communication and cryptology, especially if we are successful in demonstrating entangled photons or slow light.

A Revolution in Micropower: The Catalytic Nanodiode

117827
Year 2 of 3
Principal Investigator: J. R. Creighton

Project Purpose

Micropower sources have numerous applications for microelectromechanical systems (MEMS) and microsensors. Microsensor systems are of interest for a variety of applications such as remote sensing of chemicals, radioactivity, or biological agents to address issues related to the detection, location, and composition of weapons of mass destruction and to assist in various nonproliferation efforts of DOE. Our ability to field useful, nano-enabled microsystems that capitalize on recent advances in sensor technology is severely limited by the energy density of available power sources. We will develop an alternative revolutionary source of micropower; the catalytic nanodiode (see http://pubs.acs.org/cen/news/83/i15/8315notw1.html). Like a fuel cell, this device utilizes a fuel and oxidizer, but unlike a fuel cell, the fuel and oxidizer combine at the same surface (the catalyst) on the catalytic nanodiode. A sizable fraction of the chemical energy is harvested via hot electrons (or ballistic electrons) that are created by the catalytic chemical reaction. These electrons are collected on the semiconductor side of the metal-semiconductor (Schottky) diode structure. Unlike a fuel cell, there is not a second electrode, and the transport of other charged species (e.g., H^+) across an aqueous or solid media is not required. The fuel and oxidizer may be in the gaseous or liquid state. In this respect, the catalytic nanodiode is a simple, compact, and robust technology. This technology maps extremely well onto Sandia's expertise in semiconductor device fabrication at the Microsystems and Engineering Sciences Applications (MESA) facility, micropower applications, solid-state physics, and surface chemistry and catalysis. The goal of this project is to validate the concept, then use Sandia scientific and engineering expertise to significantly advance nanodiode technology. The final project goal will be to demonstrate a functional catalytic nanodiode micropower device that operates near room temperature (< 50 °C) using a convenient fuel source (e.g., ethanol vapor).

Summary of Accomplishments

Our major accomplishments are:

1) Determined the true nature of the nanodiode chemical signal. Chemical testing results as a function of nanodiode impedance have conclusively demonstrated that the supposed chemicurrent is in fact derived entirely from a voltage source. The catalytic chemical reaction releases heat (up to ~ 25 mW/cm^2) which significantly alters the nanodiode temperature and temperature gradient. The chemical signal is primarily derived from the thermoelectric voltage generated by the temperature gradient. A second signal component is generated by the temperature dependence of the nanodiode impedance. This second component can be amplified by adding an external bias, and its polarity can also be changed. All qualitative features of the chemical signal can be explained by these two components. Unfortunately, these results demonstrate that the catalytic nanodiode will not serve as a viable micropower source.

2) Greatly improved our diode fabrication procedure. We developed a new shadow mask and whole-wafer processing procedure that is much more robust and reproducible. The procedure also generates diodes with varying area of catalytic metal.

3) Expanded CO_2 rate measurements. In order to map out the CO oxidation kinetics over a wider operating range (particularly at lower temperatures) we established a flow-through tube furnace reactor with in-line micro-GC capability. The system was modified to accommodate the small surface areas of the nanodiodes and enhance

their contact with the impinging gas stream. Oscillations or rate instabilities were often observed, especially at low CO/O_2 ratios near the kinetic transition. Most Pt/GaN nanodiodes were found to be much more catalytically active than a Pt foil of similar dimensions.

Significance

DOE has several programs in sensors and long term operations that must currently work with commercially available power sources, namely batteries. In most of these systems, the batteries consume more than 95% of the system volume, due to the need for long duration. A revolutionary micropower source would enable vast reductions in the size of fieldable systems for deployment into strategic weapons, nonproliferation technologies, national security defense systems, and space applications.

Although this project demonstrated that the catalytic nanodiode will not serve as a viable micropower source, the work advances the scientific discovery mission of DOE, building foundational knowledge that should guide future efforts toward more fruitful paths.

Efficient Multi-exciton Emission from Quantum Dots

117829
Year 2 of 3
Principal Investigator: T. S. Luk

Project Purpose

We propose to control the radiative processes of multiple excitons in quantum dots (QDs) by engineering the photonic density of states (PDOS) surrounding the QD utilizing 3D photonic crystals (3DPCs). QDs hold tremendous promise for enhancing the efficiency of light emission and light conversion for applications including solar energy harvesting and low threshold lasers, to name a few. However, nonradiative processes dominate multi-exciton decay in QDs resulting in inefficient light emission. Since a photonic crystal is a man-made material, the dispersion properties, bandgaps and bandedge locations, and the density of states function can all be tailored for a specific application. It has been shown that by controlling the lattice structure of 3DPCs the PDOS can be controlled resulting in accelerated, slowed down, or completely inhibited radiative decay. In this way, the photonic crystal density of states can be engineered to control radiative rate of single and multi-excitons to harvest their energies and reduce the significance of non-radiative relaxation processes.

Previous experimental efforts in 2D photonic systems lacking 3D control have not demonstrated sufficient quantitative understanding of PDOS enhancement nor resulted in substantial modification of the radiative decay rate. Therefore, a theoretical effort and a systematic experimental validation will be performed on QD infiltrated 3DPCs. Two approaches will be explored, both using large density of states enhancement at the emission wavelength of the radiative transition. The first method employs a nanocavity in the 3DPC with low loss and small volume to control PDOS. The second approach utilizes the bandedge effect of photonic crystals. The main objective of this project is to enhance radiative emission properties of QD nanomaterials by factors of 10^3 to 10^4. With this fundamental understanding the groundwork will be laid to exploit QDs in light absorption and emission systems important to national security applications.

Summary of Accomplishments

The main milestone planned for the first year was to demonstrate enhancement of spontaneous emission from 2D nanocavities due to the Purcell effect. We have met the major part of this objective and are in the process of improving enhancement performance.

For the second year milestones, the main objective is to demonstrate enhanced spontaneous emission from 3D photonic crystals. We are in the process of fabricating these crystals. Although this was started in Dec 2008, there are fabrication issues related to the chemomechanical polish that needed to be worked out.

During the first eighteen months of this project, we have accomplished the following:

1. Successfully fabricated high quality 2D Si photonic crystals with L3 and double heterostructure nanocavities, and waveguides.
2. Observed high Q cavity resonance with Q factors of about 3000.
3. Demonstrated an enhancement factor of 116 in the emission of colloidal PbS quantum dots on photonic microcavity in a 2D photonic crystal. This enhancement factor is larger than previously reported results using colloidal quantum dots by an order of magnitude. A manuscript is being prepared to report this result.

4. Designed 3D Si and SiN photonic crystals to enhance PbS emission.
5. Began fabrication of 3D Si and SiN photonic crystals.
6. Presented the results in 3 conferences, and seminar presentations to two universities.

Significance

This project is about controlling radiative behavior of nano and quantum systems. It is an important milestone toward harvesting free and clean solar energy. It is also a steppingstone toward development of a unique single photon source on demand for quantum encryption and communication, a method of communication which cannot be eavesdropped to ensure protection of national security interests.

Programmed Assembly of Nanoscale Three-Dimensional Networks of Inorganic Materials

117830
Year 2 of 3
Principal Investigator: D. Robinson

Project Purpose

Photolithography is not economical below 50 nm, and exhibits poor vertical scaling. Achievement of precise, three-dimensional geometric control in the 1 to 50 nm range is best obtained through the highly selective affinity of sequence-specific synthetic macromolecules that act as scaffolding for inorganic materials. Effective control of nanomaterials in this manner is unrealized, but tools are now within reach, and Sandia has an opportunity to assume leadership of these efforts. We will use synthetic polymers with programmable sequences to control the assembly of nanomaterials. Poly(N-functionalized glycine)s (NFGs), with 15 years of development, are well characterized and easily synthesized with high molecular weight and yield. Their supramolecular assemblies are now under study at Lawrence Berkeley National Laboratory's Molecular Foundry, with whom we collaborate. These polymers form stable, helical rigid rods with lock-and-key surfaces that facilitate specific assembly into designed structures. We will develop these materials to encapsulate inorganic materials and assemble them into branched networks, as needed for nanoscale electronic, optical or fluidic circuitry. This enabling technology will allow us to address several mission-critical applications. This work directly addresses the Nanoscience to Microsystems investment area goals: to control, manipulate and integrate matter to attain unique properties and functions and realize novel complex systems. We expect the assembled materials to perform functions with greater speed and lower energy consumption, and allow more versatile transduction of nanoscale phenomena (physical, chemical and biological) to larger-scale devices. The project will develop a fundamental and disruptive technology, most appropriately funded by the LDRD program, and will provide new capabilities for a wide range of mission areas.

Summary of Accomplishments

Polymer synthesis: We developed a way to tune charge on the hydrophilic, outside-facing region of the molecule of the DNA-encapsulating N-functional glycine oligomer created in FY 2008. The successful design uses a chiral methoxypropyl sidegroup, along with chiral or achiral carboxylate sidegroups. Spectropolarimetry demonstrated that it is helical in water. Gel electrophoresis showed that it interacts with nucleic acid without causing conformational changes such as coagulation that would dramatically affect its mobility, and that the assemblies are resistant to pH changes.

Assembly with inorganic nanoparticles: We have developed tetrahedral nucleic acid cages for encapsulation and oriented interconnection of inorganic particles. Expanding the cage with at least one single-stranded segment allows efficient assembly using only sodium chloride. We observed specific assembly with 5-nm gold particles: the particles only attach to the thiolated tetrahedra.

Metallic nanoparticles are generally unstable under the high-salt conditions necessary for construction of elaborate double-stranded DNA structures, which usually require magnesium ion. However, by using our oligomers to cap gold particles, they become tolerant of the required magnesium concentrations. We have had similar success by tuning charge on 5-nm CdS particles, but they nonspecifically bind to DNA. We propose ways to correct this in our FY 2010 work.

Oligomer Characterization: We have collected neutron scattering data on a dicationic NFG oligomer in a concentrated aqueous solution and observed that it forms a cylindrical micelle structure with diameter ~ 30 Å and length ~ 90 Å, and also indicate that the cylindrical micelles associate into a higher order structure that is yet to be determined. The structure is stable with respect to temperature from 25 – 55 °C. Preliminary small-angle neutron scattering (SANS) data has also been obtained for two control peptoids with similar primary structure that imply distinct structural differences between the three peptoids.

Significance

This work offers fundamental improvements in the control of matter on the nanoscale. This degree of control would provide benefits to key energy and security applications, such as further miniaturization of components crucial to weapon systems and mobile threat detection. The DOE Office of Basic Energy Sciences has placed an "increased emphasis on the synthesis of new materials with nanoscale structural control," particularly "molecular assemblies with unique properties and specific functions."

Templated Synthesis of Nanomaterials for Ultracapacitors

117832
Year 2 of 3
Principal Investigator: B. C. Bunker

Project Purpose

This project is exploring the extent to which nanoscale templates can be used to produce solution-derived nanocomposites for ultracapacitors. Ultracapacitors incorporate electroactive materials such as those found in batteries into electrolyte-filled electrical double layer capacitors to produce materials with exceptional capacitance, power and energy densities, charge/discharge rates, and reversible cycling capability. However, achieving the ultimate performance characteristics requires that materials for ultracapacitors be engineered at nanometer length scales to maximize electrode:electrolyte contact and minimize diffusion distances for charge-compensating carriers such as protons. The goal of this project is to combine electroactive oxides having the maximum charge storage capabilities with electroactive polymers having enhanced proton conductivities to produce hybrid nanocomposites that are ideal for preparing on-chip ultracapacitors. The key to producing desired nanoarchitectures involves the use of low-temperature, solution-based processing on nanoscale templates, resulting in regular arrays of oxides, polymers, and electrolyte solutions distributed at length scales ranging from 1–150 nm. The two complementary strategies we will use for preparing nanoscale architectures are the following: 1) using self-assembled polymer precursors as templates for the solution deposition of a porous oxide matrix, and 2) using nanoporous oxides as templates for the in-situ polymerization of conducting polymers. In both cases, the compositions and architectures of the resulting nanocomposites will be extensively characterized using techniques such as solid state nuclear magnetic resonance spectroscopy, transmission electron microscopy, and both x-ray and neutron scattering. Performance characteristics of the ultracapacitors will be determined using cyclic voltammetry and electrochemical impedence spectroscopy. Correlations between charge storage characteristics and nanocomposite structures will be developed to optimize ultracapacitor performance. In addition, knowledge obtained on the template-based solution synthesis of oxide-polymer nanostructures for ultracapacitors will have a major impact on Sandia's core capabilities in self-assembled nanomaterials for other applications including batteries, fuel cells, solar collectors, and sensors.

Summary of Accomplishments

Most research activities during the past year involved a transition from developing new compositions and nanoarchitectures for ultracapacitors to in-depth characterization and mechanistic studies of a few key materials that were developed during the first year of the project. Highlights include the following:

1) Oxide Nanostructures: A metal chelating agent consisting of an alkane thiol was used as a templating agent for ruthenium oxide ultracapacitors. The template produced an architecture consisting of molecular clusters, achieving high capacitance by keeping transport distances for ions and electrons to their ultimate limit. A nanocomposite containing both ruthenium oxide and niobium oxide was created in which the ruthenium oxide provides redox activity and electron conduction, while the niobium oxide provides proton conduction. This composite was deposited as thin films and around soluble zinc oxide nanorod templates to maximize electrolyte access. Nickel hydroxide nanorods were produced by electrodepositing nickel metal within the pores of anodized aluminum.

2) Polymeric Nanostructures: Conducting polymers such as polyaniline were electrochemically deposited within the nanoporous arrays in anodized aluminum. Results show that deposition conditions can be varied to create nanorods, nanocylinders, or thin films, with conformal cylinders providing the maximum performance. New monomers were synthesized and polymerized to tune redox potentials and provide higher capacitance than

has been reported previously in the literature. A new task was added to explore 3D nanoarchitectures of carbon created using photolithography. This year, this nanocarbon will be used as templates for both electroactive oxides and polymers.

3) Theory and Modeling: Mathematical models were developed to extract materials property information from performance data such as cyclic voltammetry and electrochemical impedence data. These models have been used to determine parameters such as proton diffusion coefficients, as well as to evaluate the impact on performance of different structural elements at the nanoscale.

Significance

This project engages basic nanomaterials science and electrical energy storage technologies for microelectronics, portable electronics, and wireless communication as well as for vehicles and the power grid. This nanotemplate approach can also be used for batteries, fuel cells, hydrogen storage, solar collectors, and sensors.

Refereed Communications

M.E. Roberts, D.R. Wheeler, B.B. McKenzie, and B.C. Bunker, "High Specific Capacitance Conducting Polymer Supercapacitor Electrodes Based on Poly(tris(thiophenylphenyl)amine)," to be published in the *Journal of Materials Chemistry*.

Anomalous Suppression of Fatigue and Wear Through Stable Nanodomains

117833
Year 2 of 3
Principal Investigator: B. L. Boyce

Project Purpose

Fatigue and wear are pervasive problems in engineering designs: fatigue-induced failures alone cost the US economy an estimated $178 billion annually (based on a 1982 Department of Commerce report). There are numerous Sandia designs from nuclear weapons (NW) stronglink components to satellite flexures that have fatigue and/or wear concerns. The development of engineering alloys that are impervious or strongly resistant to fatigue and wear would open a new chapter in structural reliability. One approach to eliminate a material's susceptibility to fatigue and wear is by perturbing the requisite dislocation-length scales. Preliminary experiments at Sandia suggest that persistent slip bands (PSBs), the cyclic-dislocation precursor to fatigue-crack initiation, can be suppressed by incorporating stable arrangements of dislocation-pinning obstacles (i.e., grain boundaries) at less than the required PSB length-scale (~100 nm). These preliminary experiments have shown that a Ni alloy with a sub-50 nm grain size, locked through Zener pinning, will not fail at maximum cyclic stresses of 1.5 GPa (217 ksi) during 10,000,000 cycles! This is a > 3000× increase in lifetime compared to conventional alloys, with similar gains expected in wear life. The locking aspect is critical: other nanocrystalline metals suffer from stress-induced grain growth, and commensurate loss of anomalous fatigue and wear resistance.

Summary of Accomplishments

The past year accomplishments fall into six categories:

1. Processing. We have employed electrodeposition to fabricate a wide range of nanocrystalline Ni-based alloys. While these alloys provide the basis for fundamental deformation and failure studies, third year effort will investigate possible alternative commercially viable production methods for nanocrystalline alloys.
2. Thermal Stability. Annealing experiments have compared the thermal stability of four electroplated Ni-based alloys. Ni-0.5Mn was found to have the best resistance to thermally driven grain growth. These studies not only provide insight into the role of alloying content on thermal stability, but also provide a processing pathway for future studies of performance as a function of grain size.
3. Fatigue Behavior. To date, three nanocrystalline Ni-based alloys have shown enhanced fatigue behavior compared to conventional microcrystalline Ni. Using focused ion beam dissection, we have shown that crack initiation in all three alloys is preceded by anomalous grain growth. Surprisingly, the alloy that appears most susceptible to fatigue-driven grain growth (Ni-0.5Mn) is the most thermally stable alloy.
4. Wear Behavior. Low-friction behavior of nanocrystalline alloys has been connected to the formation of a tribological bilayer which includes both an ultrananocrystalline (grains < 5nm) superlayer and a coarsened, elongated interlayer. Under conditions of high stress and strain-rate, the ultrananocrystalline superlayer is thicker and prone to delamination, resulting in poor wear performance.
5. Mesoscale Dislocation Simulations. To model collective dislocation-mediated behaviors such as cyclic persistent slip and wear, a dislocation dynamics framework has been embedded into a generalized finite element framework. This novel approach will permit, for the first time, the study of grain-size effects on progressive damage accumulation.

6. Grain Stabilization Modeling. Thermodynamic grain growth models predict, surprisingly, that second-phase particles encourage anomalous coarsening rather than prevent it as by a Zener pinning mechanism.

Significance

This project addresses fatigue and wear, pervasive concerns in a wide range of Sandia designs from stronglink to satellite components. Additionally, this project facilitates (a) new nanoengineered materials for micro-, meso-, and conventional-scale systems; (b) familiarity with an emerging class of commercial alloys; (c) bringing a needed dislocation dynamics modeling capability to Sandia while benefiting from prior development at other laboratories; (d) productive partnering with the Center for Integrated Nanotechnologies (CINT), a DOE Basic Energy Sciences (BES) nanoscience center; and (e) improved electroplating materials characterization for other DOE programs.

Refereed Communications

H.A. Padilla and B.L. Boyce, “A Review of Fatigue Behavior in Nanocrystalline Metals,” to be published in *Experimental Mechanics*.

Impact of Defects on the Electrical Transport, Optical Properties and Failure Mechanisms of GaN Nanowires

117834
Year 2 of 3
Principal Investigator: A. Armstrong

Project Purpose

GaN-based nanowires are attractive for applications requiring compact, high-current density devices such as nanoscopic ultraviolet laser arrays. However, understanding GaN nanowire failure at high-current density is crucial to developing a new generation of nanowire devices. GaN nanowires are fraught with point-defects that contribute to breakdown through degraded electrical and thermal transport properties. Understanding the impact of defects on nanowire properties and failure mechanisms is the first step toward rational control and mitigation of defect activity. However, investigating defects in GaN nanowires is extremely challenging because nanowires are difficult to probe and conventional defect spectroscopy techniques are unsuitable for wide-bandgap nanostructures. Nevertheless, studying GaN nanowires is scientifically interesting because the combination of dislocation-free growth and sample geometry amplifies the impact of controllable defect introduction, enabling investigation of their influence at a sensitivity beyond that achievable in thin films. Defect introduction will be monitored as a function of electrical and mechanical stress. The influence of preexisting and emergent defects on degraded nanowire properties will be investigated. An outstanding problem is an acute sensitivity of nanowire thermal conductivity k_T to point-defect density due to the lack of gettering sites such as threading dislocations and enhanced phonon-surface scattering. Creation of defects due to excess Joule heating of nanowires could further degrade k_T, producing a viscous cycle culminating in catastrophic breakdown. To investigate such issues, a unique panoply of electron microscopy, scanning luminescence and photoconductivity implemented at the nanoscale will be used in concert with sophisticated molecular-dynamics calculations of surface and defect-mediated nanowire thermal transport. This proposal seeks to elucidate long-standing material science questions for GaN while addressing issues critical to realizing reliable GaN nanowire devices. This work is expected to advance nanowire-based compact chemical- and bio-sensor and solid-state lighting technologies, which are fundamental to a variety of DOE and DHS missions.

Summary of Accomplishments

FY 2009 achievements include development of a photoconductivity technique applicable to nanowires to quantify the properties and density of deep level defects. This ability enables quantitative study of defect evolution in nanowire devices during electrical stress to identify defects that are key to device breakdown. The thermal conductivity of individual nanowires devices was measured using a micro-photoluminescence technique. Nanowires were confirmed to have a reduced thermal conductivity compared to bulk films, likely due to enhanced surface- and point defect-phonon scattering. Based on the strongly peaked temperature profiles in some nanowire devices, localized thermal decomposition was considered a likely cause for device failure. Using in-situ scanning tunneling microscopy- transmission electron microscopy (STM-TEM), the breakdown mechanism for nanowire devices was confirmed to be Ga droplet formation at the nanowire surface followed by Ga and N evaporation. The mobility of defect clusters in nanowires was observed, confirming that vacancy-interstitial clusters forming in the nanowire bulk can readily migrate to the surface. This finding indicates that defects in as-grown nanowires could instigate the thermal decomposition process leading to breakdown. To better understand the influence of surface and defects on nanowire thermal conductivity, molecular dynamics of finite nanowire devices were undertaken. Due to computational limitations, tractable sizes of simulated nanowires were much smaller than actual devices. Surface-related phonon scattering dominated for simulated nanowires, so results from direct simulation did not scale correctly to actual device size, where both bulk and surface-limited thermal conductivity are important. A new method that treats the nanowire as a thin film is being pursued to maintain surface effects while also including pseudo-continuum properties.

Significance

GaN nanowire devices promise compact, highly sensitive biological and chemical sensor devices as well as more versatile solid-state lighting technologies. These components are critical to core DOE and DHS missions. The basic science revealed in this work is expected to enable more efficient lighting and new sensing technologies for homeland defense.

Refereed Communications

A.A. Talin, F. Léonard, B.S. Swartzentruber, X. Wang, and S.D. Hersee, "Unusually Strong Space-charge-limited Current in Thin Wires," *Physical Review Letters*, vol. 101, p. 076802, August 2008.

A. Armstrong, G.T. Wang, and A.A. Talin, "Depletion-mode Photoconductivity Study of Deep Levels in GaN Nanowires," *Journal of Electronic Materials*, vol. 38, pp. 484-489, April 2009.

T. Westover, R. Jones, J.Y. Huang, G. Wang, E. Lai, and A.A. Talin, "Photoluminescence, Thermal Transport, and Breakdown in Joule-heated GaN Nanowires," *Nano Letters*, vol. 9, pp. 257-263, December 2008.

X.W. Zhou, S. Aubry, R.E. Jones, A. Greenstein, and P.K. Schelling, "Towards More Accurate Molecular Dynamics Calculation of Thermal Conductivity: Case Study of GaN Bulk Crystals," *Physical Review B*, vol. 79, p. 115201, March 2009.

A. Armstrong, Q. Li, K.H.A. Bogart, Y. Lin and G.T. Wang, and A.A. Talin, "Deep Level Optical Spectroscopy Investigation of GaN Nanowires," *Journal of Applied Physics*, vol. 106, p. 053712, September 2009.

K.K. Mandadapu, R.E. Jones, and P. Papadopoulos, "A Homogeneous Nonequilibrium Molecular Dynamics Method for Calculating Thermal Conductivity with a Three-body Potential," *Journal of Chemical Physics*, vol. 130, p. 204106, May 2009.

Energy Conversion using Chromophore-Functionalized Carbon Nanotubes

117835
Year 2 of 3
Principal Investigator: A. Vance

Project Purpose

The conversion of optical energy to electrical energy is a topic of great interest, with much research and development invested in conventional materials such as silicon. Nanomaterials such as quantum dots and nanowires offer promise for optical energy conversion, due to their unique electronic, optical, and mechanical properties. Among nanomaterials, carbon nanotubes are especially attractive for optoelectronics because all the bandgaps in carbon nanotubes are direct, and also because of the possibility of ballistic electronic transport. While photocurrent generation in carbon nanotubes has been demonstrated, these experiments were done at high light intensities. Furthermore, direct photon-current conversion is hindered in pristine carbon nanotubes because of the unusually strong exciton binding energy. We propose to circumvent these issues by using chromophore-functionalized carbon nanotubes to convert low-intensity optical radiation into electric current. With collaborators at the University of Wisconsin, we demonstrated that azobenzene/nanotube transistors can be optically switched using UV light. We will expand upon this initial study and use such chromophore/nanotube hybrids for energy conversion and develop a fundamental understanding of their behavior. Throughout the life of this project, experiments and simulation will be closely linked. We will explore factors such as chromophore density, the role of electrical contacts, and time dependence of light-induced conductance changes. Carbon nanotube devices are clearly a popular area of research; however, there are few groups studying the conversion of low-intensity optical energy into electronic current. The ability to use light to modulate the conductance of carbon nanotube devices through minimally intrusive, noncovalent modification of the nanotubes could lead to significant advances in areas such as nanoscale electronics, solar energy and photodetectors.

Summary of Accomplishments

We demonstrated the use of chromophores to selectively tune the sensitivity of single carbon nanotube field effect transistors (SWNT FETs) to different wavelengths of low-intensity visible light, resulting in devices that are sensitive to almost the entire visible spectrum. We were able to demonstrate a direct correlation between device threshold voltage shifts and the optical spectra of the chromophores. This effort included extensive experimental results and in depth theoretical studies of the device physics, and was published in *Nano Letters*. Our experiments and theory support the conclusion that light-induced chromophore isomerization and subsequent dipole moment changes are responsible for the observed threshold voltage shifts in the devices. This project also supported a summer undergraduate researcher who carried out synthesis of additional polyaromatic functionalized chromophores. She isolated x-ray quality crystals of an anthracene-functionalized chromophore, and a crystal structure was obtained and published in *Acta Crystallographica*. In addition to publications, this work was presented at the March meeting of the American Physical Society.

Significance

The DOE has been interested in nanoscience-based approaches to energy conversion. This proposal directly addresses this interest. The proposed work is also relevant for Sandia's interest in photodetectors where carbon nanotubes may provide advantages over existing technologies.

Refereed Communications

X. Zhou, T. Zifer, B.M. Wong, K.L. Krafcik, F. Léonard, and A.L. Vance , "Color Detection Using Chromophore-Nanotube Hybrid Devices," *Nano Letters*, vol. 9, pp. 1028-1033, February 2009.

M.A. Rodriguez, J.L. Nichol, T. Zifer, A.L. Vance, and F. Léonard, "(E)-4-[(4-Nitrophenyl)diazenyl]phenyl Anthracene-9-carboxylate," *Acta Crystallographica*, vol. E64, p. 2258, November 2008.

Studies of the Viscoelastic Properties of Water Confined Between Surfaces of Specified Chemical Nature

117837
Year 2 of 3
Principal Investigator: J. E. Houston

Project Purpose

The provocative and unique earlier findings of an extraordinary viscosity for water confined at the nanometer level between hydrophilic surfaces has prompted an intense search for the fundamental interfacial physics involved. The measurements were made using the Sandia-developed interfacial force microscope (IFM), which is presently the only instrument capable of obtaining such detailed information. From the experimental perspective, the only path available, in order to get a handle on the fundamental nature of the phenomenon, is to systematically change the parameters of the experiments in order to narrow the number of possible sources — for example, the chemical nature and crystalline structure of the two interfacial surfaces, the external parameters of the experiments, e.g., bulk water or humidity, temperature, water salinity, etc. Also, there is considerable latitude available in the area of advanced development of the IFM measurement techniques: for example, normal and lateral creep and relaxation measurements, the effect of interfacial electrical fields, etc. These are particularly important to obtain viscoelastic properties. In addition, although considerably more risky, is the development of the theoretical tools necessary to model the structure of water at and near surfaces. Water is famously complex and computational methods for handling this complexity are presently under broad and intense development. The potential impact of this effort extends to several important Sandia missions, including the flow behavior in microfluidics and desalination membranes as well as, environmental “stiction” problems in microelectromechanical-device development.

Summary of Accomplishments

In the first half of our second year, we have made critical improvements to the IFM’s capabilities for characterizing interfacial water. An exciting outcome has been a ~15× increase in force sensitivity and improved displacement control, both necessary for characterizing subnanometer fluid flows. This work enabled what we believe is the first measurement of the forces required to squeeze a nanoscale meniscus. The meniscus forms when water vapor in the air condenses between the tip and substrate, which are initially just barely touching. When the tip pulls back and then pushes on the meniscus, the fluid resistance is manifested as a repulsive force that increases when the tip approaches the surface more quickly, a clear indication of fluid flow. As with earlier IFM work where fluid drainage could only be measured between very hydrophilic surfaces, this experiment again shows that the chemistry at the Si-water interface determines the boundary condition for fluid flow. We plan to detail this observation and publish our findings within the next few months.

Significance

Science and technology are the DOE’s principal tools in the pursuit of its national security mission and water itself may shortly become a national-security issue. The knowledge of the behavior of water at interfaces is key to the success of several DOE missions, including programs which deal with corrosion, water conservation and purification and various emerging micro-fluidic technologies. The work outlined here will provide a narrow but important contribution to the overall problem area.

Refereed Communications

M.P. Goertz, X.-Y. Zhu, and J.E. Houston, “Exploring the Liquid-like Layer on the Ice Surface,” to be published in *Langmuir*.

Low Dislocation GaN via Defect Filtering, Self-Assembled SiO_2-Sphere Layers

118735
Year 2 of 2
Principal Investigator: G. T. Wang

Project Purpose

GaN heteroepitaxial layers necessarily grown on foreign substrates possess a high density of dislocations due to poor lattice and thermal expansion match. These dislocations have been correlated with reduced internal quantum efficiency and lifetimes for GaN-based light-emitting diodes (LEDs). We propose to develop a novel, elegant, low-cost technique using self-assembled SiO_2 microspheres to create multilayered, defect blocking layers for the growth of ultralow dislocation density GaN at a cost far below that of current, multistep epitaxial lateral overgrowth schemes. This technology will provide a revolutionary advance needed for inexpensive, efficient, high power LEDs for solid-state lighting (SSL). This technique could also potentially be extended to other heteroepitaxially mismatched systems, such as high quality Ge, III-V (including GaN), or II-VI films on Si.

Summary of Accomplishments

This project was viewed as being high risk but extremely high payoff, with several significant risks due in part to the uniqueness of the approach. We successfully demonstrated that single crystalline GaN can selectively be grown through self-assembled 3D templates of silica spheres, with the sphere layers functioning as a defect reduction template. Through our research and development efforts, we demonstrated an approximately fifty fold reduction in dislocations in GaN layers grown on sapphire by this technique to the $10^7/cm^2$ range. Additionally, an almost three orders of magnitude improvement in the dislocation density was demonstrated for GaN on Si growth. A Langmuir-Blodgett technique was successfully implemented to uniformly deposit sphere layers over wafer-scale areas. We also successfully tested a method for “decorating” dislocations immediately following growth which allows for an accurate count of dislocation density using atomic force microscopy, and confirmed a one-to-one correlation of dislocations with cathodoluminescence images of the same film areas. A journal article on our technique was published and a patent application was filed.

Significance

This project will impact all aspects of the DOE SSL mission by providing a novel technique that will enable high-quality, low-cost GaN buffers for III-nitride based devices. This would provide a ready source of substrates for a wide range of applications in energy and national security, including solid state lighting, photovoltaics, UV LEDs and lasers for chem-bio detection and water purification, and high-power high-frequency transistors for lightweight synthetic aperture radar applications.

Refereed Communications

Q. Li, J.J. Figiel, and G.T. Wang, “Dislocation Density Reduction in GaN by Dislocation Filtering Through a Self-Assembled Monolayer of Silica Microspheres,” *Applied Physics Letters*, vol. 94, p. 231105, June 2009.

Nanolithography by Combined Self-Assembly and Directed Assembly

120711
Year 2 of 3
Principal Investigator: D. L. Huber

Project Purpose

A detailed molecular understanding of directed and self-assembly on the nanoscale will be required to realize the potential of nanoscience. We propose to develop the scientific understanding necessary to control and direct self-assembly of polymers at the nanoscale in order to create precisely controlled, periodic nanostructures. Our novel approach is to direct the phase separation of mixed polymer brushes by engineering the interfacial interactions at the micron scale. The salient idea, which has not been demonstrated experimentally or theoretically, is to use boundary interactions to orient nanoscale assemblies into long range ordered patterns. A polymer brush is obtained when long polymer molecules are covalently bonded to a substrate. The synthesis of mixed brushes is surprisingly simple and uses inexpensive reagents. The two components can phase separate almost instantaneously (no component needs to diffuse more than a few tens of nanometers), and can have their phase separation directed. We will develop the synthetic methodology to produce mixed polymer brushes and will investigate the physical processes governing their directed assembly using numerical modeling and experimental characterization. The modeling will be used to predict the phase-separated morphologies and mechansims as a function of the important parameters in the system, such as the polymer molecular weights, grafting densities, and energetic interactions between all molecular components with each other and with the substrate. The results of this numerical exploration of phase space will be used to guide synthesis by providing parameter sets to obtain the desired properties. The outcome of this project will be an understanding of how to direct nanoscale self-assembly using microscale patterning to create large-area nanopatterns. In addition to the new science, technological impact will come from creating new functional surfaces by templating off the polymer nanopatterns for applications such as molecular electronics, nanostructured solar cells, and extremely high-density data storage.

Summary of Accomplishments

We have a joint theoretical and experimental approach to this work. On the theory side, we have developed a density functional theory (DFT) code capable of simulating mixed polymer monolayers with random graft locations. We have begun studying the effects of molecular weight, graft density, and polymer interactions in this system. The resulting structures confirm that the experimental system chosen will yield patterned nanoscale features as expected, and that these features will follow the lithographically defined micron scale features. We have also shown new phases that are not achievable with diblock copolymers and are in the process of confirming these results using experiment.

On the experimental side, we have demonstrated the phase separation of mixed monolayers of polystyrene and poly(methylmethacrylate). This phase separation occurs without annealing, though annealing improves the structure. This is in contrast to the diblock copolymer system, where many hours of annealing are required to achieve any horizontal phase separation of any kind. This is a major advantage over diblock copolymers and may lead to this approach being commercialized as a method of nanoscale lithography. We have also developed the chemistry to pattern polymer initiators through a variety of methods including stamping and photolithography. Patterned polymers have also been produced and their phase separation is being studied and compared to theory.

Significance

The understanding of nanoscale self-assembly gained from this project will be applicable to applications that impact national missions in energy and security. Applications include improved photovoltaics, nanoelectronic and nanophotonic devices, sensors, and nanofluidic systems. This proposal addresses several research areas outlined in the National Nanotechnology Initiative, in particular the design and synthesis of structured nanomaterials and in reliable, cost-effective nanomanufacturing.

Development of Novel Porous Nanocomposites for National Security Applications

125854
Year 2 of 2
Principal Investigator: S. M. Dirk

Project Purpose

Porous polymers have impacted many areas of science and engineering over the last 40 years including catalyst supports, scaffolds for tissue engineering in order to regenerate damaged or missing tissues, low K polymer dielectrics, and membranes and ion-exchange resins for separation technologies. Porous polymeric materials also have potential broad utility in the defense and national security community, which has not been adequately explored. While porous polymers are widely available in the commercial sector, the materials are typically limited to a few specific polymer chemistries that are not easily modified to meet emerging needs. We will continue to identify the physical and chemical factors that control the average porosity, pore size, and pore size distribution, enabling porous materials technology to be exploited with any polymeric resin. This will enable skip-generation technology for the defense and security sector, particularly in the area of sensor technology and protective membrane materials, which require dramatic improvements in selectivity and sensitivity to meet future needs. Many of these future needs will require both porosity and conductive particle fillers. Sandia and North Dakota State University (NDSU) Coatings and Polymeric Materials department are in the unique position of having the appropriate combinatorial tools, polymer physics, and polymer chemistry expertise to develop polymeric nanocomposites with controlled pore volume and size. The knowledge gained from this project will be critical for developing next-generation sensor and membrane platforms for national security needs. In FY 2009, we will collaborate with NDSU using a combinatorial research approach to produce a library of nanocomposites with the intention of identifying the physical factors that control both conductivity as well as porosity, such as porogen loading, polymer-porogen interactions, filler size, filler loading, filler surface chemistry, and polymer crosslink density.

Summary of Accomplishments

A typical method to produce porous polymers involves the use of porogens like sodium chloride, particulate fillers, or a solvent that that can be selectively removed after resin cure leaving a porous structure. While these techniques can produce porous materials with a wide variety of total porosity, and average pore size, they have not been evaluated in nanocomposites, where nanosized fillers are present. In collaboration with NDSU, we have identified, via combinatorial chemistry, several factors that control both pore size and nano- and microparticle distribution within the polymer matrix materials. In addition, we have developed, fabricated, and demonstrated the use of a gradient temperature combinatorial device to study the effects of temperature on poragen containing resin systems loaded with nano- and microparticles.

Significance

Conducting porous polymeric materials have potential broad utility in the defense and national security community enabling the formation of highly sensitive sensors. Furthermore, conductive porous polymers may provide lightweight electrodes for use in energy storage devices like ultracapacitors.

Architecturally Controlled Nanocathode Materials for Improved Rechargeable Batteries

130767
Year 1 of 3
Principal Investigator: E. D. Spoerke

Project Purpose

The purpose of this project is to exploit chemical synthesis, computer modeling, and both structural and electrochemical characterization to create high-capacity, moderate voltage electrode materials for lithium ion battery technologies. Concentrating on improving cathode materials, whose poor capacities continue to limit cell performance, our specific approach will aim to extract moderate to high capacities from inexpensive, moderate voltage ceramic materials (e.g., iron oxides), specifically focusing on nanoscale morphologies believed to enhance stability and capacity. By developing a detailed understanding of the relationships between electrochemical activity and variables such as material phase, nanoscale morphology and atomic doping, we expect to be able to engineer improvements in the performance and cyclability of moderate voltage metal oxide phases. This alternative "capacity-based" approach will enable us to produce cathodes capable of attaining high energy densities while avoiding the host of serious, often dangerous, side-effects (e.g., electrolyte degradation, current collector corrosion, binder deterioration, and other deleterious side reactions) associated with higher-voltage cathodes popular in current battery research. Achieving this technical goal will require a comprehensive, collaborative approach wherein atomistic modeling, designer chemical synthesis, and in situ crystallographic and electrochemical characterization will all support one another in a system of integrated feedback that will drive the continual refinement and improvement of developing materials. This multidisciplinary approach will exploit our team's expertise in materials synthesis, computational modeling, in situ characterization, and electrochemistry to create the next generation of lithium ion cathode materials, with the potential to revolutionize a stalwart industry and address critical national energy needs.

Summary of Accomplishments

We have applied an integration of synthesis, modeling, and characterization to develop a baseline understanding of the chemistry and properties of iron oxides as they relate to rechargeable lithium iron oxides.

Synthetically, we have developed a suite of capabilities that have not only enabled us to generate the scale, purity, and select phases desired, but they will be adaptable to the synthesis of novel phases and morphologies of lithium iron oxides as we move forward. More specifically, we have synthesized large-scale quantities of numerous phases along the Fe_2O_3-Li_2O tie line as well as less common phases such as rare polymorphs of Fe_2O_3 and alkaline ferrates containing hypervalent iron cations. In addition, we have made significant progress developing custom iron alkoxide precursors and using these precursors to develop novel iron oxide nanoparticles.

Computer modeling has dramatically enhanced our understanding of both the structure and the properties of the different materials phases. Structural models have helped identify interesting synthetic targets and synthetic strategies that may yield optimal results. In addition, developing models of properties such as electronic structure, generated from familiar iron oxides, will continue to prove valuable as we attempt to understand and predict behaviors of new materials phases in the upcoming fiscal year.

On the characterization front, we have used x-ray diffraction (XRD) capabilities extensively, not only to identify the phases of materials synthesized, but using variable temperature XRD, we have identified critical processing parameters required to synthesize specific oxide phases. Electrochemically, we have adapted existing electrode assembly methods to our new materials, allowing for critical electrochemical characterization of materials synthesized. These measurements both confirmed the expected performance of familiar iron oxides, and provided initial insights into the potential of alternative phases, such as polymorphs of Fe_2O_3 and the potassium ferrates.

Significance

This battery materials research seeks to develop new science and technology related to energy storage, an important national and global topic. Our approach, integrating synthesis, characterization, and modeling, offers promise in creating a new, low-cost, environmentally friendly, and safer lithium ion battery system. In addition, project success will provide valuable new insight into battery materials research with potentially significant impact on energy storage for transportation, capturing renewable energy, improving power grid efficiency, and powering both consumer and military portable electronics.

Atomic Mechanisms Governing Interface Formation in Nanostructured, Phase-Separated Thermoelectric Alloys

130768
Year 1 of 2
Principal Investigator: D. L. Medlin

Project Purpose

Expanding the use of thermoelectric devices for waste heat recovery and more-efficient cooling will require new bulk materials with dramatically improved energy conversion efficiencies over the current state of the art. The central materials challenge is to balance the competing requirements of high electrical conductivity, high Seebeck coefficient, and low thermal conductivity. Overcoming this challenge is difficult because these properties are highly interrelated in traditional, single-phase, solid-solution alloys. However, recent work has shown it is possible to decouple these transport properties by introducing nanometer-scale distributions of interfaces that, for instance, preferentially scatter phonons, reducing the thermal conductivity, or selectively filter low-energy charge carriers, enhancing the Seebeck coefficient. One promising route to introducing the necessary interfaces in bulk materials is to control the solid-state phase-separation processes in multiphase alloys to produce a nanometer-scale distribution of heterophase interfaces. In particular, recent work at the California Institute of Technology (Caltech) has demonstrated that the phase-decomposition in the Pb-Sb-Te system can be controlled to produce a bulk, self-assembled, layered material consisting of nanometer-scale lamellae of PbTe and Sb_2Te_3. We propose to collaborate with the Caltech researchers to explore the atomic-scale mechanisms that govern this self-assembly process, in order to understand the science underpinning these nanostructured thermoelectric alloys.

Summary of Accomplishments

Our primary technical objectives during the initial stage of this project have been to prepare materials, to initiate our microstructural study, and to begin analyzing the defect structures at the relevant interfaces. We have begun by investigating interfaces between the tetradymite structured compound, Sb_2Te_3, and two different rock-salt structured tellurides, PbTe and $AgSbTe_2$. We are synthesizing our materials through solid-state routes: decomposition of $Pb_2Sb_6Te_{11}$, which is also a layered, tetradymite structured compound, into PbTe and Sb_2Te_3 lamellae, and precipitation of Sb_2Te_3 plates in supersaturated solid-solutions of PbTe and $AgSbTe_2$. We have established the specimen preparation protocols to reliably prepare specimens for microscopic analysis have begun analyzing the detailed interfacial structure of PbTe/Sb_2Te_3 and $AgSbTe_2$/Sb_2Te_3 interfaces using transmission electron microscopy. Our work is showing how misfit strain and phase transformations are connected to the interfacial line defects. These issues are important because local strain and interfacial defects likely affect the formation and morphological stability of the interfaces as well as their electronic and thermal transport properties. We have completed an invited review article on interfaces in thermoelectric materials.

Significance

Thermoelectrics have diverse energy conversion and cooling applications that span much of Sandia's mission space. Existing and potential future applications include long-term, high-reliability power sources, localized cooling devices, low-temperature power scavenging, and high-temperature waste heat recovery.

Refereed Communications

D.L. Medlin and G.J. Snyder, "Interfaces in Bulk Thermoelectric Materials," *Current Opinion in Colloid and Interface Science*, vol. 14, pp. 226-235, August 2009.

Bio-inspired Nanocomposite Assemblies as Smart Skin Components

130769
Year 1 of 3
Principal Investigator: S. M. Brozik

Project Purpose

The Defense Threat Reduction Agency (DTRA) is interested in the development of sophisticated materials that can automatically detect and respond to chemical and biological threats without the need for human intervention. In living systems, cell membranes perform such functions on a routine basis, detecting threats, communicating with the cell's interior, and triggering automatic responses such as the opening and closing of ion channels. The purpose of this project is to learn how to replicate simple threat detection and response functions within artificial membrane systems. The key attributes that we intend to explore to make such a "smart skin" include the following: 1) a lipid bilayer host matrix with sufficient mobility to allow components to reconfigure themselves in response to specific stimuli; 2) recognition sites that both adsorb "threats" and trigger membrane responses; 3) functionalized nanoparticles that can be reconfigured to reversibly switch the membrane between an open, permeable state and a closed, impermeable state; 4) ion channels that can be programmed to switch interactions to make the membrane "open" or "closed"; and 5) an underlying substrate that provides the stimuli for programming the membrane once threats are detected. This work will provide the scientific underpinning for developing a wide range of responsive membrane-based nanocomposites for both homeland defense and energy applications.

Summary of Accomplishments

Our FY 2009 milestones were aimed at determining the mechanism of insertion of nanoparticles in lipid bilayer assemblies, synthesizing and characterizing monolayer functionalized nanoparticles, and characterizing the effect of surface charge on nanoparticle insertion and aggregation in lipid assemblies. Briefly, using a new version of fluids density functional theory we have assigned a more accurate description of the single site solvent we are using to model water. We have begun studies to calculate free energy cost to insert nanoparticles into our new model bilayer as a function of increasing hydrophobicity. Experimentally, we have begun evaluating the interaction of quantum dots with lipid bilayers based on surface chemistries, and we see distinct differences between amine, carboxylic acid, polyethylene glycol (PEG), and streptavidin terminated quantum dots. Utilizing imaging capabilities built in-house, we have tracked single nanoparticles in a supported lipid bilayer and automated the analysis of single particle data to reduce the time and cost required for data reduction and determination of diffusion coefficients. We have also developed an imaging method to measure membrane potentials in supported bilayers while measuring ion conductance. This information will be used to investigate the role of membrane potential on lipid-nanoparticle interactions. Finally we have synthesized gold nanoparticles with cyclodextrins and are characterizing the host-guest interaction between the cyclodextrin hosts and ferrocene derivatives in bilayer assemblies. We have also completed synthesis of 11-mercaptoundecanoic acid, terpyradine lipoic acid, and naphthalene functionalized nanoparticles and tetrathiofulvene (TTF) nanoparticles. Neutral TTF will not interact with the naphthalenes but, when oxidized to the dication, will bind via aromatic stacking interactions forming pores within the bilayer system.

Significance

This work will provide the scientific underpinning for developing a wide range of responsive membrane-based nanocomposites for both homeland defense and energy applications. DTRA has called out specific research dealing with responsive materials for chemical and biological defense. For Sandia and DOE science missions, the development of biomimetic nanocomposites is one of the frontier areas in nanoscience.

Characterization and Control of the Thermal Fluctuations of Nanosensors for Next-Generation Sensitivity and Robustness

130770
Year 1 of 2
Principal Investigator: R. E. Jones

Project Purpose

Nanoelectromechanical systems (NEMS) are spawning a new generation of novel devices. For example, a NEMS beam-like oscillator's small size promises smaller activation energy and greater sensitivity than traditional sensors. The greater sensitivity, however, comes at the price of greater susceptibility to thermal "noise." Our aim is to characterize and ultimately filter or control this noise. The effects of thermal fluctuations on small structures have been observed in recent experiments. For example, an atomic force microscope (AFM) with an attached molecule of DNA was used to measure binding energies and function as a biosensor. These experiments demonstrated that the resolution of this device was limited only by the thermal noise. Without some means of characterizing the noise such limits will persist. In fact, current device design and characterization methodologies are often based on simple linear continuum approaches with little or no modeling of the stochastic nature of nanoscale dynamics. These traditional methods become inadequate at the typical dimensions of NEMS, especially given the fact that these devices have relatively large thermal fluctuations and are employed in nonequilibrium regimes. Recent fluctuation theorems (FTs) provide a framework for understanding the dynamics of these devices far from equilibrium, but they require experiments and simulations to fully model the system. Using a combined experimental, theoretical, and modeling effort, we intend to quantify and control this limiting behavior which is not predicted by the simplified design techniques and up to now left as uncharacterized system noise. Specifically, we intend to discover means of improving the sensitivity of the sensor through filtering and control based on a detailed model of the thermal noise. The main outcomes of this project will be exactly this model of thermal noise, as well as direct estimates of device sensitivity through free energy measurements.

Summary of Accomplishments

This year, we were able to make substantial progress in fabricating suspended single carbon nanotube devices that can be electrically sensed and actuated. The device we are creating is novel to Sandia and will be a platform for measurements in the next fiscal year as well as potential proposals to DARPA (Defense Advanced Research Projects Agency) in the out years. Also we have made relevant, publishable discoveries about the frequency content of the thermal noise in carbon nanotubes using molecular dynamics and statistical mechanics. The structure of the noise is quite remarkable and can be exploited in our future efforts to improve the signal-to-noise ratio of carbon nanotubes used as mechanical resonance sensors. This work is ready for submission to the high impact journal *Physical Review Letters*, with a fuller exposition to be submitted to *Physical Review B* or *Journal of Chemical Physics*.

Significance

Characterization of short-time fluctuations will improve the fundamental understanding of NEMS. This will lead to means of effectively filtering and possibly controlling thermal noise. These methods will enable the detection of molecules with extremely short binding duration or at very low concentrations, for example. Ultimately, this project will enable novel, extremely sensitive NEMS sensors to be designed and employed in several of the Laboratories' strategic management units (SMUs) and defense missions.

Enabling Graphene Nanoelectronics

130771
Year 1 of 3
Principal Investigator: S. W. Howell

Project Purpose

We are combining a complete array of expertise and resources toward investigating three innovative and synergistic synthesis approaches for advancing reproducible fabrication and fundamental scientific understanding of high quality graphene films on technologically relevant substrates (Si and SiC). Recent work has shown that graphene, a 2D electronic material (with 1D nanoribbon semiconducting properties) amenable to planar semiconductor fabrication processing, possesses tunable electronic material properties potentially far superior to metals and other standard semiconductors. Despite its phenomenal electronic properties, focused research is still required to develop techniques for depositing/synthesizing graphene over large areas, enabling the reproducible mass-fabrication of graphene-based devices. For this project, we are focusing synthesis efforts toward three complementary techniques: 1) a novel non–ultrahigh vacuum (UHV) annealing-based synthesis approach for dramatically improving the quality and lateral size of graphene on SiC (medium risk); 2) novel graphene-on-Si approaches using directed assembly Si-H thermolysis strategies for a possible pathway for complementary metal oxide semiconductor (CMOS) integration (high risk); 3) transfer or directed assembly of graphene from Si-C or Si(111) onto MOS-relevant Si(100) using diazonium attachment/transfer chemistry (high risk). To develop vital fundamental understanding of these fabrication processes, characterization techniques such as low energy electron microscopy (LEEM), Raman spectroscopy, and scanning probe microscopy (SPM, especially atomic force microscopy/ scanning capacitance microscopy (AFM/SCM) will be utilized to provide deeper insight towards anneal-driven domain size, thickness, morphology, work function characteristics, and defects. Electronic characterization will also be conducted to gauge the quality of the graphene materials. If successful, our efforts will develop a suite of available synthesis strategies for addressing the unsolved challenging problems prohibiting the realization of next-generation graphene-based devices (i.e., disruptive CMOS-based devices, novel high-frequency devices). Our team possesses an unrivaled “complete package” of complementary expertise and capabilities (synthesis, characterization, integration, and modeling) necessary for high-impact mission-related graphene research results in this emerging competitive field.

Summary of Accomplishments

The group made numerous key accomplishments in the project’s first year synthesis and transfer goals: (1) we have established the synthesis route for single layer graphene film on SiC(0001) with mobility of ~9,000 cm^2/Vs and domain size of 50 μm^2 (which is close to the state-of-the-art reported values); (2) we developed a scalable method to pattern novel diazonium/iodonium attachment chemistry on Si substrates (necessary for directed assembly and transfer of graphene); (3) we have demonstrated attachment of acetylene molecules onto Si as a precursor for annealing into graphene via the thermolysis approach; (4) we have used low-energy electron microscopy (LEEM) to monitor in real-time the nucleation of graphene islands and their growth into sheets that completely cover Ru(0001), Ir(111), and Ni(111) substrates (by controlling the nucleation density and growth rate, single graphene domains of up to 1 mm in extent were achieved). Raman and LEEM characterization accomplishments were also made, and the group is preparing additional complementary x-ray photoelectron spectrometry (XPS) characterization of graphene materials to support the needs of the various synthesis approaches. Using density functional theory (DFT) calculations, we found that the (2x2) C reconstruction on the (000-1) (carbon-face) silicon carbide surface with one graphene layer on top has favorable free energies (driven by the Si ad atom reconstruction). We also performed preliminary calculations on a (11-20) SiC step edge with a graphene layer draped across it. We have also developed lithographic processes to fabricate simple graphene devices for characterization of electronic transport properties. We have made important contributions toward the understanding of quantum transport properties in epitaxially grown graphene films and observed the integer quantum Hall effect, and obtained exciting results on electron heating.

Significance

Despite the relative frenzy of research activity elsewhere, there is presently insufficient organized research aimed towards realizing next-generation high-speed and high-frequency graphene devices. This project will enable Sandia to establish proven graphene expertise and capability for meeting anticipated national security and DOD (e.g., Defense Advanced Research Projects Agency [DARPA]) needs. This expertise/capability will also advance the scientific discovery and innovation goals of DOE, in particular those of the Office of Basic Energy Sciences (BES).

Refereed Communications

K.V. Emtsev, A. Bostwick, K. Horn, J. Jobst, G.L. Kellogg, L. Ley, J.L. McChesney, T. Ohta, S.A. Reshanov, J. Röhrl, E. Rotenberg, A.K. Schmid, D. Waldmann, H.B. Weber, and T. Seyller, “Towards Wafer-Size Graphene Layers by Atmospheric Pressure Graphitization of Silicon Carbide,” *Nature Materials*, vol. 8, pp. 203-207 , March 2009.

E. Loginova, S. Nie, K. Thürmer, N.C. Bartelt, and K.F. McCarty, “Rotational Domains of Graphene on Ir(111),” to be published in *Physics Review B*.

Hierarchical Electrode Architectures for Electrical Energy Storage and Conversion

130772
Year 1 of 3
Principal Investigator: K. R. Zavadil

Project Purpose

This proposal will develop, through the discovery process, the fundamental knowledge base necessary for the creation of stable hierarchical electrode architectures for electrical energy storage and conversion. Hierarchical electrodes are the enabling technology necessary to produce revolutionary improvements in the performance characteristics of electrochemical devices capable of storing electrical charge (i.e., ultra- or redox capacitors) or interconverting electrical charge and chemical energy (i.e., batteries and reversible fuel cells). Such revolutionary improvements are necessary to ensure a secure energy future for the nation. An important barrier to achieving stable hierarchical electrodes is Ostwald ripening of these nanoscale structures driven by dissolution and redeposition dynamics. As a consequence, constructing stable hierarchical electrodes requires a fundamental understanding of the impact of overall geometric shape, surface energetics, and environmental factors on the ripening dynamics.

We propose to address the problem of electrode stability by studying ripening-resistant metal structures recently discovered and developed at Sandia. In situ measurement diagnostics will be used to study the evolution of nanostructure topography as a function of electrode morphology and electrochemical factors. Local metal dissolution and redeposition rates will be measured and used in computational simulations to develop a mechanistic understanding of the origins of stability. Computational methods will be expanded to take into account the electrochemical double layer contribution to nanoscale stability. Synthetic methods will be developed to produce new hierarchical electrode architectures to enhance and explore the limits of stability. The role of alternate metals, chemical passivation schemes, and the inclusion of functional charge storage materials on structure stability will also be explored. In addition, new in situ diagnostics for characterizing charge storage mechanisms at electrode surfaces will be developed. Discoveries made using this tightly coupled synthesis, characterization and computation approach are anticipated to impact a wide range of electrochemical charge and energy storage technologies.

Summary of Accomplishments

A hierarchical electrode was fabricated from foam-like Pt spheres and subjected to repeated oxidative stress by cycling 6000 times over a potential range of 0.6 to 1.1 V versus the reversible hydrogen electrode. This electrode exhibited a 55% reduction in electrocatalytic response to the oxygen reduction reaction. Electron microscopy showed that the dendritic substructure of the spheres had undergone ripening to form rope-like ligaments. These results established a baseline ripening resistance for this material. Work was initiated on decorating the basic building block of these materials with gold to improve the ripening resistance. A gold nanoparticle synthesis process was developed and demonstrated as effective at depositing nanoparticles on dendritic Pt sheets. A method for covalently binding metal nanoparticles and mesoscale ripening-resistant structures to planar electrodes was developed and demonstrated. Use of this attachment technique allows for the stable imaging of nanostructures using electrochemical scanning probe microscopy and ensures the electronic coupling of bound structures with the underlying electrode, such as graphite. An outcome of this work is new knowledge about the mechanism of nucleation and growth of aryl moieties on graphene surfaces and the electronic and mechanical consequences of this functionalization on graphene. Molecular dynamics simulations have been run on infinite Pt slabs and on Pt polyhedral nanoparticles to establish the relationships of surface melting and particle shape change with temperature. Thermal ripening is considered a starting analog for the electrochemical environment where a metal undergoes partitioning between the solid and vapor (liquid for electrochemical case) phases. Relationships were established between surface orientation and the onset for reconstruction, shape change (for particles) and eventual surface melting. The molecular dynamics (MD) code was applied to simulate shape change for individual dendrite structures under thermal stress. A predictive x-ray scattering code was written to support planned in situ measurements of ripening.

Significance

This project addresses the DOE mission to provide energy security for our nation. Discovered knowledge is anticipated to impact a range of energy storage technologies including ultracapacitors, batteries and fuel cells. Revolutionized energy storage capability will enable vehicle electrification allowing for a shift toward domestic fuel sources, point of generation storage facilitating a shift to carbon neutral or renewable energy sources, and expanded flexibility in transmission grid design.

Refereed Communications

Y.J. Song, M.A. Hickner, S.R. Challa, R.M. Dorin, R.M. Garcia, H.R. Wang, Y.B. Jiang, P. Li, Y. Qiu, F. van Swol, C.J. Medforth, J.E. Miller, T. Nwoga, K. Kawahara, W. Li, and J.A. Shelnutt, “Evolution of Dendritic Platinum Nanosheets into Ripening-Resistant Holey Sheets,” *Nano Letters*, vol. 9, pp. 1534-1539, April 2009.

Hierarchical Morphology Control for Nanocomposite Solar Cells

130773
Year 1 of 3
Principal Investigator: J. W. Hsu

Project Purpose

Solar energy has the potential to meet future power demands with minimal environmental impact. However, current photovoltaic (PV) solar harvesting technologies are too expensive for broad usage. New materials and technologies must be developed to lower the manufacturing and deployment costs while maintaining good performance (> 10% power conversion efficiency). Organic and organic-inorganic hybrid photovoltaics have the potential to meet these performance goals because these systems offer the ability to tailor an individual material's optoelectronic properties via chemical synthesis. In addition, they meet the critical requirement of inexpensive manufacturing (e.g., ink-jet printing and roll-to-roll printing) on novel substrates (e.g., textile) because they require only low temperature processing. Most importantly, the large internal interfacial area of these nanostructured material systems is critical for high photocurrent generation, and appropriate interfacial material engineering should lead to enhanced device performance. Currently, organic photovoltaics (OPVs) based on polymer-fullerene nanocomposites have demonstrated > 5% efficiency. Performance of these OPV devices depends critically on the morphology of the interpenetrating domains that separate the polymer (donor) and fullerene (acceptor) phases, which so far have been studied only in an entirely trial-and-error fashion. To make significant advances going forward will require unprecedented understanding and control in manipulation of donor-acceptor morphology at the nanoscale, to enhance photocarrier separation and transport. The purpose of this project is to understand how the connectivity of the electron donating phase (conjugated polymer) and that of the electron accepting phase (inorganic nanoparticles) affect the performance of the solar cells. The hierarchical structures of the network will be tuned through interfacial chemistry, guided by modeling.

Summary of Accomplishments

We have successfully made ZnO, ZnMgO, and TiO_2 nanoparticles, demonstrated the feasibility of linking nanoparticles via surface functionalization, and shown the effect of nanoparticle-solvent interaction strength on the nanoparticle network morphology through molecular dynamic simulations. To perform the simulations, we had to add a new routine into the C++ large-scale atomic/molecular massively parallel simulator (LAMMPS) code that will create bonds between pairs of particles. We added a new approach, in which Zn precursor is added to the polymer solution, and a film is cast from the mixture and annealed in humid environment to convert to ZnO embedded in the polymer matrix. We have also applied atomic force microscopy (AFM) to characterize surface topography of nanoparticle blended polymer films. Bilayer solar cells made of a ZnO or ZnMgO nanoparticle layer and a poly-3-hexylthiophene (P3HT) layer have shown three fold enhancement in efficiency compared to similar devices made of a ZnO sol gel film. We have also attempted to make bulk heterojunction solar cells with ZnO nanoparticles and precursors. However, the inorganic materials tend to aggregate in the organic solvents and the resulting films are too rough for devices. We have identified surface functionalization routes to better disperse nanoparticles in organic solvents.

Significance

Energy independence and security have become a key DOE mission and national urgency. The success of this work will position Sandia to contribute to future generations of solar cell technologies. The collaboration among researchers with a wide range of expertise enables the team to attack an important energy problem that cannot be done by each researcher alone. Collaborating with the National Renewable Energy Laboratory (NREL) will position us to move to the technology forefront.

Refereed Communications

E.D. Spoerke, M.T. Lloyd, E.S. Martin, D.C. Olson, Y.-J. Lee, J.A. Voigt, and J.W.P. Hsu, "Improved Performance of P3HT/ZnO Hybrid Photovoltaics Modified with Interfacial Nanocrystalline Cadmium Sulfide," to be published in *Applied Physics Letters*.

Y.-J. Lee, M.T. Lloyd, D.C. Olson, R.K. Grubbs, R.J. Davis, J.A. Voigt, and J.W.P. Hsu, "Effect of ZnO Nanorod Array Morphology on the Performance of Nanostructured Hybrid Photovoltaic Devices," *Journal of Physical Chemistry C*, vol. 113, pp. 15778-15782, September 2009.

E.D. Spoerke, M.T. Lloyd, Y.-J. Lee, T.N. Lambert, B.B. McKenzie, Y.-B. Jiang, D.C. Olson, T.L. Sounart, J.W.P. Hsu, and J.A. Voigt, "Nanocrystal Layer Deposition: Surface-Mediated Templating of Cadmium Sulfide Nanocrystals on Zinc Oxide Architectures," to be published in the *Journal of Physical Chemistry C*.

High-Temperature, Large Format FPAs for Emerging Infrared Sensing Applications

130774
Year 1 of 3
Principal Investigator: J. K. Kim

Project Purpose

Mission requirements continue to drive up the size and resolution of mid-infrared focal-plane-arrays (FPAs), but the scaling trend is now severely challenged. This problem has been traditionally addressed by improving HgCdTe sensor quality, as well as cooler and solar-cell efficiencies, but these incremental improvements are slowing and are not expected keep up with the demands of emerging infrared applications. Other persistent problems are unreliability of two-stage cryocoolers and low FPA operability resulting from fundamental HgCdTe material limitations.

We propose to develop a disruptive photosensor technology that can offer a significant advantage over HgCdTe in mission capabilities, enabling a higher FPA detectivity at the same operating temperature or the same detectivity at a higher temperature as required when using very large FPAs. The basis of this technology is the InAs/Ga(In)Sb strained-layer superlattice (SLS) whose bandstructure is engineered at the nanoscale to manipulate material properties, such as bandstructure and carrier lifetime, to achieve sensor performance unattainable with bulk materials. The overall structure is strain free on the GaSb substrate, which is available in a significantly higher quality compared to CdZnTe, permitting higher operability than HgCdTe. For these reasons, SLS is considered to be a promising technology to fill the HgCdTe technology gap and has received significant attention.

We will tackle two key challenges required to realize the superiority over HgCdTe as predicted by theory: improving SLS materials to reduce dark current and efficient pixel-scaling to high FPA resolutions using nBn technology. Success will serve to enhance Sandia's role in the areas of intelligence and strategic/tactical military systems.

Summary of Accomplishments

Activity to date has been to establish a robust theoretical scientific basis for assessing ideal and actual material and device performance and validating theoretical models with measurements of material and device characteristics, followed by FPA demonstrations. This overall goal has been pursued through four interdependent tasks: SLS bandstructure modeling, SLS carrier lifetime measurement, nBn device modeling, and nBn FPA demonstration. All proposed goals and milestones for FY 2009 have been achieved. We have significantly extended Sandia's modeling and experimental capabilities and expanded the fundamental scientific understanding of SLS and nBn. Accordingly, two invention disclosures were filed in FY 2009 and one paper was published.

We have implemented a robust SLS bandstructure model based on the empirical pseudopotential method which can take into account every relevant nonidealities by treating SLS atom-by-atom. This tool forms the basis of evaluating and optimizing SLS by not only predicting material behavior but also identifying deficiencies in actually grown materials. Carrier lifetime measurement — originally proposed as an FY 2010 goal for characterizing the effects of defects in SLS — was also performed in FY 2009. Carrier lifetime measurement allows direct probing of the quality of SLS material, layer-by-layer, to reveal the effects of each constituent of

SLS, as a method of troubleshooting. Great progress was also made in understanding the physical mechanisms of nBn operation, which is currently poorly understood in the community. We have also made and demonstrated a 640 x 512 nBn FPA.

Significance

This project will impact satellite-based, airborne and ground-based mid-wavelength/long-wavelength infrared (MWIR/LWIR) imaging systems that are vital in nonproliferation assessment, tactical surveillance, missile defense and combat support. High-temperature MWIR/LWIR detectors developed through this project will enhance the performance and functionality of infrared imaging systems that are currently limited by the excessive cooling requirements of the focal plane array.

Refereed Communications

J.F. Klem, J.K. Kim, M.J. Cich, G.A. Keeler, S.D. Hawkins, and T.R. Fortune, “Mesa-Isolated InGaAs Photodetectors with Low Dark Current,” *Applied Physics Letters*, vol. 95, p. 031112, July 2009.

Narrow-Linewidth VCSELs for Atomic Microsystems

130775
Year 1 of 3
Principal Investigator: D. K. Serkland

Project Purpose

Vertical-cavity surface-emitting lasers (VCSELs) are the laser of choice for photonic microsystems due to their low power consumption, ease of integration, and single frequency operation. For example, the 1 mW power consumption of a VCSEL is more than an order of magnitude lower than the nearest alternative: traditional edge-emitting lasers. However, the typical VCSEL linewidth (100 MHz) is approximately ten times wider than the natural linewidth of atoms used in atomic beam clocks and trapped atom research, which degrades or completely destroys system performance.

We propose to develop a new external-cavity VCSEL (EC-VCSEL) having a linewidth narrower than 1 MHz, specifically for use in emerging atomic microsystems, such as primary frequency standards and atom traps. In order to reduce the VCSEL linewidth, we must simultaneously increase the Q of the laser cavity and decrease the linewidth enhancement factor of the active region. We will increase the stored optical energy and thus cavity Q by extending the cavity length to 50 microns (over 10 times longer than normal), terminating the extended cavity with an external high-reflectivity dielectric mirror. The 10-fold increase in cavity length precludes an all-semiconductor structure, but is still small enough to permit wafer-scale microfabrication of the device. Significant metal organic chemical vapor deposition (MOCVD) epitaxial growth development will be undertaken to allow the extended cavity geometry, minimize free-carrier absorption losses, and develop active quantum wells that achieve minimum linewidth enhancement (alpha) factor. VCSELs have long been a differentiating technology for Sandia, due to the complexity of VCSEL design, epitaxial growth, and microfabrication. If we are successful in wafer-scale fabrication of narrow-linewidth VCSELs, these new devices and our advances in scientific understanding could enable future development to tailor these devices for use in specific high-performance atomic-physics microsystems.

Summary of Accomplishments

We have accomplished our overall first-year goal of understanding the scaling of EC-VCSEL linewidth versus key laser parameters, such as cavity length, cavity losses, and linewidth enhancement factor (alpha). We built and operated an 850-nm electrically-injected EC-VCSEL, thereby completing our first FY 2009 milestone, using appropriately designed epitaxial structures and a modified VCSEL fabrication process. The EC-VCSEL achieves laser threshold at current densities comparable to standard VCSELs, which is important for retaining the low power consumption that VCSELs uniquely provide.

We also built an apparatus to measure the linewidth and the linewidth enhancement factor (alpha) of our VCSELs, which enabled us to complete the second FY 2009 milestone to measure the linewidth of our EC-VCSELs versus cavity length. To our knowledge, our measurement of VCSEL linewidth enhancement factor is the first at Sandia. We have theoretically modeled the linewidth enhancement factor of two alternative quantum-well gain regions, and we are in the process of comparing his predictions with our measurements and we plan to publish the results in late 2009.

In keeping with the first-year goal to understand linewidth scaling versus VCSEL cavity length, we have designed, grown, and fabricated an all-semiconductor extended-cavity VCSEL. Although not specifically designed to achieve a record linewidth, the extended-cavity VCSEL yielded a linewidth of 23 MHz, which is considerably better than our previous record of 50 MHz. We presented two invited talks on the extended-cavity-VCSEL results, and a Society of Photographic Instrumentation Engineers (SPIE) manuscript was submitted and published in February 2009.

Significance

Sandia's differentiating capabilities in compound semiconductor epitaxial growth, VCSEL microfabrication, and optical microsystem integration will be enhanced by this research project. Success in making a narrow linewidth VCSEL could impact a variety of areas: primary frequency standards, neutral atom and ion traps, and quantum information research. Applications range from improved military communication and navigation to quantum encryption.

Phonon Manipulation with Phononic Crystals

130777
Year 1 of 3
Principal Investigator: I. F. El-Kady

Project Purpose

We propose to develop a fundamental understanding of, and a methodology for, deterministic phonon spectrum control at the THz region (100 K-phonons) using a top down phononic crystal (PhonC) approach. Present approaches to phonon control are based on texturing the surface to increase phonon scattering or shrinking the diameter of the material to prevent bulk propagation much like a cutoff waveguide, or phonon scattering off grain boundaries. All such approaches are either highly nondeterministic or are capable of only targeting a narrow spectral range. In contrast, PhonCs utilize physics similar to Bragg-scattering. In a fashion reminiscent of photonic lattices, spectrally wide bandgaps can be deterministically produced in which phonons are inhibited, accompanied by a redistribution of the phononic density of states (DOS). This offers a unique vehicle for tailoring the phonon spectrum for a variety of applications and awards a larger degree of control. For example by selectively enhancing the efficiency of phonon propagation in specific spectral bandwidths, enhanced thermal-to-RF frequency tags and microcoolers can be realized. Conversely, by selectively suppressing THz phononic spectral bands, exceptionally high-ZT materials can be achieved. Furthermore, other important processes, such as the electron-phonon interaction that cap the performance in high-T_c superconductors, and phonon-photon interaction essential for quantum-well or dot based solid state lighting could potentially be impacted by the profound phonon control provided by PhonCs. If successful, this approach will lead to a wide range of new thermal applications such as efficient and directional heat removal from integrated circuits, thermoelectric materials with improved efficiency, and new approaches to thermal harvesting. Finally, by extending the existing phononic-photonic crystal homomorphism this program will lay the foundation for realizing the first phononic metamaterials essential for high-precision focusing and manipulation of vibrational energy for a wide range of ultrasonic imaging devices and deep-sea cloaking.

Summary of Accomplishments

In the theoretical area we were able to develop a better understanding of the physical origins of phononic bandgaps. We developed two new modeling capabilities, plane wave expansion (PWE) and the planes approximation method, for better understanding the Bragg and Mie scattering conditions that form phononic crystals. The results of these new models correlate well with previous measurements and finite difference time domain (FDTD) models. One very important accomplishment was extending the FDTD models to include phononic crystal thickness which becomes very important at high frequencies. We have also developed methods for modeling the mode shapes of propagation outside the phononic bandgap and correlated these modes with results from PWE. In the Microsystems and Engineering Sciences Applications (MESA) facility, we have fabricated Si/W and Si/air phononic crystals and phononic crystal based cavities at frequencies as high as 8.5 GHz and with minimum feature sizes of 150 nm using optical (mass producible) lithography. Our partners at the University of New Mexico (UNM) have fabricated Si/air phononic crystals using focused ion beam (FIB) lithography with minimum feature size of 26 nm, corresponding to a bandgap center frequency/temperature of 100 GHz/5 K. UNM has also developed FIB masking techniques that results in vertically etched sidewalls which is important when realizing phononic crystals. In the experimental area, measurement techniques for characterizing phononic crystal modification of the thermal phonon distribution have been extensively researched. A Brillouin light scattering (BLS) system for characterizing thermal phonons in 1–100 GHz (0.05 – 5 K) phononic crystals has been researched and purchased. In addition an oxford dilution refrigerator based setup has been developed for measuring thermal phonon transport in phononic crystals at temperatures as low as 10 mK.

Significance

This research could result in a new class of thermal materials for heat control and thermal energy scavenging and will lay the foundation for realizing the first phononic metamaterials essential for high-precision focusing and manipulation of vibrational energy for a wide range of ultrasonic imaging devices and deep-sea cloaking. Furthermore, it promises to put Sandia at the forefront of a new branch of science of direct interest to our DOE and DOD customers.

Refereed Communications

I. El-Kady, M.F. Su, Y. Soliman, D. Gottler, P. Hopkins, P. Rakich, Z. Lesseman, and R.H. Olsson III, "Origin of Reduction in Phonon Thermal Conductivity of Microporous Solids," to be published in *Applied Physics Letters*.

I. El-Kady, M.F. Su, Y. Soliman, D. Gottler, P. Hopkins, P. Rakich, Z. Lesseman, and R.H. Olsson III, "Band Structure of Bulk Modes in Two-Dimensional High-Contrast Solid-Solid Phononic Crystals," to be published in *Physical Review E*.

R.H. Olsson III, S.X. Griego, I. El-Kady, M. Su, Y. Soliman, D. Goettler and Z. Lesseman, "Realizing the Material fQ Limit in Phononic Crystal High Q Cavities," to be published in *Applied Physics Letters*.

I. El-Kady, M.F. Su, Y. Soliman, D. Gottler, P. Hopkins, P. Rakich, Z. Lesseman, and R.H. Olsson III, "Physical Origins of Deep Wide Phononic Bandgaps," to be published in *Physical Review B*.

Real-Time Studies of Battery Electrochemical Reactions Inside a Transmission Electron Microscope

130778
Year 1 of 3
Principal Investigator: J. P. Sullivan

Project Purpose

In this project we will develop a capability to investigate lithium-ion (Li-ion) battery electrochemical processes in real time inside a transmission electron microscope (TEM). This unique capability could have impact in a number of research areas, including the science of catalysis, electrodeposition, corrosion, capacitive energy storage, and electrochemical energy storage (i.e., batteries), which is the focus of this study. Currently, there are serious fundamental issues in Li-ion batteries regarding performance degradation during cycling and aging that are unresolved and poorly understood. Furthermore, the fundamental study of these problems has been hampered by the lack of experimental and theoretical techniques that can identify structural changes in battery electrodes with atomic to nanoscale resolution during actual battery operation. We will develop both a sealed silicon micromachined fluidic platform as well as a simple open platform using a vacuum-stable ionic liquid (IL) electrolyte to measure structural changes within and at the surfaces of battery cathodes and anodes. We will explore the mechanism of Li intercalation in carbon-based anodes and phase changes that occur as Li inserts and de-inserts in nanoscale cathodes. We will identify and characterize solid-electrolyte-interphase (SEI) compounds that form on the electrode surfaces during polarization and potential cycling. We will use molecular dynamics (MD) and ab initio MD (AIMD) to model the Li intercalation in ideal carbon nanotube (CNT) electrodes and the formation of SEI compounds on carbon-based anodes. We will also develop versatile silicon-based electrochemical platforms that should have great utility for both in situ as well as ex situ electrochemical investigations. To our knowledge, this would be the first real-time study of battery reactions inside a TEM and potentially the first study that demonstrates atomic resolution of electrochemical processes inside a TEM.

Summary of Accomplishments

In the first year of this project we have generated several key accomplishments, and we have firm confidence that the approach that we are pursuing will generate exciting breakthroughs in the understanding of lithium-ion batteries. These accomplishments include the following:

1. We have demonstrated a simple battery electrode-electrolyte system for use inside a transmission electron microscope (TEM) that is based on a holey carbon grid coated with a vacuum-stable ionic liquid electrolyte. We have tested the ability to probe individual nanoscale battery anodes (carbon nanotubes [CNTs]) and cathodes (a vanadium dioxide nanowire) using an in situ scanning tunneling tip, and we have manipulated ionic liquids in situ, thus completing the testing of the necessary components of our in situ electrochemical platform.
2. We have devised an experimental means of fixing two CNT electrodes to electrical contacts with a narrow gap in between that permits electrochemical and structural measurements of lithium intercalation into CNTs. We have also developed the framework and initial simulations of the experimental geometry using classical molecular dynamics (MD) modeling.
3. We have performed ab initio MD on graphite/ethylene carbonate + lithium systems and have seen preliminary evidence for solid-electrolyte-interphase formation.
4. We have completed the design of a versatile MEMS (microelectromechanical system) chip that not only enables high-resolution TEM imaging using conventional battery electrolytes but also provides a vast array of electrode geometries for in situ and ex situ electrochemical testing. We have met all milestones to date, and we are on track to meeting our overall ambitious project objectives.

Significance

This project impacts lithium-ion battery and novel electrical energy storage technologies. These are critical for remote and mobile energy systems (remote sensors, vehicle propulsion, off-grid solar). The DOE has requested new research that focuses on renewable and alternative energy technologies, and research on electrochemical energy storage is a critical component of that initiative. In addition, this work could aid the development of electrochemically based chem/bio sensors to support defense, intelligence, or homeland security needs. Our research in electrochemical energy storage will reveal fundamental mechanisms associated with charge storage, interfacial transport, and electrochemical cycling. Understanding of these phenomena is essential in order to develop novel battery materials and architectures with performance that far exceeds current systems (factors of 2 to 5 times greater in storage or power than existing technology). These revolutionary performance improvements are needed to meet the nation's goals for alternative and "green" energy generation and storage.

Refereed Communications

A. Subramanian, A.R. Alt, L. Dong, B.E. Kratochvil, C.R. Bolognesi, and B.J. Nelson, "Electrostatic Actuation and Electromechanical Switching Behavior of One-Dimensional Nanostructures," to be published in *ACS Nano*.

Science-Based Solutions to Achieve High Performance Deep UV Laser Diodes

130779
Year 1 of 3
Principal Investigator: M. H. Crawford

Project Purpose

A number of mission-critical applications would greatly benefit from a compact, deep ultraviolet (< 340 nm) laser diode (LD), however commercial LDs are currently limited to longer UV wavelengths. AlGaN semiconductor alloys are the most promising materials for deep UV LDs, with potential for emission across the 200–365 nm region and the recent demonstration of mW-level 275–300 nm AlGaN light-emitting diodes (LEDs) by our Sandia team. To date, realization of deep UV LDs has been thwarted by the lack of fundamental insight and solutions to key AlGaN materials challenges. These challenges include (1) nanoscale point defects, (2) p-doping limitations, and (3) high internal optical losses and limitations to optical gain. Through previous internal (LDRD) and external (Defense Advanced Research Projects Agency [DARPA]) investments, our team has established a world-class capability in AlGaN materials and has developed the infrastructure and materials/device fabrication experience to elucidate and overcome these challenges. We propose a science-based approach that will apply our state-of-the-art AlGaN metal-organic vapor-phase epitaxy capabilities, innovative materials growth and heterostructure design strategies, differentiating materials characterization techniques and advanced device modeling to gain fundamental insight into these three critical challenges. We will apply those insights and Microsystems and Engineering Sciences Applications (MESA) microfabrication (Microfab) processing capabilities to design and fabricate AlGaN LDs in the 300–340 nm region. If successful, our project will yield the world's first 340 nm and shorter wavelength LDs, relevant to a range of applications including fluorescence-based bioagent sensing and trapped-ion-based quantum computing. Materials insights gained from this project could be applied to a range of III-Nitride materials and devices, enabling advances in deep UV light emitting diodes (LEDs) for water purification, visible LEDs for solid-state lighting, photovoltaics for power-over-fiber applications and high-electron-mobility-transistors for synthetic aperture radar applications. This project therefore offers a unique opportunity to leverage Sandia strengths and achieve both science and technology breakthroughs with strong relevance to DOE missions.

Summary of Accomplishments

Our FY 2009 accomplishments include the application of deep-level optical spectroscopy (DLOS) to AlGaN films to quantify point defect energy levels and densities. Our first study focused on epilayers grown under quantum well (QW) growth conditions and evaluated different Al compositions corresponding to different laser wavelengths. DLOS spectra and modeling revealed two dominant acceptor defect levels in each epilayer. The deepest level is tentatively assigned to be a cation vacancy complex and displays an increased density of states for the higher Al composition alloy. Extensive growth studies combined with photoluminescence and Hall measurements were conducted to map out growth conditions for on-going DLOS studies on QWs and p-AlGaN epilayers. P-type short-period superlattice (p-SPSL) structures were grown to assess their potential in achieving effective hole injection. The structures demonstrated excellent deep UV transmission and lateral resistivities as low as 1.6 ohm-cm. Vertical resistivities were assessed by a vertical transmission line model method to be at least 1000× the lateral resistivities and dependence of vertical resistivity on template composition was explored. Proof-of-concept hole injection was demonstrated through electroluminescence at ~280 nm from a QW LED structure employing a p-SPSL with average Al composition of 0.61. Aspects of this work were presented at three professional conferences. Multiple bulk and SPSL structures were grown, with and without p-type doping, to quantify sub-bandgap optical loss through transmission spectroscopy. Laser process development included optimization of an etched facet process as well as the development of a ridge waveguide laser process that incorporates this new facet process. High-reflectivity facet coating development achieved greater than 90% reflectance at 320 nm.

Significance

This project supports DOE's strategic goal of providing world-class science to address mission needs. Nitride materials insights from this project could lead to advances in solid-state lighting, a major Sandia investment area aligned with DOE's Energy mission. Deep UV laser diodes will enable a new technology applicable to compact systems for fluorescence-based bioagent sensing and trapped-ion-based quantum computing, applications of interest to DHS and agencies including the Defense Advanced Research Projects Agency (DARPA) and the Intelligence Advanced Research Projects Activity (IARPA).

Refereed Communications

M.A. Miller, M.H. Crawford, A.A. Allerman, K.C. Cross, M.A. Banas, R.J. Shul, J. Stevens, K.H.A. Bogart, "Smooth and Vertical Facet Formation for AlGaN-Based Deep-UV Laser Diodes," *Journal of Electronic Materials*, vol. 38, pp. 533-537, January 2009.

Transport Mechanisms for Charge Transfer Processes at Electrode-Solid-Electrolyte Inferfaces

130780
Year 1 of 3
Principal Investigator: K. F. McCarty

Project Purpose

The purpose of this project is to develop and apply new in-situ spectroscopies to understand and improve electric charge transfer in electrochemical devices such as fuel cells. Electrochemical technology will play an increasingly critical role in meeting the nation's energy challenges in both stationary power applications and transportation. The essential physical phenomenon occurring in all electrochemical devices is the transfer of electrical charge across material interfaces. How this charge transfer occurs and its relationship to the device's performance and reliability is largely unknown. This project develops fundamental understanding of interfacial charge transfer by characterizing it in real time during electrochemical operation. We are studying the charge-transfer process in solid-oxide fuel cells (SOFCs) for three reasons: (1) SOFC interfaces are more accessible for in-situ characterization than in other electrochemical devices; (2) Within the same technology platform, electricity can be generated from fuels and vice versa when run as fuel cells or as electrolyzers; (3) SOFCs can operate on a variety of fuels, including hydrogen and hydrocarbons.

Thus, SOFCs could potentially contribute significantly toward low-carbon energy systems for both fixed and portable (transportation) applications. But like all electrochemical-based technologies, they suffer from performance and cost issues. The advances needed, especially those for lower-temperature vehicular operation, have been hampered by inadequate understanding of elementary processes. In particular, detailed, microscopic measurements of interfacial species concentrations, their spatial distributions, and transport rates under operating conditions have not been made. We are determining this information by characterizing the species present on SOFC materials during operation. We are using micro- and nanofabrication to develop a new experimental "platform" with accessible surfaces and enhanced performance. We then characterize operating SOFC surfaces at realistic pressures and temperatures using ambient-pressure x-ray photoelectron spectroscopy.

Summary of Accomplishments

We have made significant progress in designing and fabricating unique experimental platforms providing high-purity materials, optical access, and compatibility with the x-ray photoelectron spectroscopy (XPS) end station at the Advanced Light Source (ALS). To better define the three-phase-boundary (TPB) region where electrochemistry occurs, we initially fabricated electrochemical cells (ECs) using thin-film patterned electrodes. Electrodes are deposited on the upper surface of the electrolyte [single-crystal yttria-stabilized zirconia (YSZ)]. A key difficulty overcome was making reliable, convenient, and reproducible electrical contact to the electrodes. We solved this problem by using custom-designed, spring-loaded miniature probes mounted on the sample transfer platen. We also constructed an experimental chamber that allows operation of ECs for electrochemical characterization and testing under appropriate temperatures and gas mixtures.

We conducted experiments on Ni/YSZ/Pt and Ni/YSZ/Ni cells with dense thin-film electrodes to investigate the ability of XPS to monitor chemical species at the TPB. Using the new spatial imaging capability at APS, we were able to see electrochemically generated species that spillover between the Ni and Pt electrodes and the YSZ electrolyte. Furthermore, we used the imaging capability to map the electrical potential across the electrodes and the electrolyte. In this manner, we quantitatively measured the electric overpotentials, that is, the voltage drops between the electrodes and the electrolyte. Our research has produced the first direct measurements of the overpotentials, which critically control the efficiency of fuel cells.

Significance

This work will benefit DOE's mission by contributing to the following strategic goals:

- Energy security — Promotes the availability of diverse sources and delivery methods of domestically produced, environmentally sound energy supplies, and advances technology needed for utilization of hydrogen energy infrastructure.
- Science — Advances knowledge of fundamental processes involved in electrochemical devices.
- Environment — Will allow significant reductions in carbon emissions.

Feasibility of Nano-Optomechanical Systems (NOMS) for Extreme Environment-Capable Silicon Photonics

138703
Year 1 of 1
Principal Investigator: P. T. Rakich

Project Purpose

Despite remarkable advances in silicon photonics, a solution to the dimensional and environmental sensitivities of this technology is urgently required because such sensitivities present a serious barrier to yield and stable operation of silicon photonic devices. We investigate a solution to the problem of microcavity thermal and dimensional sensitivities through a new class of integrated silicon photonic devices with nanomechanical movable parts (broadly termed nanooptomechanical systems, or NOMS), whose motion is powered-by-light. Under illumination by modest (mW) optical-powers, recent research has shown that forces produced by light can generate nanomechanical adjustments in the moving parts of the microcavity, allowing the cavity frequency to be controlled and stabilized using an incident optical signal. (This previous theoretical work was done at Massachusetts Institute of Technology (MIT), by the PI of this project). The result is a self-adaptive optically controlled "smart-microcavity," which is completely thermally insensitive. This all-optical a-thermalization method has the distinct advantage that it requires no local power source; it dissipates negligible on-chip power, and is robust in extreme environments.

To date, the compelling self-adaptive functionalities of such NOMS designs have been explored through basic theoretical models in the context idealized systems. Through this feasibility study, we will adapt these device designs to "real" microelectromechanical system (MEMS) fabrication processes and perform size, weight and power (SWAP) analyses to better understand the impact of such devices in various military and high-performance computing applications.

Summary of Accomplishments

To date, the compelling self-adaptive functionalities of such NOMS designs have been explored through basic theoretical models in the context idealized systems. In this project, we have developed a much simplified and tractable physical model for the forces within such systems which allow us to much more elegantly predict the effect that fabrication tolerances might have on the real-world performance of such devices. The theory that we have developed, which is termed the response theory of optical forces (RTOF) has been published in a peer reviewed journal paper in *Optics Express*. Through this theory, one is able to relate the optically induced forces within an optomechanical device to the optical phase and amplitude response of the device as a function of the mechanical degree of freedom present within.

In addition, through application of the newly developed RTOF theory, we have been able to simplify the analysis and design of complex optomechanical systems. We have filed two invention disclosures based on the outcome of this research.

Significance

This project investigates the feasibility of first-in-class "smart" self-adaptive photonic elements for ultrawidely tunable resonators and precision all-optical nanopositioning in integrated optical interconnections, sensors, and nanoactuators. If feasible, such "smart" systems will enable the application of high-performance integrated optics in the extreme environments found in weapons systems, satellites, novel sensors, and other key national security applications.

Refereed Communications

P.T. Rakich, M.A. Popovic, and Z. Wang, "General Treatment of Optical Forces and Potentials in Mechanically Variable Photonic Systems," *Optics Express*, vol. 17, pp. 18116-18135, September 2009.

Coupled Femtosecond Spectroscopy

138916
Year 1 of 1
Principal Investigator: T. E. Beechem

Project Purpose

The performance and reliability of many microsystems ranging from high-power electronics utilized in radar and satellites to microelectromechanical systems (MEMS) serving in sensory and actuating applications is directly linked to the device's operational temperature. Consequently, optimization and even realization require that the mechanisms governing the thermal dissipation be clearly understood. Due to the electronic nature of these devices, thermal dissipation occurs via energetic transfer from the electrical to lattice environments thus inherently coupling these systems. Despite these systems being implicitly linked, device characterization has continually focused on singularly probing either the (i) electronic or (ii) lattice (phonon) carriers, making it impossible to directly observe their coupling and hence the full nature of the thermal transport.

In response, this study provides an initial step in spanning the gap between operation and investigation, while in conjunction, providing a paradigm shift in device characterization, by seeking to analyze each energetic carrier concurrently. Specifically, the project attempts to prove the viability of such a concurrent approach through the observation of both subpicosecond resolved thermoreflectance (TTR) and Raman signals in a manner that allows for their simultaneous collection. As this project is intrinsically a "proof of concept" endeavor, effort is then focused not on the motivating thermal phenomena, but rather on the equipment and optical arrangement that would permit the observation of ultrafast TTR and Raman signals first individually and, if time permitted, simultaneously.

Summary of Accomplishments

This project is an initial effort to develop a capability to simultaneously perform transient thermoreflectance (electrons) and Raman spectroscopy (phonons) at subpicosecond timescales with the long-term goal of developing a tool that is uniquely suited to probe and decipher the cascade of energy through a material. As a first step then, the project's goals centered not on the analysis of these thermal processes but rather on the acquisition of subpicosecond TTR and Raman signals. TTR signals have been acquired in a robust, rigorous, and repeatable fashion on a time scale of ~100 fs using a colinear pump probe arrangement for a variety of materials including silicon. The employed optical arrangement is currently being utilized to measure and quantify such parameters as thermal conductivity, thermal boundary conductance, and the electron-phonon coupling factor. Acquisition of an ultrafast Raman signal was only demonstrated in an unrepeatable fashion using with this set up, however, due in large part to the spectral broadening inherent in the use of a 90 fs laser pulse. Analysis of this difficulty bounded, for the first time, the capability of performing ultrafast Raman at decreasing timescales. From this analysis, it was concluded that Raman signals may only be resolved when they are spectrally separated from the laser line by at least 3 times that of the bandwidth limited pulse. Therefore, future efforts focused on the acquisition of simultaneous Raman and TTR signals will utilize 150-fs pulses in order to balance the requirements of temporal and spectral resolving power.

Significance

This project addresses the DOE mission of scientific discovery for national security applications. The mechanisms driving thermal transport influence performance for a variety of systems including thermoelectrics and high-power electronics. In response, this project has taken initial steps to develop a unique capability devoted to examining these transport mechanisms. Upon full realization of such a capability, the exact thermal processes most pertinent to performance will be identified with greater fidelity, thereby allowing for device design to mitigate these effects.

Extreme Solid State Refrigeration using Nanostructured Bi-Te Alloys

138917
Year 1 of 1
Principal Investigator: P. A. Sharma

Project Purpose

Thermoelectric refrigerators that can spot-cool a circuit from room temperature to cryogenic temperatures eliminate the need for bulky liquid cryogens and compressors. Materials are desperately needed for solid-state refrigeration below ~150 K, the current practical cooling limit of the best Bi_2Te_3 based thermoelectrics. We have found that nanostructured Bi-Te alloys are promising candidates for low temperature thermoelectric cooling due to their significantly reduced thermal conductivity relative to bulk Bi_2Te_3 at ~77 K. In this project, we will (1) synthesize and structurally characterize specific promising Bi-Te nanostructured alloys; (2) investigate the figure-of-merit for cooling at 77 K using both theory and experiment; and (3) demonstrate that practical cooling is possible in these alloys with a prototype. Cooling existing IR detectors to 77 K with thermoelectrics could potentially double their sensitivity without further design changes.

The Bi-Te alloys under investigation form Bi_2Te_3/Bi_2 superlattices with nanometer spacings, which probably lead to the reduced thermal conductivity we have discovered. Our measurements of the electronic properties and first principles theory show that these alloys may be semimetals (similar numbers of electrons and holes). The combination of electronic and thermal properties should be useful for Ettingshausen cooling, a close relative of thermoelectric cooling. When subjected to the magnetic field of a permanent magnet, combined electron and hole transport can be used to pump heat. As few semimetals exist, the only material used for Ettingshausen cooling is elemental bismuth, but it only reaches a temperature of ~128 K in the laboratory. The nanostructured superlattice materials have a strongly reduced thermal conductivity compared to bismuth at low temperatures, potentially improving the figure of merit for an Ettingshausen cooler in the 77 K range.

Summary of Accomplishments

We investigated the potential of Bi-Te alloys for Ettingshausen refrigeration applications at the boiling point of liquid nitrogen. In order to accomplish this goal, we built up two new capabilities: 1. flux growth of single crystals and 2. Nernst effect measurements. Single crystal flux growth is a very important synthesis tool for research of new materials. Nernst effect measurements are important for understanding the coupling between heat and charge transport, which underpins thermoelectric applications.

We gained a significant understanding of carrier transport in polycrystalline Bi_4Te_3, and supplemented our measurements with ab initio electronic structure calculations. Bi_4Te_3 is a layered semimetal with a reduced thermal conductivity. It has nearly 100 times more p-type relative to n-type carriers with rather low mobility. The particular sample under study had a poor figure of merit for Ettingshausen cooling relative to bismuth, the standard material for this type of refrigeration. We could link the poor figure of merit to poor carrier mobility and speculate that this may be due to the layered nature of the material.

Single crystal growth of the Bi-Te system was heavily investigated. We found a new phase with the stoichiometry $Bi_{10}Te_9$ that has not yet been reported in the literature.

Significance

Cooling existing IR detectors to 77 K with thermoelectrics could potentially double their sensitivity without further design changes. Sandia's interest in detection ranges from nondestructive testing, biometrics, night vision, and satellite-based imaging. The ability to cool circuits without liquid cryogen could also dramatically expand the use of superconducting electronics, which have many defense and commercial uses. Our results will be useful in new searches for Ettingshausen materials.

Viscoelastic Coupling of Nanoelectromechanical Resonators

139071
Year 1 of 1
Principal Investigator: R. J. Simonson

Project Purpose

This work will leverage an unprecedented "top down" nanofabrication capability to create novel methods of materials characterization at 10–50 nanometer dimensions. Collaborators at California Institute of Technology (Caltech) have designed nanoelectromechanical (NEMS) single clamped beam resonators for gas sensor applications. Pairs of these devices separated by reproducible gaps in the 10–50 nm range can now be fabricated through process development advances made by collaborators at the *Laboratoire d'Electronique et de Technologie de l'Information* (Electronics and Information Technology Laboratory [LETI - Grenoble, France]). By depositing polymeric or inorganic materials as free-standing films that bridge the gap between pairs of such resonators, the devices can be mechanically, electrically, and/or thermally coupled. One side of a coupled NEMS pair can be mechanically driven by thermoelastic, piezoelectric or other excitation, while the mechanical and thermal response of the other NEMS device is monitored. The mechanical response will depend on variations in the viscoelastic moduli of the coupling film. Concerted measurements could eventually be made of electrical and thermal conductance of the bridging materials as well, seeking correlations between those properties and aging due to frequency-dependent mechanical strain, contaminant exposure, thermal history, and electrical bias. Successful development of this novel material characterization platform will supplement and extend existing methods of nanoscale measurements, e.g., measurement of local conducting properties by scanning tunneling microscopy or viscoelastic properties by atomic force microscopy-based nanoindentation. In particular, the latter method measures materials properties at low displacement frequencies while the proposed coupled resonators will measure high-frequency responses. By enabling material properties measurements at the "mesoscale," this work will help provide necessary data to bridge the length scale gap between atomistic and continuum simulations of materials properties. Thus, this research will potentially impact both the design of new "micro to nano" devices, and provide data in the modeling gap between atomistic and continuum length scales.

Summary of Accomplishments

We have set up the capability for excitation and measurement of the resonance of single and paired nanoelectromechanical single-clamped beam cantilevers at Sandia. These devices are fabricated at Caltech or at CEA-LETI (Electronics and Information Technology Laboratory of the French Atomic Energy Commission). Test devices have nominal in-plane dimensions of 2.5 microns x 0.7 microns. The devices are electrothermally driven following methods developed at Caltech. We have fabricated drive/readout systems that include RF synthesizers, RF mixers, and lock-in signal amplification enabling the detection of frequency, phase, and amplitude of the mechanical resonance of single and coupled oscillators. In addition, we have initial results on spray-coating of SU8 polymer solutions in cyclopentanone solvent onto gold and SiN substrates. We have chosen SU8 as the initial test system for evaluation of mechanical properties of polymeric materials at length scales less than 50 nm. This system was chosen due to its relatively controllable crosslinking rate as a function of ultraviolet radiation exposure. In addition, since SU8 is widely used as a photoresist, a series of mechanical property measurements are available in the literature for bulk samples of the material, as well as nanoindentation results that provide mechanical property measurements at the approximately 100 nm length scale. The latter measurements are made at slow nanoindenter tip displacement rates and therefore correspond to low-frequency (<100 Hz) excitation of the material. However, those measurements are expected to provide a comparison for our high-frequency measurements on samples with similar dimensions.

Significance

Success in this project will benefit the science mission by creating a new tool that will directly probe the behavior of matter in the gap between atomistic-to-micro length scales. By providing concerted measurements of mechanical, electrical, and thermal energy transport across 10–50 nm material samples, improvements to both microsystem design and materials aging relevant to stockpile lifetime monitoring will be enabled. In particular, at present, there are no existing techniques that can probe mechanical responses at these distances. Recent advances in peridynamic materials modeling at Sandia and elsewhere have begun to bridge the gap in materials simulation capability between atomic-level modeling and traditional continuum-based materials modeling. The development of a tool to make empirical measurements in this dimensional gap will benefit future materials modeling efforts.

Nanostructures from Hydrogen Implantation of Metals

139135
Year 1 of 1
Principal Investigator: M. D. Ong

Project Purpose

With many renewable energy sources of intermittent nature, energy storage will be important for the implementation of clean energy. We propose to investigate a recently discovered pathway to nanoporous structures created by hydrogen implantation in metals. Nanoporous materials have high specific surface areas, making them ideal as supercapacitor electrodes. We will apply the approach to aluminum, a material of proven value for this purpose, and gain a deeper understanding of the properties of these materials and the mechanism of their formation.

In experiments for fusion applications, formation of nanoporous films several micrometers thick was observed in tungsten and beryllium surfaces exposed to helium or hydrogen plasmas. Preliminary observations suggest that this effect also can occur on aluminum. We will create aluminum nanostructures, vary formation conditions, and study the reaction to test the hypothesis that volatile alane (AlH_3) is formed in the porosity generated by the radiation damage, and assists the restructuring of the material. Alane is known to be produced when atomic hydrogen is exposed to an unoxidized aluminum surface. Monte Carlo modeling will provide evidence to support or refute this mechanism.

The potential benefit of this project is an increase in our understanding of synthesis of nanostructures and possibly the demonstration of a novel alternative route to nanoporous aluminum. In addition, the modeling component of this project will give a theoretical description of the creation of these voids and may also shed light on the mechanics of surface rearrangement in nanoscale structures. We also expect that this project will allow team members and collaborators to advance their materials characterizations skills that will be beneficial to other related projects in the future. This project is well-suited for the LDRD program because it is a creative scientific idea that can lead to potentially high-value research and development in the future.

Summary of Accomplishments

Our results described the evolution of the near surface morphology of aluminum when implanted with hydrogen. Small bubbles are initially formed that will eventually coalesce to make larger bubbles and blisters as additional hydrogen ions are implanted. We also observed that void growth is preferential along grain boundaries and other microstructural defects in the aluminum, and faceting within voids indicates that some crystallographic planes are likely being etched preferentially. We noted that the chemical reaction of hydrogen and aluminum appears to play an important role in the reconstruction of the bombarded region of aluminum because helium, a chemically inert species, produces significantly different morphologies from those produced by hydrogen despite the fact that both gases are virtually insoluble in the aluminum matrix. Moreover, we found that helium implantations in aluminum resulted in the smallest pore sizes and smallest ligaments of aluminum in the resulting morphology. The relatively high concentration of oxygen in the energy dispersive x-ray spectroscopy analysis indicated that more new surface area was formed from the helium implantations than from the hydrogen implantation. The helium implantations appear to be a more promising route to the synthesis of nanostructured metals than the hydrogen implantations.

Complementary modeling of the evolution of the aluminum surface in the presence of hydrogen indicated that alanes readily form and that their desorption can etch the (111) surface of aluminum. However, the theoretical binding energies of alanes to the surface calculated from density functional theory are too great to allow this to happen. This project suggests that subsurface hydrogen significantly affects the binding energy of alanes to the aluminum surface, possibly leaving them in a physisorbed state.

Significance

We hope to advance our ability to control and manipulate ion implantation techniques to acquire high surface area materials that could potentially be used for supercapacitors and fuel cells for green grid and vehicle electrification applications. These applications are important components of Sandia's mission to develop clean renewable energy sources and greater national energy security.

Study of III-Nitride Based Photovoltaics

139242
Year 1 of 1
Principal Investigator: J. Wierer

Project Purpose

The purpose of the project is to discover ways in which III-nitrides can be used to enable very-high-efficiency photovoltaic (PV) structures. III-nitrides are attractive because they are direct bandgap, can absorb the entire solar spectrum, are radiation hard, and have low surface-recombination rates; yet are relatively unexplored in PV. Leveraging Sandia expertise in III-nitride materials, the feasibility of creating multijunction cells containing III-nitride cells alone or in combination with traditional high-quantum-efficiency III-V compound cells was investigated. InGaN/GaN core-shell nanowires was also investigated for new PV designs, because of their unique properties such as strain- and dislocation-free growth, ease of compositionally graded structures enabling absorption of the entire solar spectrum, and ultraefficient carrier generation and collection.

Summary of Accomplishments

This feasibility study explored potential ways in which III-nitrides can contribute to future high-efficiency solar cell designs. First, we researched methods of creating a wide band-gap III-nitride cell for use in a mechanically stacked multijunction solar cell in combination with other traditional high-quantum-efficiency III-V compound cells for high efficiency. The typical growth of InGaN on c-plane GaN layers cannot achieve the necessary indium concentrations because of lattice mismatch strain between the GaN and InGaN layers. We found various methods for creating high indium concentration InGaN layers, all using strain relief techniques. These include creating strain-reduced InGaN template layers on patterned m-plane substrates, porous GaN, and on oxidized AlInGaN layers. A second area researched was exploring methods of creating InGaN/GaN nanowires to enable strain relief, and hence higher critical thickness and indium composition InGaN layers for a wide-gap solar cell. Promising methods that we discovered included growing InGaN layers on the top of GaN nanowires, or covering the core GaN nanowires with InGaN shell layers. Lastly, bandstructure modeling for potential III-nitride solar cells was performed. We found that III-nitrides with GaN-InGaN heterointerfaces have large piezoelectric polarizations, adding complexity to the III-nitride layer design. The polarization fields can create situations where carriers are forced to drift in the wrong direction lowering the efficiency of the solar cell. We found solutions to the polarization problem that include growing on nonpolar surfaces or growing all InGaN structures.

Significance

A comprehensive III-nitride photovoltaic capability will beneficially impact energy security and national security. We have shown ways III-nitrides could improve multijunction PV cells, increasing their efficiency. Also III-nitrides are radiation-hard and operate at high temperatures so they are useful for future PV devices in space/satellite missions. High-quality, high-composition InGaN layers will not only improve PV, but also nitride light emitting diodes (LEDs) and lasers.

THz Transceiver Characterization

139363
Year 1 of 1
Principal Investigator: M. Lee

Project Purpose

The purpose of this project was to quantify the performance characteristics of monolithically integrated Schottky diode + quantum cascade laser (QCL) heterodyne mixers at terahertz (THz) frequencies. These integrated mixers are the first all-semiconductor THz devices to successfully incorporate a diode mixer directly into the optical waveguide of a QCL, obviating the conventional optical coupling between a THz local oscillator and rectifier in a heterodyne mixer system. As a result, coupling inefficiencies and the need for precise mechanical stability are eliminated, and the entire local oscillator/diode package can be built into a tiny form factor via microfabrication methods. The goal of this project was to measure limits of performance and utility. In particular, we aimed to demonstrate that the integrated device could function as a compact THz heterodyne receiver of an external THz signal.

Summary of Accomplishments

Using prototype monolithically integrated mixer devices, we found that the diode was an excellent tool to characterize detailed QCL behavior that could not be observed previously, such as sensitivity to feedback dependence, which is of significant importance to many different applications. During this project, we used the diode to measure precise QCL mode shifting in response to temperature, bias, and external feedback. We found that internal frequency locking can improve differential but not common mode stability. Most importantly, we showed that this integrated mixer functions as a true heterodyne receiver of an externally received THz signal. A manuscript on the heterodyne detection results has been submitted to *Nature Photonics*.

Significance

We completed measurements fully and quantitatively characterizing a THz monolithically integrated mixer. Publication and dissemination of these results will help make this technical advance more broadly accepted in application areas relevant to DOE's missions, such as defense (THz telecommunications and radar), homeland security (toxic gas sensing and concealed weapons imaging), and environmental monitoring (atmospheric composition assaying).

Electrospun Nanowires for Improved Lithium Ion Battery Anodes

139459
Year 1 of 1
Principal Investigator: T. J. Boyle

Project Purpose

Silicon is an excellent metal for Li ion battery anodes since it can store significant volumes of lithium. however, only upon going to the nanoregime can the material withstand the expansion/contraction that the cycling undergoes. This proposal plans to focus on the production of M(0) nanowires (M = Sn, Ge, Li) nanowires and use these materials to determine the characteristics that effect the final conductivity of these alloy systems. Electrospinning (ES) methodologies will be used to generate these materials wherein the solvent in these systems is necessarily polar. The initial materials of interest will be precursors that can generate Sn(0), Ge(0), and Li(0) wires at Sandia or encapsulated wires through an ES process and Si(0) wire at North Dakota State University (NDSU). The conversion to M(0) will be challenging but can be overcome by postprocessing under reducing conditions. Optimization of these precursors for the production of M(0) wires will be undertaken. Additionally, it is believed that the alternative dopants may require higher-temperature processing for conversion. Of particular interest for cation dopants are the group 14 congeners (i.e., Ge and Sn), as well as group 13 (Al, Ga, In) cations. The Li^+ transport of the understudied alloys will be investigated to optimize the properties of these critical anode materials.

Summary of Accomplishments

Electrospun nanowires of:

1. SnO without polymer — tadpole shaped. Homoleptic tin(II) 2,6-di-isopropylphenoxide ($Sn(DIP)_2$) yielded wires with some dots. Heteroleptic tin(II) bistrimethylsilylamide, 2-mono isopropoxidephenoxide ($Sn[NR_2(oPP]$)) yielded similar materials that beryllium dome x-ray diffraction (BeD-XRD) indicates may be Sn metal.
2. Ge wires with the use of 0.25 polyvinylpyrrolidone (PVP), otherwise only electrospray
3. AlO_x not formed.
4. Li not pursued due to time constraints.
5. Si nanodots formed by electroreduction. Electrospinning not attempted.

Significance

Improvements in battery components will impact energy related problems, including programs to improve the capacity and rate capability of existing battery chemistries for transportation, and improvements for small, thin-form-factor batteries. If successful, results of this project could also be used to provide for large-scale energy storage since the capacity of this anode would also benefit grid energy storage.

Plasmonic Filters

139466
Year 1 of 1
Principal Investigator: E. A. Shaner

Project Purpose

Metal films perforated with subwavelength hole arrays have been show to demonstrate an effect known as extraordinary transmission (EOT). In EOT devices, optical transmission passbands arise that can have up to 90% transmission and a bandwidth that is only a few percent of center wavelength. We have demonstrated over 1 micron of passive tuning in structures designed for an 11 micron center wavelength. If a suitable midwave (3–5 micron) tunable dielectric ($BaTiO_3$ or $LiNbO_3$) were integrated with an EOT mesh designed for midwave operation, a fast voltage tunable filter solution could be demonstrated with a several hundred nanometer passband. Such an element could replace filter wheel components for imaging applications.

To the best of our knowledge, no group has performed imaging experiments through an EOT structure. This is likely because most work in plasmonics focus on visible wavelengths, where a wide array of agile optical elements already exists; there simply is no need. In the midwave band and longwave (8 microns to 12 microns) there are fewer options. Here we look to plasmonic devices, where optical properties can be tailored through structuring of metal and the surrounding dielectric environment, to bring new functionality to the infrared portion of the spectrum.

Summary of Accomplishments

We performed mid-infrared imaging experiments through plasmonic filters that were comprised of perforated metal hole arrays. We have not seen any such study performed in the literature, and it was unknown if imaging through such structures would be problematic. Using a micro-bolometer camera and filters designed for 10 micron wavelength, we successfully imaged hot objects through the filters. To first order, there was no significant distortion observed.

Significance

Sandia has a long history in developing sensors for a wide variety of national security and nuclear weapons applications. Plasmonic concepts represent a new class of frequency-selective elements that must be investigated further in order to determine their long term potential for meeting defense related needs.

Macro-Ions Collapse Leading to Hybrid Bio-Nanomaterials

139586
Year 1 of 1
Principal Investigator: K. Achyuthan

Project Purpose

The purpose of this investigation was to understand macro-ions collapse to form compacted yet functional structures as exemplified by deoxyribonucleic acid (DNA). Consider that the total length of human DNA is approximately 140 astronomical units or about 70 round trips between the Earth and the Sun, yet it is packed inside cells that are only 10 microns in size. Each human cell contains DNA approximately 3 meters in length. Clearly, biological systems have figured out how to use higher-order structures (self-assembled folding) to optimize the properties and function of biomolecules such as DNA and proteins. An understanding of these processes will provide significant insight and direction to the formation of synthetic nanomaterials. Hybrid nanomaterials composed of natural and synthetic molecules offer new properties absent in constituent components; however, the design and control of such nanohybrids has proved daunting. The self-assembly of DNA macro-ions and synthetic materials in order to form useful hybrid bio-nanomaterials is therefore a formidable challenge. The theoretical understanding of reversible complexation/de-complexation transitions could be useful for understanding the assembly of more complex structures in controlled environments at a macro level. Our studies will enable the prediction of how nanomaterials organize, self-assemble and function, based upon the molecular properties of the constituent components. In this effort we take a page out of nature for the study of self-assembling nanomaterials. This is a key step toward end-use driven designer nanomaterials and aligns with the Nanoscience to Microsystems (NTM) mission to "control and manipulate" matter "to attain unique properties and function."

Summary of Accomplishments

We used supramolecular self-assembling cyanine and the polyamine spermine binding to *Escherichia coli* genomic DNA as a model for DNA-drug interactions during high throughput screening (HTS). Spermine competitively inhibited the self-assembly of cyanine upon DNA scaffold as signaled by decreased fluorescence from DNA-cyanine ensemble. Sequence of DNA exposure to cyanine or spermine was critical in determining the magnitude of fluorescence diminishment. Methanol potentiated spermine inhibition by > 10-fold. The IC_{50} for spermine inhibition was 0.35 ± 0.03 M and the association constant K_a was 2.86×10^{-6} M. Reversibility of DNA-model drug interactions was evident from the mitigation of fluorescence decrease at higher concentrations of cyanine. Spermine interactions with Lambda bacteriophage DNA demonstrated system flexibility. The choice and rationale regarding the model drug, the dye and the effects of methanol are discussed. Cyanine might be a safer alternative to the mutagenic toxin ethidium bromide for investigating DNA-drug interactions.

In conclusion, we executed DNA-model drug-dye displacement studies using 384-well microplates in order to demonstrate assay miniaturization and HTS capabilities. Spermine dissociation by cyanine leads to DNA de-condensation that could be a conformational probe for studies of gene expression or shut-off. Our studies are broadly applicable since although collapsed or relaxed DNA structures might be different for different ligands, the overall condensation mechanism is likely to be similar and can be studied in a HTS environment using supramolecular self-assembling cyanine. Studies are in progress to explore the reciprocal binding sites on different types of DNA scaffolds for cyanine and the various polyamines of spermine, spermidine, putrescine and cadaverine in order to further evaluate the macro-ion collapse.

Significance

Our project broadens nanofabrication in a fundamental area that is important to nanotechnology development by studying the scientific principles of self-assembly using DNA collapse as a model system. This is a key step toward end-use driven designer nanomaterials and aligns with the scientific discovery and innovation mission of DOE.

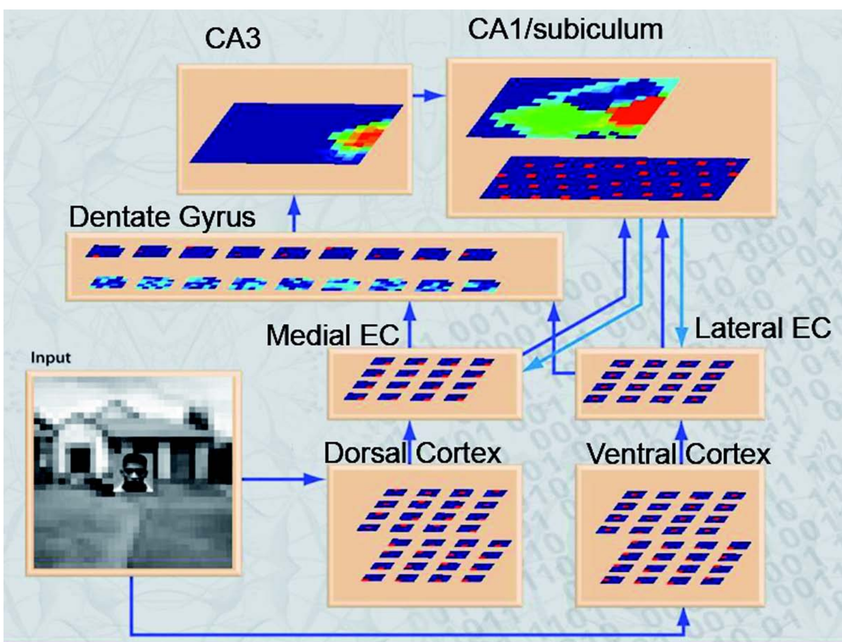
NEW DIRECTIONS INVESTMENT AREA

This investment area (IA) focuses on research areas in which Sandia is newly embarking or has recently embarked, and hence, tends to encompass national security initiatives that seek to draw existing Laboratory expertise into new applications for national security. Best exemplifying such initiatives are projects in biological sciences — with emphasis on alternative energy and biothreat reduction — projects at the nanotechnology-bioscience interface, and those in the cognitive sciences — particularly as applied to support for decision-makers.

Modeling Aspects of Human Memory and Reasoning for Scientific Study

Project 105938

While great strides have recently occurred in the field of human cognition, there is no unified theory regarding the neural network dynamics in the brain that underlie human memory and reasoning. To assist in approaching such a unified conceptual framework, this project is creating a computational architecture to simulate human cognitive processing pathways within the brain, during memory consolidation, and to compare the results of human study participants and computational model at memory retrieval. For example, the research has indicated that contextual memories — those based on association of objects within a particular context — provoke quite similar responses in human brain and computational model. According to evaluations from the academic neuroscientists affiliated with the project, the Sandia research has produced a simulation environment able to accomplish these ends. The potential impact of a more-thorough understanding of the brain extends beyond neuroscience into several national security areas.

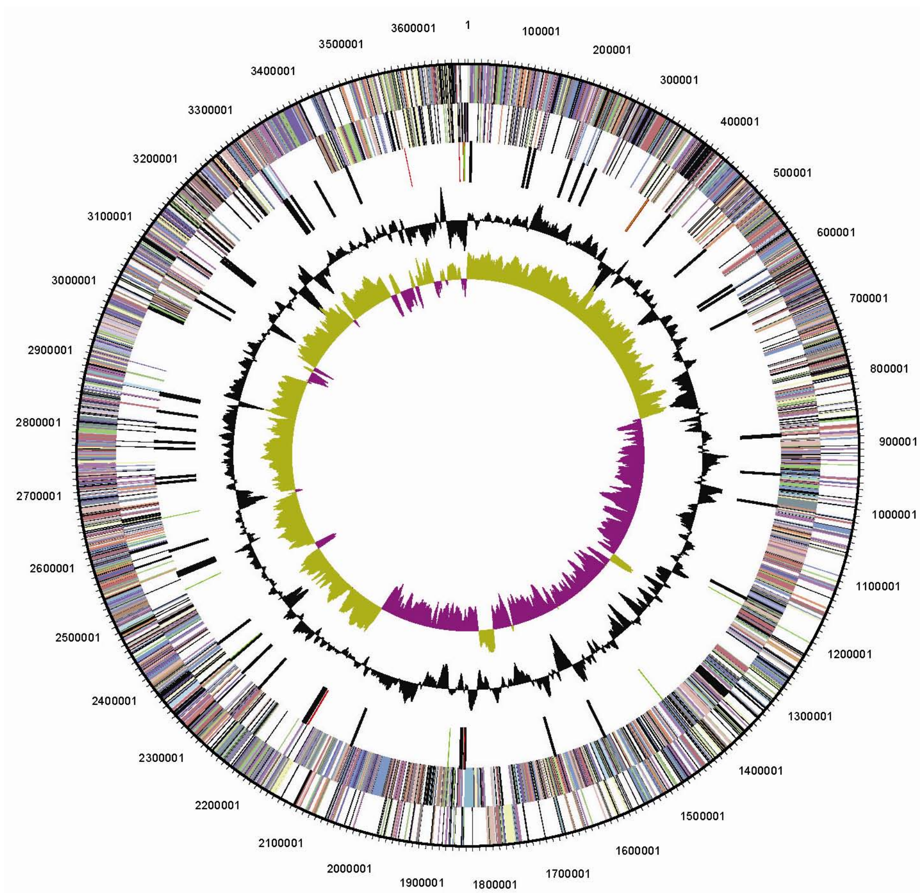


Map of interconnections of brain areas involved in processing memory consolidation.

Synthetic Biology of Novel Thermophilic Bacteria for Enhanced Production of Ethanol from 5-Carbon Sugars

Project 105944

A critical component of our energy future could be biofuels from plant wastes, but only if adequately efficient processes can be devised and implemented. To this point, a problem has been the reaction-condition mismatch between the process of saccharification — the breakdown of the lignocellulose fibers in plant wastes to sugars — and fermentation, the biological process by which bacteria and certain fungi form the biofuel ethanol from these sugars. Additionally, saccharification yields a mix of five- and six-carbon sugars, but many popular fermenting organisms are unable to use five-carbon sugars for ethanol fermentation. This project has characterized a novel thermophilic bacterium, *Geobacillus thermoglucosidasius*, which can accomplish simultaneous saccharification and fermentation (SSR) at high temperature (60 °C). A detailed map of the bacterium's circular chromosome has been published by this project, and flux analysis of its metabolic pathways using ^{13}C-labelled metabolites has pointed the way toward optimization of ethanol production. The bacterium is tolerant to 10% ethanol, while most other thermophiles only tolerate 4%, and it ferments both five- and six-carbon sugars.



Genetic map of the circular chromosome (DNA molecule) of *G. thermoglucosidasius*.

NEW DIRECTIONS INVESTMENT AREA

Neural Assembly Models Derived through Nanoscale Measurements

105936
Year 3 of 3
Principal Investigator: H. Fan

Project Purpose

Neuroscience experimental techniques allow brain activity to be measured at the cellular level (e.g., microelectrode implants) and the large-scale systems level (e.g., electroencephalography [EEG], functional magnetic resonance imaging [fMRI]), however existing methods offer limited insight bridging these scales. For instance, there is little understanding of the mechanisms by which individual neurons are organized into assemblies that correspond to specific memories. Significant scientific advances would be attainable given technology that enables measurement of the activity of individual neurons for large volumes of brain tissue *in vivo* (i.e., living animal).

This project addresses this objective through development of self-assembling nanocrystals or nanoelectrode arrays that may be injected or implanted in an animal's brain to provide data concerning neuron activation prior to, during, and subsequent to performance of a laboratory task. Additionally, methods will be developed that utilize data from nanosensors to train a computational model of the dynamic patterns of neural activation corresponding to the memory processes underlying observable behavior.

Summary of Accomplishments

This project successfully demonstrated that nanoprobes could be engineered that were biocompatible, and could be biofunctionalized, that responded within the range of voltages typically associated with a neuronal action potential. Furthermore, the Xyce parallel circuit simulator was employed and models incorporated for simulating the ion channel and cable properties of neuronal membranes. The ultimate objective of the project had been to employ nanoprobes in vivo, with the nematode *Caenorhabditis elegans*, and derive a simulation based on the resulting data. Techniques were developed allowing the nanoprobes to be injected into the nematode and the neuronal response recorded. To the authors' knowledge, this is the first occasion in which nanoparticles have been successfully employed as probes for recording neuronal response in an in vivo animal experimental protocol.

Significance

This research will provide an enabling capability to develop new sensing technologies that are important for a range of national security applications. This research represents a building block in the integration of nanotechnology, biology, and cognitive science. This project helps establish a laboratory technology base in neurotechnologies that may be transitioned to national security mission areas.

Modeling Aspects of Human Memory and Reasoning for Scientific Study

105938
Year 3 of 3
Principal Investigator: M. L. Bernard

Project Purpose

Working with leading experts in the fields of psychology, neuroscience, and computational intelligence, we propose to create a scientifically rigorous computational architecture for embodied human modeling. A fundamental aspect of this endeavor is to create a mechanism to test and derive new and innovative theories and questions within cognitive science so as to move the scientific community closer to understanding how, why, and when we make decisions. While great strides have been made in understanding these aspects of cognition, there is no unified theory of human thought. Achieving a more unified understanding will permit a better grasp of how humans conceptualize, incorporate, and reason about information. This will, in part, be accomplished by integrating the latest research and theories of memory and reasoning into a single computational architecture. Working with academia, research experiments will be conducted to empirically validate the psychological architecture, as well as theories behind the architecture, while highlighting future enhancement opportunities. Scientists will be able to help assess the validity of various psychological assumptions by using this framework as a generally comprehensive experimental test bed. Doing so should generate complementary theories to help explain and predict aspects of cognition. Moreover, scientists will be able to compare the model's predictions to actual human performance, allowing for both model validation and theoretical development. This construct will integrate semantic (facts-based) and episodic (event-based) declarative memories, as well as basic reasoning in an abstraction architecture. The framework will have parallel and distributed processing of persistent representations of concepts and events that predict patterns of behavior. The processing of information will occur through a network topology that integrates information upward from sensory inputs and downward from reasoning processes.

Summary of Accomplishments

We created a neurocognitive computational model to support the ability to do classification/categorization of a range of visual inputs, to remember the prior occurrence of each of those inputs individually, to do pattern completion permitting recovery of those items based on partial or incomplete cues, to represent different locations in the visual environment, to remember which individual items occurred in which locations, and to bind together in memory representations of any arbitrary collection of items with one another and with their spatial or other contexts. All of these capabilities are implemented in a model with biological realism greater than in any previously implemented model. Finally, it is done in a way that permits us to test the contributions of each of the individual components of the model and to compare that with what is seen in humans and animals.

Significance

This project is unique in its scope and its ambition. Simply put, constructed and extensively validated a cognitively based, computational architecture to serve as a test bed to answer questions that are currently not fully understood in the scientific community, such as, "what are the specific processes integrating episodic memory?" Working with academia, we designed a cognitive framework to at least partially answer these questions by designing neurocognitive computational models of memory. Working with experts in memory, we have integrated subsystems that have not been modeled as part of a larger system.

This project benefits the science and defense national security mission of the DOE and other federal agencies by increasing the understanding of key aspects of cognition as well as by creating a higher-fidelity human modeling architecture. This will enable better understanding of the thought processes underling human behavior, as well as enhance human modeling in areas such as action/counter-action predictive simulations, co-evolutionary training, and assistive decision-making.

Psychologically Plausible Learning Mechanisms for Sandia's Cognitive Framework

105939
Year 3 of 3
Principal Investigator: A. E. Speed

Project Purpose

Currently, the ability of software to recognize isomorphic problems that do not share surface likeness is very limited. That is, software is not able to make analogies between situations in different domains the way humans can. The goal of this work is to develop a software model capable of learning from experiences by enabling it to create analogies in a human-like manner. To accomplish this, we are building a framework that will discover the structural aspects of the source and target analogies on its own, rather than hand-coding those relationships into the model, a priori. Our primary assertion is that to accomplish this goal, we must understand how the brain represents knowledge, and how environmental feedback influences these representations. Specifically, we assert that analogy emerges from connectivity between and within different cortical areas — it is something we get for free, rather than being a specific algorithm or module that has evolved. If successful, this will be the first physiologically based computational analogical capability to integrate sensory processing into analogical processing, and will be able to detect analogies not explicitly programmed in by the modeler, thereby increasing the variety of problems to which computational architectures in general can be applied. It will also provide a theory, implemented in computational code, about how lower-order sensory processing links to higher-order cognition in the human brain.

Summary of Accomplishments

We learned a significant amount about the nature of the physiology underlying analogy — and we also learned there are still significant gaps in the experimental literature that would be necessary to wholly inform a computational model of virtually any higher-order cognitive process if that model is to account for not only that process but also for the physiological method for knowledge representation underlying that process. We demonstrated the ability to measure very complex operations in prefrontal cortex using electroencephalography (EEG). We developed a method for automatically generating stimuli based on a standard measure of analogical ability (and IQ) and we normed a subset of over 800 such stimuli against the standard measure in humans. We developed and refined a computational model that links unimodal sensory processes (based on mammalian ventral visual stream) and prefrontal cortex — something that has not been done before. We developed and proposed a novel theory of prefrontal cortical function that accounts for analogy as well as numerous other empirical findings in the published literature.

We have two peer-reviewed publications to date and expect to have at least 4 additional peer-reviewed papers resulting from this research, including at least one paper on the model itself, papers describing the dynamical characteristics of the model, a paper on the visual input portion of the model, and a paper describing our capability for automatically generating the stimulus set we are using in addition to papers resulting from our collaboration with Jim Kroger at New Mexico State University.

Significance

This work supports the DOE mission in several ways. It enhances basic science understanding and establishes our standing in the cognitive neuroscience community. It enables numerous applications in the longer term, e.g., enhanced human emulation capabilities, cognitive modeling capabilities, and human-machine interfaces. All are relevant to national security as they enhance human capabilities to make decisions under uncertainty using huge amounts of information in highly dynamic environments.

Refereed Communications

L.E. Matzen, Z.O. Benz, K.R. Dixon, J. Posey, J.K. Kroger, and A.E. Speed, “Recreating Ravens: Software for Systematically Generating Large Numbers of Raven-Like Matrix Problems with Normed Properties,” to be published in *Behavior Research Methods*.

A. Speed, “Computational Modeling of Analogy: Destined Ever to Only be Metaphor?” *Behavioral and Brain Sciences*, vol. 31, pp. 397-398, 2008.

Resolving Dynamics of Cell Signaling via Real-Time Imaging of the Immunological Synapse

105940
Year 3 of 3
Principal Investigator: J. A. Timlin

Project Purpose

The interaction between a cell and a pathogen begins at the "immunological synapse," the contact region between the cell and its adversary. Cellular response to infectious agents is a signal transduction process that is determined not only by the presence of specific receptor proteins in the membrane, but also on the dynamics of interaction of those proteins with other key components in the signaling network. Although many proteins have been identified in the signaling machinery of various cell systems, little is known about the overall organization and dynamics of protein interactions at the synapse during stimulation. This lack of knowledge severely limits our understanding of the critical initial phase of infectious disease processes. We propose to provide this spatiotemporal data by using recent technological advances that enable us to optically detect and track in real time protein migration and clustering at membrane interfaces. Specifically, with total internal reflection microscopy (TIRF) we selectively excite fluorophore-labeled proteins at the synaptic contact region. By coupling TIRF with advanced analysis techniques such as image correlation spectroscopy and single particle tracking, we will be able to capture subtle changes in membrane organization that characterize immune responses. Multi-labeling will allow us to directly monitor specific protein-protein interactions leading to cellular signaling. To help interpret these measurements, a modeling effort will connect the protein motion with underlying protein and lipid interactions. We will use this approach to elucidate the initial stages of cell activation in the immunoglobulin E (IgE) signaling network of mast cells and the toll-like receptor (TLRY) response in macrophages stimulated by bacteria. This work will provide a deeper understanding of the initial stages of cellular response to external agents.

Summary of Accomplishments

Overall, this has been a very successful project. We designed, built, and characterized a total internal reflection (TIRF) microscope capable of simultaneous dual color detection and excitation. This microscope configuration gives us the ability to probe two proteins specifically at the membrane interface at the same time with video rate temporal resolution. We have integrated and optimized quantitative image analysis algorithms to extract information from our images. We have used this new instrument to investigate the early events in cell signaling in both innate and adaptive immune systems: studying TLR4 and IgE receptor systems, respectively. We have discovered the formation of mast cell synapse and provided the first-ever characterization of the spatial reorganization and downstream signaling. We have determined IgE receptor cluster formation occurs via diffusion limited trapping at cell protrusions. We have simultaneously visualized the dynamic behavior of the TLR4 receptor and its lipopolysaccharide stimulatory molecule. In addition, we have improved molecular modeling capabilities for proteins in lipid environments.

Significance

In its broadest aspect, this work strengthens the competency of DOE in cell biology, biophysical imaging and analysis, and advanced computation capabilities for the life sciences. More specifically, it will impact missions in biodefense and infectious diseases by significantly enhancing the fundamental understanding of the early stages of cell stimulation, which could lead to improved, noninvasive detection technologies, better diagnostics, and new therapeutic agents.

Microalgal Biodiesel, Feedstock Improvement by Metabolic Engineering

105943
Year 3 of 3
Principal Investigator: T. W. Lane

Project Purpose

The displacement of liquid petrochemical transportation fuels with renewable biofuels is a growing national priority (DOE Energy Efficiency and Renewable Energy and United States Department of Agriculture [USDA]). While biofuel production alone is not expected to rival established sources of power generation near term on a whole-scale level, it is believed that it can be an important part of an efficient and robust national energy policy mid- to long-term that reduces dependence on foreign oil. Of the alternative feedstocks being investigated (e.g., biodiesel, bioethanol), one holds the promise of displacing a significant portion of its petrochemical alternative: biodiesel produced through harvesting of algae. Diatoms produce triacylglycerides (TAGs): the feedstock for biodiesel production. The per-cell production of TAGs is greatest under nutrient limitation; conditions that result in a low growth rate. To achieve high overall TAG production we will decouple the metabolic pathways for TAG synthesis from regulation by starvation. This project will be driven by Sandia's strengths in computational analysis, molecular biology and chemical analysis. Taking advantage of the sequencing of diatom genomes, we will identify the genes encoding the enzymatic pathway for the production of TAGs. We will correlate the expression of these genes with growth state and TAG production. We will model the flow of material through these pathways and identify competing pathways, which divert material into non-target products. We will manipulate the expression of genes in these pathways to optimize production of TAGs. This is a problem with two major technical challenges, the scope of the metabolic engineering and the difficulty in manipulating diatoms. Rather than inserting one or two genes we will alter the regulation of entire metabolic pathways.

Summary of Accomplishments

We conducted a digital transcriptomic analysis of gene expression during the transition from exponential growth to nutrient starvation and triacylglycerol accumulation in the model species *Thalassiosira pseudonana*. During this analysis we measured the transcript abundance for 21,000 putative genes; approximately 8,000 more than were previously identified. We focused not only on the analysis of the genes encoding enzymes in the triacylglycerol biosynthesis pathway but also on those encoding enzymes involved in ancillary pathways. We identified the genes that display increased transcript levels under conditions of starvation when compared to that found during mid-logarithmic growth. We utilized the data from the transcriptomic analysis, computational modeling of the biosynthetic pathways, and the results from work in higher plants to select genes for overexpression as part of our effort in metabolic engineering. We generated transgenic microalgae using a biolistic transfection system. The DNA constructs that were inserted were designed to result in the overexpression of specific genes encoding enzymes thought to contribute to the production of triacylglycerol and the targeting of the resulting protein to the chloroplast of the genetically modified cell. The insertion of these constructs resulted, in some cases, in an increase in triacylglycerol abundance and thus met the primary goal of this project. We carried out a detailed analysis of these transgenic strains including a mass spectrometric analysis of the triaclyglycerols. We also carried out a classical mutagenesis of *Thalassiosira pseudonana* and screened for and identified mutants that displayed an increase in triaclyglycerol accumulation. Finally we characterized the transesterification of triacylglycerols extracted from our model algae grown under nutrient limitation conditions.

Significance

This project addresses the DOE mission to increase the energy security of the United States. Reducing national dependence on imported petroleum has become an important national priority. The production of biomass derived transportation fuels is an important element of an overall national energy policy. Of the alternative feedstocks being investigated, only biodiesel, produced through harvesting of algae, holds the promise of displacing a significant portion of its petrochemical alternative.

Refereed Communications

E.Yu, F. Zendejas, P.D. Lane, S. Gaucher, B.A. Simmons, and T.W. Lane, "Triacylglyceride Accumulation in the Model Diatoms *Thalassiosira Pseudonana* and *Phaeodactylum Tricornutum* During Starvation," to be published in the *Journal of Applied Phycology*.

Synthetic Biology of Novel Thermophilic Bacteria for Enhanced Production of Ethanol from 5-Carbon Sugars

105944
Year 3 of 3
Principal Investigator: R. Sapra

Project Purpose

The sustained high price of petroleum has greatly increased interest in bioderived fuels like ethanol. Most evaluations of ethanol's economic feasibility have shown that ethanol must be derived from cellulosic biomass. However, there are two major hurdles for the low-cost production of bioethanol: conversion of plant biomass into fermentable sugars and conversion of both hexose and pentose sugars into ethanol. The most promising production process combines the enzymatic hydrolysis and fermentation steps into a single bioreactor, termed simultaneous saccharification and fermentation (SSF). SSF's usefulness is limited in practice because the optimal process conditions for the individual steps differ. We have proposed to use synthetic biology tools to optimize ethanol production from a thermophilic bacterium, *Geobacillus thermoglucosidasius* M10EXG to address the problem of efficient fermentation of C5 sugars at high temperature, thus enabling cost-effective ethanol production. This bacterium ferments C6 and C5 sugars and is tolerant to ethanol concentrations of up to 10% (v/v), but in nature, produces a low yield of ethanol. Our technical approach relies on synthetic biology combined with fermentation optimization. We propose to sequence the genome of the bacterium, and map key metabolic pathways to design optimal pathways for ethanol. The genomic and metabolic tools will complement traditional genetic mutation methods to make mutants to maximize the flux of carbon to the ethanologenic pathways while minimizing the production of carbon byproducts (e.g., acetate, lactate). Computational tools like flux balance analysis will also be used to guide pathway changes and fermentation conditions toward designing more efficient pathways for ethanol production. Our approach has distinct advantages of using an organism that is ethanol tolerant and thermophilic, properties that are very difficult to engineer.

Summary of Accomplishments

A recently discovered thermophilic bacterium, *Geobacillus thermoglucosidasius* M10EXG, ferments a range of C5 (e.g., xylose) and C6 sugars (e.g., glucose) and is tolerant to high ethanol concentrations (10%, vol./vol.). We have investigated the central metabolism of this bacterium using both in vitro enzyme assays and ^{13}C-based flux analysis to provide insights into the physiological properties of this extremophile and explore its metabolism for bioethanol or other bioprocess applications. Our findings show that glucose metabolism in *G. thermoglucosidasius* M10EXG proceeds via glycolysis, the pentose phosphate pathway, and the tricarboxylic acid (TCA) cycle; the Entner-Doudoroff pathway and transhydrogenase activity were not detected. Anaplerotic reactions (including the glyoxylate shunt, pyruvate carboxylase, and phosphoenolpyruvate carboxykinase) were active, but fluxes through those pathways could not be accurately determined using amino acid labeling. When growth conditions were switched from aerobic to microaerobic conditions, fluxes (based on a normalized glucose uptake rate of 100 units (g DCW)/ hr through the TCA cycle and oxidative pentose phosphate pathway were reduced. The carbon flux under microaerobic growth was directed to ethanol, L-lactate (>99% optical purity), acetate, and formate. Under fully anaerobic conditions, *G. thermoglucosidasius* M10EXG used a mixed acid fermentation process and exhibited a maximum ethanol yield of 0.38 ± 0.07 moles per mole of glucose. In silico flux balance modeling demonstrates that lactate and acetate production from *G. thermoglucosidasius* M10EXG reduces the maximum ethanol yield by approximately threefold, thus indicating that both pathways should be modified to maximize ethanol production.

Significance

Ethanol produced from lignocellulose is the only known short-term resource that can displace a significant amount (> 30% on a volumetric basis) of the petrochemical transportation fuels used today. Achieving this goal will require processes and refineries where cellulose pretreatment and deconstruction can be combined with fermentation at high temperatures. Metabolic engineering of *G. thermoglucosidasius* will provide insights and discoveries towards making a high-temperature ethanol-tolerant organism.

Refereed Communications

Y.J. Tang, R. Sapra, D. Joyner, T.C. Hazen, S. Myers, D. Reichmuth, H. Blanch, and J.D. Keasling, "Analysis of Metabolic Pathways and Fluxes in a Newly Discovered Thermophilic and Ethanol-Tolerant *Geobacillus* Strain," *Biotechnology and Bioengineering*, vol. 102(5), pp. 1377–1386, 2009.

Efficient Breakdown of Lignocellulose Using Mixed-Microbe Population for Bioethanol Production

105946
Year 3 of 3
Principal Investigator: A. J. Powell

Project Purpose

Energy independence is paramount for economic recovery and national security. Scaleable, sustainable advanced biofuels production can potentially eliminate reliance on imported petroleum, and will likely also yield net reductions in greenhouse gas emissions. In the United States, corn-derived starch remains the principle input for industrial scale fermentation and biofuels production; current production methods have no advantage economically, because they compete with agricultural food commodities, nor environmentally, because total carbon input and output are at least as high as those associated with petroleum production and use. More significantly, corn-based biofuels production methods do not result in substantial net energy gains, i.e., energetic outputs are similar to inputs. Efficient, scaleable and environmentally sustainable conversion of lignocellulosic biomass, such as agricultural residues, is both the principal technical challenge and the prerequisite for a renewable fuels-based economy.

Our research efforts will use genome sciences-enabled approaches to deliver novel biotechnology-based solutions to the key bottleneck in advanced biofuels production: efficient deconstruction of lignocellulose. We will isolate thermophilic fungi, organisms that grow at greater than 50 °C, from two different extreme environments: a carbon-poor aridland ecosystem (ALE) of central New Mexico (NM) and thermal features from Yellowstone National Park. These extremophilic organisms will enable identification of novel, high-efficiency enzyme systems that are robust to harsh biorefinery production processes, which include high temperatures, extreme pH and osmolarity values for biomass pretreatment stages. Thermophilic fungi have established utility in industrial-scale bioconversion processes, and are thus highly relevant to lignocellulose deconstruction applications.

Summary of Accomplishments

To deliver novel, efficient enzyme systems and gene products to drive transformational advances in lignocellulose deconstruction, we have employed culture-based methods and a high throughput sequencing approach. Using culture-based methods, we have isolated and generated preliminary genotypic and phenotypic characterization for 42 different strains of thermophilic fungi from two distinct extreme environments (the central NM ALE and thermal features in Yellowstone National Park). Our first results indicate that these microbes frequently outperform the current industrial cellulolytic organisms (*e.g.*, *Trichoderma reesei*, *Aspergillus niger*, *A. nidulans*, *Thielavia terrestris*, *etc.*) in assays relevant to biomass deconstruction. Molecular genotyping data indicate that thermophilic fungi in our collection belong to phylum Ascomycota and are associated with either the Eurotiales or the Sordariales. The 42 strains are comprised of at least seven species that are known to contain thermophilic lineages; species in our collection include *Aspergillus fumigatus*, *Scytalidium thermophilum*, *Thermomyces lanuginosus*, *Talaromyces thermophilus*, *Myceliophthora* sp., *Thermoascus aurantiacus,* as well as strains associated with undescribed taxa sampled from compost heaps. Further, initial phylogenetic analyses of strains in our collection show within-species diversity, i.e., different strains are present within a species, signaling the presence of recombining populations. Preliminary phenotypic screening indicated that numerous strains have comparable or even greater growth rates than the currently deployed industrially-relevant species on lignocellose-containing media. Similar trends were evident in growth rate screens on defined lignocellulose-containing media at extreme pH and osmolarity values, and temperatures greater than 50 °C, with strains in our collection frequently outperforming industry standards.

Significance

Our main research goal is to identify novel, robust, high-efficiency lignocellulolytic enzyme systems that are known to be prevalent in organic carbon-limited ALEs. This work is anticipated to lead to catalytic technologies that will significantly reduce biomass breakdown costs, and advance DOE's energy security mission.

Biomolecular Transport and Separation in Nanotubular Networks

117838
Year 2 of 3
Principal Investigator: D. Y. Sasaki

Project Purpose

A new pathway in cellular communication that uses lipid nanotubes to transfer biomolecules and organelles between cells has been discovered in macrophages, lymphocytes, and neural cells. These recent findings could completely alter our concept of cell communication and immune response. We propose to develop platforms, models, and methodology that will enable us to study nanotubule networks with live cells and cell models systems using micro- and nanoscale characterization tools. We shall develop lipid nanotube constructs that would couple into optical and electronic probes to investigate: 1) the formation of lipid nanotubes, 2) chemical/physical/biological phenomena that dictate selectivity of transported biomaterial, 3) the origin of forces used to shuttle biomaterials across the nanotube, and 4) the biological significance of the nanotubule connections.

Our approach brings together several strengths developed at Sandia to provide a thorough understanding of the role of lipid nanotubes in cellular networks and how they might be exploited for mediating immune response and cell communication. A proposed cell immobilization array platform coupled to a confocal microscopic imaging system and micromanipulator system could precisely interrogate the cellular processes leading to nanotube formation and cell activation by controlling cell spacing and biomaterial transport while monitoring cellular response. Sandia is particularly suited to address this important biological problem through its expertise in lipid membrane assemblies, theory of membrane structure and dynamics, unique 3D imaging methods, and transport via microelectrophoresis and motor proteins. The proposed work will advance the biochemical analyses, measurement technologies, and modeling of cell responses to pathogens. Understanding cell-pathogen interactions and the resultant cellular processes are critical to national security. This research is exploratory in nature and can immediately address a new area of research that could lead to very high scientific impact in the biosciences.

Summary of Accomplishments

Over the past year, we have discovered that tubular membrane structures spontaneously form upon strong binding interactions between His-tagged protein and Cu(II)-iminodiacetate (IDA) functionalized membranes. Through experiments with supported lipid bilayers we determined that Cu(II)-IDA functionalized lipid components phase separated into domains that strongly ($> 5 \cdot 10^8$ M_e^{-1}) bound His-tagged proteins. The protein complexation induced spontaneous curvature of the domain that, depending upon the matrix phosphatidylcholine lipid, formed lipid nanotubes with lengths of up to tens of microns.

In an effort to understand the roles that cytoskeletal fibers and motor protein activity play in lipid nanotube formation we employed a synthetic system composed of a kinesin-driven inverted motility assay of microtubules interacting with giant lipid vesicles. Lipid tubules were observed in linear and branched structures covering distances of up to 0.5 mm. Studies performed with lipid membranes with a range of bending energies found that the inverted motility afforded pulling forces which extended tubule formation up to six times higher in energy (24×10^{-20} J) compared to protein-membrane interactions alone.

Simulations of nanotubes with different lipid types have been performed. Molecular dynamics simulations in the NPT ensemble were run so that the geometry (tubule length and radius) could self-adjust. Lipids with varying tail length and saturation have been treated to date, all producing at least metastable nanotubes. We have progressed towards distinguishing the preference of different lipid types for the curved nanotube structure.

We have studied nanotube formation of murine and human macrophage cells by exposure to lipopolysaccharide (LPS). In addition to a robust innate immune response, the cells also form a variety of projections with a significant fraction forming high-aspect-ratio nanotubes (< 1 μm diameter). A number of the nanotubes observed were found connecting two or more cells forming cell-nanotube networks.

Significance

The proposed research is relevant to several DOE missions: 1) national security (biodefense) — understanding cell-pathogen interactions and subsequent cellular processes; 2) development of diagnostic tools — cell-cell network interfaced with spectroscopic and nanoscale imaging tools will enable new detection/imaging platforms; and 3) advance nanoscale science — novel materials developments and nanoscale transport systems will provide new foundations for nanoscience impacting energy and environment.

Initiation of the TLR4 Signal Transduction Network — Deeper Understanding for Better Therapeutics

117839
Year 2 of 3
Principal Investigator: M. S. Kent

Project Purpose

The innate immune system represents our first line of defense against microbial pathogens. Toll-like receptor 4 (TLR4) is the cell-surface receptor primarily responsible for initiating the innate immune response to lipopolysaccharide (LPS), a major component of the bacterial cell envelope. TLRs represent a means by which we can effectively control inflammatory responses. However, relatively little is known about the molecular mechanisms underlying TLR activation. Design of small molecule therapeutics to modulate immune activation will benefit greatly from a better understanding of TLR4 activation and membrane proximal events. Resolution of the molecular mechanisms requires direct structural information for the TLR4 receptor complex, including the ability to detect ligand-induced conformational changes in the components and TLR4 dimerization. To acquire structural information at the required level of detail, we will reconstitute the system in model membranes and analyze the TLR4 receptor complex and its dynamics during the transition from quiescence to activation at high resolution using specialized biophysical characterization tools. These tools include neutron reflection (NR), x-ray scattering, cryoelectron microscopy, lifetime and spectrally resolved confocal microscopy, and total internal reflectance fluorescence (TIRF) microscopy. Molecular modeling will complement the experimental studies. This work will allow testing of molecular mechanisms at an unprecedented level of detail. This collaborative work with University of Texas Medical Branch (UTMB) will provide fundamental understanding of the first step in immune cell activation, and facilitate the rational design of inflammation modulators. Study of the specificities and structures of ligand-receptor interactions during this critical first stage in innate immunity is missing in other Sandia work. Together, these efforts will establish Sandia as a world leader in the structural biology of innate immunity. In addition, the new methodology developed in this project for studying the structure and dynamics of transmembrane receptors will apply to a host of other systems.

Summary of Accomplishments

1. Structural studies of MD-2 and TLR4/MD-2 to resolve the mechanism of dimerization.

   Neutron reflectivity (NR) studies of MD-2 upon binding lipid A indicated a large conformational change in MD-2, consistent with one of the hypothesized models for TLR4 dimerization. However, this was later revealed to be due to the presence of a reducing agent in the buffer.

   Further NR work involved TLR4/MD-2. Due to delays in in-house expression of these proteins and the high cost of purchasing large quantities, it was decided to do NR at solid-liquid interface rather than liquid-air to reduce the amount of protein needed by 1/6. This required several preliminary steps due to the need to deposit bilayers with high fractions of distearyl iminodiacetate (DSIDA).

   CryoEM was used to image liposomes and free TLR4/MD2 in solution.

2. Express recombinant MD2 and the soluble portion of TLR4.

   Plasmid for human TLR4-10xHis expression is now in hand that can be used for cell-free expression; plasmid has been verified.

3. Determine the equilibrium and dynamics of TLR4/MD2 dimerization for lipid A and lipid IVa.

Fluorescence correlation spectroscopy (FCS) studies examined iminodiacetate (IDA)-functionalized model membranes regarding lipid mobility, domain formation, and protein affinity.

1,2-dioleylglycero-3-triethyleneoxideiminodiacetic acid (DOIDA), a fluid-phase lipid with a metal-chelating IDA headgroup, was synthesized. DOIDA avoids domain formation that occurs with the gel-phase lipid DSIDA in the absence of ligand. This is crucial for developing diffusional studies of ligand-induced dimerization of TLR4/MD2.

TLR4/MD2 was labeled with amine-reactive dyes, essential for FCS, cross correlation, and fluorescence resonance energy transfer (FRET) measurements of dimerization.

FCS studies were performed with labeled TLR4/MD2 with confocal and TIRF microscopes. Some results showed a decrease in diffusion of labeled TLR4/MD2 after addition of lipid A consistent with dimerization of TLR4. However, first two color cross-correlation studies by TIRF did not show LPS-induced dimerization. More studies are ongoing.

Significance

Understanding TLR4 activation will lead to improved design of adjuvants of vaccines and small molecule therapeutics to modulate immune responses. The biodefense and emerging infectious disease research community is actively investigating how to manipulate TLRs in order to control inflammatory responses by boosting the immune system in anticipation of a bioweapon attack and down-regulating inflammation to prevent septic shock associated with systemic bacterial infection.

Refereed Communications

C.C. Hayden, J.S. Hwang, E.A. Abate, M.S. Kent, and D.Y. Sasaki, “Directed Formation of Lipid Membrane Microdomains as High Affinity Sites for His-Tagged Proteins,” *Journal of the American Chemical Society*, vol. 131, pp. 8728-8729, July 2009.

“Trojan Horse” Strategy for Deconstruction of Biomass for Biofuels Production

117840
Year 2 of 3
Principal Investigator: M. Z. Hadi

Project Purpose

The production of biofuels to displace fossil fuels is a pressing national priority (DOE/EERE [Energy Efficiency and Renewable Energy] and United States Department of Agriculture [USDA]). Nearly all domestic ethanol is from corn-derived starch. “Energy crops” and agriculture waste are preferred long-term solutions for renewable, cheap and globally available biofuels. Biomass needs to be converted to fermentable sugars for biofuels production using pretreatments, disrupting cellulose cross-links (e.g., lignocellulose), allowing exogenously added recombinant microbial enzymes to access cellulose for “deconstruction” into starch. The efficiency of this process is low due to recalcitrance of cellulosic biomass, mass transfer issues during biomass deconstruction, and low activity of recombinant deconstruction enzymes. Costs are high due to low net efficiency, the requirement for enzyme reagents, and energy intensive and cumbersome pretreatment steps.

The purpose of this research is to employ synthetic biology to provide solutions to these problems. We propose to engineer plants that self-produce a suite of cellulase enzymes either freely expressing in the cell or targeted to the apoplast for cleaving the linkages between lignin and cellulosic fibers. The genes encoding these degradation enzymes will be obtained from extremophilic organisms that grow at high temperatures and extreme pH. These enzymes will remain inactive during the life cycle of the plant but become active during hydrothermal pretreatment i.e., elevated temperatures. With the success of this research, deconstruction can be integrated into a one-step process thereby increasing efficiency (cellulose-cellulase mass transfer rates) and reducing costs.

Summary of Accomplishments

Leveraging our recently established collaborative research relationship with USDA-ARS [Agricultural Research Service] facility in Albany, we first identified positive calli (plural of callus) harboring the engineered enzymes. Calli were induced to generate shoots followed by roots and after acclimatization to the growth chamber were moved to the greenhouse. Plants containing the sso1949 actuator as well as celA were moved to the greenhouse for propagation and seed-set. Tissues from these positive plants were tested for expression using zone clearing assays (a plate based rapid assay). Once enough biomass was available, it was evaluated using molecular techniques. Briefly, we started by performing the polymerase chain reaction (PCR) to confirm the presence of the actuator DNA in the transformed tissue, we then performed reverse transcriptase PCR (RT-PCR) to confirm the presence of mRNA from the coding regions. We then developed an in vitro assay to detect enzyme activity in extracts from plants containing high levels of actuator mRNA. We also performed scanning electron microscopy to visualize ultrastructure differences in plant tissue as a result of actuator expression.

Arabidopsis plants transformed using the floral dips method, as well as seeds selected on antibiotics were also genotyped using PCR and mRNA levels interrogated. Scanning electron microscopy (SEM) studies on the *Arabidopsis* plant and enzyme assays on plant extracts were also performed. We also expressed the sso1949 open reading frame (ORF) in yeast cells and, at first, saw sporadic expression of the protein. After extensive screening of yeast colonies we found that prolonged over-expression of the enzyme was resulting in cellular toxicity. We have now gone to a long growth under repressive conditions and a short time for induction of the enzyme. We then established conditions for efficient lysis of these yeast cells and assayed the extracts for enzymatic activity.

Significance

The successful completion of this research would benefit a broad spectrum of DOE and Sandia activities; especially those associated with low-carbon transportation fuels. In particular, the production of integrated systems that can reduce costs of biomass conversion into fermentable sugars is of significant interest to DOE.

Enhanced Performance of Engineered Neural Networks Using Nanostructured Probes and Predictive Computational Modeling

117841
Year 2 of 3
Principal Investigator: C. D. James

Project Purpose

Functional enhancement and repair of neural tissue circuitry requires the ability to engineer neural-tissue networks that can be designed, measured, and modified to test hypotheses regarding the relationship between network architecture and function. Our specific interest is in developing methods to enhance higher cognitive functions (learning/memory) in the central nervous system (CNS), and to restore function to damaged neural circuits in the peripheral nervous system (PNS). This will be accomplished using microfabricated chemical and topographical cues to guide dissociated neurons into functional networks. We will use conventional electrophysiology techniques to detect synaptic memory in the form of long-term potentiation (LTP) and long-term depression (LTD). The synaptic interface between two neurons will be controlled/varied with microfabricated cues in order to determine the influence of synaptic network architecture on the development of LTP and LTD. With our collaborator at the University of Texas at Arlington, we will leverage these engineering techniques to control the development of functional connections between motor neurons and muscle cells in order to restore function in PNS tissue. Optical probes currently being developed in LDRD Project 105936 will be used in conjunction with simultaneous electrophysiology measurements to aid in the development of long-term noninvasive optical probes for measuring neural activity in vitro. Experimental data will then be used to train a computational model to predict network architectures with enhanced performance, and the model will be validated with experimental measurements on the constructed neural-tissue network. In this regard, the proposed research offers a rare opportunity to generate falsifiable predictions about the structure and activity of computational models of neural-tissue networks since the engineered structure can be verified directly with microscopy rather than indirectly with conventional correlation techniques. We will fabricate and characterize cell network guidance substrates in the Microsystems and Engineering Sciences Applications (MESA) facility.

Summary of Accomplishments

We have fabricated ~1.0 micron deep trenches plasma-etched into glass for guiding neurons with a minimum width of ~1.2 microns. All three surfaces of the trenches are then coated with poly-L-lysine to provide both topographical and chemical guidance cues. We have acquired statistics on guidance efficacy of poly-L-lysine coated trenches, and have observed preliminary evidence of properly polarized neurons using simple geometrical cues. Specifically, we are able to position cell bodies, axons, and dendrites with > 60% accuracy using the proper guidance cues on the glass substrate. This quasi-3D dual guidance-cue strategy is novel, and we will submit a journal publication focusing on cell fidelity to patterns as a function of pattern geometry and chemical interface. For the electrophysiology work, we have completed the electrophysiology setup at the Center for Integrated Nanotechnologies (CINT) with full patch-clamp and fluorescence imaging capabilities. We are currently in the process of finishing up the system to handle both patch and field recordings in preparation for the heterogeneous networks grown in compartmentalized microfluidic structures. A Masters student at the University of New Mexico (UNM) is measuring LTP/LTD in corticostriatal slices for comparison to these phenomena in engineered networks fabricated in this project. For the computational modeling work, we conducted some preliminary simulations of autapses (synapses from a neuron onto itself) in order to identify conditions that could theoretically lead to neuronal self-firing. As a result, we have identified experimental protocols and data analysis methods that will be used both by the simulations and the experiments. The Xyce-

DAKOTA interface has been improved to ease automatic exploration of neuron morphology and network topology. Traditionally, DAKOTA varies numerical parameters while doing parameter sensitivity analyses or optimization. The new changes enable DAKOTA to vary circuit connectivity as well, a feature crucial for predicting changes in network activity due to changes in network topology.

Significance

This project will serve DOE and DOD missions in advancing scientific understanding in the field of neurotechnology, specifically in the application of engineering microsciences and computational modeling for enhancement and restoration of human neural circuitry. Long-term applications for the warfighter include restored motor function to limbs, augmented memory/learning, and enhanced visual perception.

Atomic Magnetometer for Human Magnetoencephalography

117842
Year 2 of 3
Principal Investigator: P. Schwindt

Project Purpose

Magnetoencephalography (MEG) is one of only a handful of noninvasive techniques for measuring electrical activity in the brain. MEG requires a magnetic field sensor with a sensitivity of a few femtotesla/$Hz^{1/2}$ and thus has historically been performed with cryogenic superconducting quantum interference devices. Recently, atomic magnetometers, based on measuring the spin precession of alkali atoms in a magnetic field, have demonstrated equivalent sensitivity but do not require cryogenic cooling resulting in a much smaller package. With an atomic magnetometer, one can envision a much more cost-effective, smaller device. We propose to develop an atomic magnetometer for human MEG measurements.

To develop the atomic magnetometer, we need to design for high sensitivity while keeping in mind the requirements of the human subject. A major component of the effort will be to collaborate with MEG experts at the Mind Research Network (MRN) and the University of New Mexico to provide us guidance in the design and use of the device for human subjects. The high spatial resolution of MEG comes from using multiple sensors around the head. Because the atomic magnetometer reads out the atomic response to a magnetic field via optical interrogation, we can readily achieve multichannel operation by simply detecting separate regions of the probe laser beam. We will first focus on achieving high sensitivity and proper magnetic shielding. Then we will develop highly sensitive, semitransportable devices that can be largely operated by the neuroscientist, culminating in a high-quality MEG measurement of a human subject at MRN.

Summary of Accomplishments

The focus of this year was the development and characterization of a magnetic sensor tailored to the MEG application. For MEG, the active area of the sensor, (the atomic vapor cell) must be as close a possible to the subject's head. In addition, the sensor must be compact to allow the sensors to be densely arrayed around the head. In a conventional atomic magnetometer, the atomic state is prepared and interrogated with a pump and a probe beam propagating perpendicularly to each other. We constructed a sensor where the pump and probe beams are combined on a single optical axis. The beams are retro-reflected after passing through the vapor cell to create a long slender sensor with the cell at one end. This geometry places the cell within 1 cm of the head and allows dense packing of sensors. To maximize sensitivity in the single-axis design, we have developed a novel two-color pump and probe scheme where the pump at 795 nm is easily separated from the probe at 780 nm for high-fidelity detection. To date, we have demonstrated a sensitivity of 14 fT/$Hz^{1/2}$ with a bandwidth of 30 Hz with excellent prospects for improvement in both metrics.

Additional results are the measurement of the magnetic field environment of the shielded room at MRN where we will be making MEG measurements of human subjects. The field in this room is too large for our sensor to operate so we have developed a multicoil system to cancel the field over a volume roughly the size a human head. This coil system will support the coils, the magnetometer, and the subject. We are in the process of getting approval from the Sandia Human Studies Board to perform MEG scans on human subjects in December 2009.

Significance

Recently, the DOE has begun to recognize the importance of human cognition to its overall missions. A key component to this mission must be the ability to measure brain function, and magnetoencephalography (MEG) provides a high-fidelity technique to do so. Because an MEG system using atomic magnetometers could become portable and miniaturized, numerous national security applications are enabled by this work. Additionally, precision magnetometry can be applied to other applications critical to DOE, such as underground detection, remote sensing, and materials reliability.

A Systems Biology Approach to Understanding Viral Hemorrhagic Fever Pathogenesis

130781
Year 1 of 3
Principal Investigator: B. Carson

Project Purpose

Arenaviruses such as Lassa cause lethal hemorrhagic fever in humans and are pathogens of bioterror concern. They may be transmitted by airborne routes and have incubation times under two weeks with mortality up to 30%. A fundamental problem in understanding their pathogenicity is that infected and uninfected cells can exchange information, reciprocally influencing their behavior. Thus, cell population-level experiments will never tell us why some people survive while others die from Lassa fever because many ill effects of viral infection are mediated by the immune system rather than by the virus itself. Excessive type I interferons (IFN alpha/beta) drive hemorrhagic symptoms, but arenaviruses paradoxically appear to block production of these cytokines. We hypothesize that this apparent contradiction is due to differential effects of the virus on the infected cell versus uninfected neighboring cells. This hypothesis is impossible to test by conventional means which asynchronously infect thousands of cells simultaneously, masking the difference between first- and second-order effects. We will deconvolute this system by isolating and infecting individual cells then performing unprecedented measurements of performing unprecedented measurements of interferon (IFN) alpha/beta; and other response-critical cytokines with novel fluorescent transcriptional reporters and in situ solid phase immunodetection. Using a microfluidic cell isolation platform, we will compare isolated cell to population level infection to discover how these viruses provoke lethal cytokine production. The devices we will use were originally developed to study toll-like receptor signaling in response to bacteria. However, with some modifications and new experimental protocols, we will use these flexible devices to address otherwise impossible fundamental biological questions. This project is high risk because we will attempt difficult high-sensitivity cytokine and transcription factor measurements on isolated cells, which has never been done. Although this may not be possible, there is currently no other way to obtain this critical information.

Summary of Accomplishments

In FY 2009, we successfully acquired viruses and developed infection and propagation protocols. We acquired and propagated a number of different cell lines required for virus assay and for subsequent experiments. We established a collaborative contract with the laboratory of Dr. Norbert Herzog, University of Texas Medical Branch. We generated fluorescent reporter constructs for tumor necrosis factor alpha (TNF alpha) and interferon beta. We produced and successfully tested cell lines stably expressing each reporter. We validated the reporters using microscopy and flow cytometry both on and off-chip. We demonstrated responsiveness of the reporters to Sendai virus infection as well as to purified viral and bacterial components. We found that the TNF alpha reporter responds rapidly (2 hours) to stimulation and is also responsive to stimulus withdrawal over a period of days. We designed and began making a plasmid encoding nuclear factor kappa B (NF-κB) p105/p50 antibody fused to cyan fluorescent protein. We rebuilt and improved pressure control and valving equipment required for our experiments and completed fabrication of our single cell array microfluidic chips. We captured and isolated individual reporter cells in a microfluidic device and measured their TNF alpha production in response to viral components. Measurements of this kind have never been done before. We generated a preliminary NF-κB network model and began predictions for the kinetic behavior of individual transcription factor subunits. We built a training set for host-virus protein-protein interactions and began validating it using a leave-one-out method. Preliminarily, we predict that Pichinde virus nucleoprotein interacts with RelA/p65 and potentially five other candidate proteins.

Significance

This project benefits the DOE scientific and DHS awareness and response strategic goals by addressing a key deficiency in our understanding of emerging infectious hemorrhagic fever virus pathogenesis. We will employ Sandia's world-class microfluidic technologies to develop biomarker assays of unprecedented sensitivity to study the response of individual cells to a National Institute of Allergy and Infectious Diseases (NIAID) category A virus, ultimately supporting therapeutic and vaccine strategies to combat these viruses. To the broader biology community, the methods and technologies we are developing in this project represent a fundamentally new way to discriminate between cell-intrinsic and -extrinsic behaviors. This is a fundamental and long-standing challenge in cell biology with wide ranging applications in human health as well as biodefense.

Biomolecular Interactions and Responses of Human Epithelial and Macrophage Cells to Engineered Nanomaterials

130782
Year 1 of 3
Principal Investigator: S. M. Brozik

Project Purpose

Nanotechnology holds a vast promise of enabling a wide range of transformational technologies, but also has inherent risks with respect to human health and environmental effects. In fact, engineered nanoparticles are already being used in a variety of commercial products including “wrinkle-free” clothing (silver nanoparticles) and sunscreen (metal oxide nanoparticles) despite the overall lack of knowledge concerning the associated health impacts. Examples such as the ability of carbon nanotubes to cross the blood-brain barrier, however, suggest that nanomaterials may represent a significant and serious risk to human health. Thus, the National Nanotechnology Initiative (NNI) has recognized that there is an immediate and critical need to establish a basic understanding of the health-related issues regarding engineered nanomaterials. A critical challenge embodied within this problem arises from the ability to synthesize nanoparticles with a wide array of physical properties (e.g., size, shape, composition, surface chemistry, etc.), which in turn creates an immense, multidimensional problem in assessing toxicological effects. We propose to address this challenge by establishing fundamental relationships between the physical and chemical properties of engineered nanoparticles and the associated biomolecular interactions and response of cells. Based on the most likely routes of exposure (i.e., inhalation, ingestion, and dermal) and highest associated risk, we investigate the cell-surface interaction and response pathways of epithelial and immune cell lines that are involved in the toxicological response to xenobiotics (e.g., nanoparticles) using advanced imaging techniques, biochemical analyses, and chip-based sensor arrays.

Summary of Accomplishments

In this year, we made significant progress in developing correlations between toxicity/response of immune cells and the size/surface functionality of quantum dots (QDs). QDs of seven different sizes and three different functionalities (i.e., amine-, carboxylic-, and polyethylene glycol [PEG]-terminated) were characterized by fluorimetry to evaluate intrinsic differences in their photoluminescence and quantum efficiency. Significant size-dependent differences were observed among the QDs. Size- and media-dependent differences in the photonic properties were also observed when QDs were prepared in the different cell culture media. These data are necessary for deriving scaling factors, and normalizing quantitative difference between QDs in uptake.

Initial analysis of QD uptake by macrophage cells confirms a size × concentration dependency. Cellular uptake was greatest when RAW macrophage cells were exposed to 100 nM concentration of QD 620 particles; a linear relationship between QD size and uptake was not observed. Total internal reflection fluorescence microscopy of cellular uptake in live RBL mast cells suggests that uptake does occur, which is in direct contrast to previous observation with fixed cells. The half-life of cellular uptake for QD 605 particles is estimated at 5.5 minutes, suggesting that uptake is rapid. The high disparity of diffusion coefficients of QDs interacting with RBL membranes suggests that a wide array of QD states exist within the media. Confocal hyperspectral imaging (HSI) of RBL cells exposed to multiple QDs also suggests that certain sizes of QDs are preferentially internalized by the cells. The ability to image cellular uptake via HSI is highly advantageous, as several different QD sizes can be evaluated simultaneously. Documentation and approvals were also obtained in this fiscal year to acquire human cell lines requiring BSL-2 facilities and practices, and we subsequently obtained one lung and two human colorectal epithelial cell lines from the American Type Culture Collection (ATCC).

Significance

In this project, Sandia has a strategic opportunity to establish a leadership position with respect to evaluating the health-related implications of nanoparticle exposure. Issues of nanotoxicology and nanomaterials safety will directly impact Sandia's mission in nanoscience (e.g., the Center for Integrated Nanotechnologies [CINT]) and national security (e.g., nefarious use of toxic nanoparticles), as well as provide fundamental science beneficial to the larger nanoscience, biological, and toxicological communities.

From Algae to Oilgae: In Situ Studies of the Factors Controlling Growth, Oil Production, and Oil Excretion in Microalgae

130783
Year 1 of 3
Principal Investigator: S. Singh

Project Purpose

Transforming algal oil into biodiesel requires solving the problems of growing large robust algae populations that produce high fractions of easily harvested specific fatty acids. Current efforts proceed in engineering fashion, ignoring the fundamental biological processes at play. As a consequence, important issues regarding cell growth, utility of the fatty acids produced, and efficiency of oil recovery have been difficult to resolve. We propose a radical new approach that will provide the biological insight needed to solve these issues. We will apply our unique experimental and theoretical expertise in cell electrophysiology and imaging to interrogate individual cells in situ to identify molecular mechanisms leading to growth, production of specific fats and their translocation. We will track channel activity in live algae stressed by various environmental factors to discover the significance of ion efflux to algal growth and to identify channels to manipulate for optimized growth. Growth also depends on photosynthesis. With hyperspectral imaging tools, we will track photosynthetic pigments responding to different growth and light conditions to learn how to optimize photosynthetic processes in algae for enhanced growth. We will use our unique in-situ imaging capabilities (fluorescence and Raman) and statistically designed experiments to develop fundamental, science-based detailed insights into triacylglyceride (TAG) production, control and translocation mechanisms in algae. Fatty acid composition and production vary between algae and in response to altered environmental conditions. We will apply Sandia imaging capabilities that enable precise location, quantification, and compositional analysis of TAGs produced by algal cells in real time to determine the molecular factors controlling fat composition and production. With this information in hand, we iteratively apply genetic and metabolic engineering methods to algae to achieve improved TAG production and composition. Knowledge of the biological mechanisms and algal cell functions will provide the missing foundation for efficient transformation of algal oil into biodiesel.

Summary of Accomplishments

This year, we established small-scale algal cultures for five different algae species. We completed collecting baseline growth curves and kinetics of lipid production for these cultures. We also initiated statistically designed experiments employing significant factors to generate multifactorial response curves required for optimizing TAG production. Using our hyperspectral confocal fluorescence microscope coupled with multivariate curve resolution (MCR) analysis, we developed a label-free method for determining the location and amount of lipids present in each cell. We demonstrated that we can quantitatively measure the lipid present in algae via the resonance enhanced carotenoid Raman signal that is present in the fluorescence images and which correlates directly with lipid levels determined from Nile Red labeling. In addition, we made great strides in setup, testing and optimization of Raman for in-vivo monitoring of lipid production and compositional analysis. We compiled Raman spectral libraries of model algal lipids and lipid extracted from algae and in single live algae for five different algae species. Degree of saturation (C=C) and relative chain lengths could be determined from the I_{1650}/I_{1440} intensity ratios, by fitting the number of C=C bonds for model fatty acids as a linear function. The average number of C=C bonds of mixed oils and extracted algal oil was predicted based upon the fitted calibration data set. The average number of C=C bonds in the extracted algal oil was calculated to be ~0.5, which demonstrates that less than half of the extracted oils are fully saturated. We also succeeded in acquiring Raman signals from live algal cells by laser trap methods, which demonstrates our ability to perform Raman investigations of live algal cells. In another major success, preliminary data of the phosphate starvation lipid trigger demonstrated enhancement in lipid accumulation in *Neochloris oleoabundans*.

Significance

Development of a robust national supply of renewable biofuels is a priority target for DOE. Our proposed work can impact Sandia's efforts to establish direct procedures for selecting, optimizing algal biomass for biofuels through detailed in-situ molecular level understanding of factors affecting fat production and composition.

Functional Brain Imaging by Tunable Multispectral Event-Related Optical Signal (EROS)

130784
Year 1 of 3
Principal Investigator: O. B. Spahn

Project Purpose

Functional brain imaging is of great interest for understanding correlations between specific cognitive processes and underlying neural activity. This understanding can provide the foundation for developing enhanced human-machine interfaces, decision aides, and can even provide mechanisms for enhancing cognition at the physiological level. Furthermore, successful miniaturization of these devices can provide dismounted applications for warfighters and can provide small footprint, noninvasive methods for real-time monitoring of decision-making in a wide variety of applications from scientists to analysts to decision makers. The functional near infrared spectroscopy (fNIRS) based event-related optical signal (EROS) technique pioneered by Professors Gratton and Fabiani at the University of Illinois at Urbana-Champaign (UIUC) is particularly promising as it provides direct, high-fidelity measures of temporal and spatial characteristics of neural networks underlying cognitive behavior, something not offered by other neuroimaging techniques such as electroencephalography (EEG) and functional magnetic resonance imaging (fMRI). However, current EROS systems are hampered by relatively poor signal-to-noise-ratio (SNR) and depth of measure, limiting areas of the brain and associated cognitive processes that can be investigated. We propose to perform a science-based study to optimize the efficacy of a multispectral fNIRS EROS system approach. Our team is uniquely qualified to investigate and potentially develop this enabling technology with expertise in optoelectronics and optical signal processing as well as cognitive science and functional brain imaging. Critical strategic partnerships and collaborative teaming will be conducted with the EROS pioneers, Gratton and Fabiani at UIUC, as well as the University of New Mexico, New Mexico State University, and the MIND Research Network. This study will provide the technical foundation for follow-on hardware development and potentially miniaturized portable neuroimaging systems; an invaluable capability for numerous military and homeland security applications.

Summary of Accomplishments

UIUC/Beckman collaboration

- Observed EROS measurement setup and data collection on subject for different project
- Reviewed theoretical work performed to date
- Concluded that a new flexible EROS model should be developed and validated with milk tank data

EROS model development

- Finite element mesh volume including variable scattering, absorption and refractive index parameters
- Monte Carlo photon migration model
- Time-dependent photon properties
- Optimization and parallelization of code
- Code validation

Detection Ideas

- Differential detection for (1) noise cancellation and (2) active volume localization and confirmation

Presenting results at Human Brain Mapping meeting in June 2009 based on modulation frequency effects in previous milk tank results and simulations.

Significance

Potential portable EROS systems could have widespread application where direct measurement of warfighter cognitive processes could have tremendous impact in operational and training environments. Homeland security interests in the motivation of unknown persons could also potentially benefit from a portable, nonintrusive functional brain imaging technology.

K-Channels: On/Off Switches of Innate Immune Responses

130785
Year 1 of 3
Principal Investigator: S. L. Rempe

Project Purpose

Infectious diseases from pathogenic microbes annually account for one-quarter of all deaths worldwide and, in a pandemic year, one single pathogenic strain can kill more than 2% of the world's population. Current efforts to stave off the "inevitable" next infectious disease pandemic focus on the traditional prescription of developing new vaccines and drugs that kill microbes, so far with disappointing results. In order to progress, a new paradigm in medical treatment is needed for fighting infectious disease. Inspired by recent work, we will look to the immune cells, not the microbes, for potential drug targets. New evidence strongly suggests that a molecular switch exists in the cell membrane that can actively modulate immune responses to pathogenic attacks. Unexpectedly, the switch exists in the form of a potassium-selective channel protein. We propose to discover the role of K-channels in innate immune responses to pathogens of importance to biodefense using a fundamental bioscience research and development strategy that capitalizes on our recent advances in molecular modeling, high-resolution optical and electronic cell interrogation techniques, and microfluidics platform development. With these unique methods, we will interrogate the relationship between K-channels and immune responses with unprecedented accuracy and scope, ranging from the atomic resolution of single protein channels, to signaling processes of individual immune cells and cell populations. The scientific insight gained should enable rational manipulation of channel activity in order to boost or suppress innate immune responses, depending on the pathogen threat at hand.

Summary of Accomplishments

We have made significant progress toward understanding the role of transmembrane potassium channels in immune response. We have obtained DNA for functional fluorescent BK channels, which enables study of conformational changes via fluorescence resonance energy transfer (FRET) in a channel repeatedly implicated in modulating immune responses to pathogen exposure. A stable human cell line (HEK) transiently expressing fluorescently labeled toll-like receptor 4 (TLR4) complexes and fluorescently labeled BK channels is being developed so we can study the physical interaction between channels and immune receptors in the membrane. We have begun tracking two events that occur within the TLR4 signaling pathway in RAW cells in response to pathogenic challenges: translocation of RelA fusion construct from cytoplasm to nucleus; transcription of the cytokine tumor necrosis factor-alpha (TNFα) (via a fusion construct). This permits monitoring of intermediate and late events in the immune response. In contrast to the normal response of RelA fusion protein in the nucleus to challenge by components of *E. coli* (lipopolysaccharide [LPS]), the oscillatory pattern is more heavily damped and the time to the first peak of the nucleus-to-cytoplasm fluorescence ratio is delayed in the presence of a nonspecific K channel modulator. To understand the connection between early phases of immune response and K-channel modulation, we have begun two investigations measuring: 1) differential TLR4 and correlated BK-channel dynamics under exposure to LPS; 2) differential TLR4 and correlated membrane potential dynamics exposed to small-molecule K-channel blockers. We observed formation of a TLR4 dimer as a member of a larger multimeric state initiated by LPS stimulation using a unique hyperspectral temporal image correlation spectroscopic analysis. Parallel efforts are being developed for monitoring the effects of channel blockers on immune receptor dynamics. Preliminary results suggest that the generic K-channel blocker, tetraethylammonium (TEA), results in transient hyperpolarization of the cell, and modulation of transcription factor waves in the secondary stage of LPS-induced immune response.

Significance

Our work impacts missions in biodefense and emerging infectious disease. Our knowledge of how a membrane protein provides on/off switching of the innate immune response will lead to new ideas for diagnostic and therapeutic treatments of malfunctioning immune cells. This work leverages recent advances in imaging techniques, cell interrogation platform developments, and biomolecular modeling strategies and complements, without overlap, current studies of host-pathogen interactions.

Refereed Communications

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S. Varma and S.B. Rempe, “Structural Transitions in Ion Coordination Driven by Changes in Competition for Ligand Binding, “*Journal of the American Chemical Society*, vol. 130, pp. 15405-15419, October 2008.

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Modeling Cortical Circuits

130786
Year 1 of 2
Principal Investigator: F. Rothganger

Project Purpose

The neocortex is the highest region of the brain, where audio and visual perception takes place along with many important cognitive functions. One path to understanding perception and cognition is to reverse engineer the circuits in this system. Some have proposed that the neocortex follows a generic circuit pattern which is repeated over its surface (with some specialization), and that we can understand the whole by decoding this generic circuit.

Rao & Ballard [1] proposed that the local circuits of the visual cortex implement a hierarchical generative model. Their model used gradient descent at multiple time scales to interpret input and learn new patterns. Dr. Tom Anastasio of University of Illinois at Urbana-Champaign (UIUC)/Beckman Institute proposed a novel learning rule, called input minimization (InMin), in which local circuits adjust their behavior in a way that minimizes the total signaling activity on their inputs. In collaboration with Dr. Anastasio, we have demonstrated that InMin can learn eye-control behavior from inputs containing mixed state and error signals.

We propose to synthesize a template neocortical circuit by combining the InMin learning mechanism with a generalization of the Rao & Ballard model. The InMin rule addresses the complex signaling environment in which a local cortical circuit operates, and provides a realistic learning mechanism in the absence of a global reward signal. It is consistent with the brain's need for signaling efficiency within a limited energy budget.

This model has tremendous potential beyond describing the processing of local circuits. It can generalize to interactions between a human and the environment, and show how every circuit in the brain participates in this process. If it proves feasible, it could be a breakthrough in both sensory and cognitive processing.

Summary of Accomplishments

In the first 12 months of this project, we have accomplished the following:

- Established a collaboration with Dr. Steve Levinson of the University of Illinois Urbana-Champaign Beckman Institute, an expert in hidden Markov models (HMMs), which are a key candidate model for cortical operation. His group has a relationship with Numenta, which gives us indirect access to expertise on hierarchical temporal models (HTMs), another key candidate model. Supported by this project, Luke Wendt, a student of Dr. Levinson, developed a system to learn control using neural networks.
- Reproduced the emergence of visual receptive fields using both the Rao & Ballard [1999] method and self-organizing maps (SOMs, also known as Kohonen maps).
- Developed software for executing neural network simulations on parallel hardware. Currently this software runs on a multicore desktop system. This is the first step towards porting the simulation to a supercomputer.
- Started to map out alternate circuits that more-closely resemble cortical architecture. We have developed a simple notation based on linear algebra to express neural networks, which we have applied to several algorithms (Rao & Ballard, adaptive resonance theory [ART]). This will allow us to easily compare algorithms and pick those that best fit the neurophysiological data.

- Developed a method for interconnecting stages of a neural network inspired by the layered architecture of the neocortex and the retina. While fundamentally the same as a traditional neural network, this approach shifts the focus to spatially dispersed computation rather than a set of parallel but separate modules.

Significance

Human modeling supports several Sandia missions by enabling such ends as characterizing adversarial behavior and predicting/enhancing human performance as part of critical systems. Beyond human modeling, a deep understanding of the principles of cognition will enable powerful technical solutions to a range of national issues, such as monitoring large amounts of sensor data for potential threats, or flexible autonomous military robots.

Reference

1. R. Rao and D. Ballard. "Predictive Coding in the Visual Cortex: a Functional Interpretation of Some Extra-Classical Receptive-Field Effects," *Nature Neuroscience*, 2:1, pp 79–87 (1999).

Robust Automated Knowledge Capture

130787
Year 1 of 3
Principal Investigator: R. G. Abbott

Project Purpose

Our customers in the national security domain need tools that enable human knowledge and behavior to be modeled at a level of individual specificity that has been largely ignored within the cognitive neurosciences. A prevailing assumption in cognitive theory has been that cognitive processes are largely invariant across individuals and across different conditions for an individual. Attention has focused on identifying a universally correct set of components and their interactions, and individual variability is generally regarded as measurement error. We propose that cognitive adaptability is a trait necessary to explain the inherently dynamic nature of cognitive processes as individuals adapt to ongoing circumstances. Cognitive adaptability does not imply a "blank slate;" instead, it is asserted that there exists inherent flexibility that may be quantified and used to predict variations in cognitive performance. Previous investments in automated knowledge capture (AKC) provide Sandia unique capabilities in using machine learning techniques to construct individualized cognitive models. Consequently, Sandia is uniquely positioned to conduct this research.

This proposal has three primary objectives:

Objective 1: Test key hypotheses of cognitive adaptability.
Hypothesis 1: For a given task, individuals will exhibit different strategies with the specific strategy employed being a product of their intrinsic skills.
Hypothesis 2: Individuals will exhibit varying levels of adaptability with an individual's adaptability determining their propensity to switch strategies in response to changing circumstances.

Objective 2: Develop automated knowledge capture techniques to characterize cognitive adaptability. We will develop techniques to: (1) model patterns of selective information retrieval; (2) detect strategic biases revealing beliefs and intrinsic skills; (3) detect shifts in strategy over time; (4) develop mathematical techniques to bound the uncertainty in the individual cognitive models derived through AKC.

Objective 3: Establish neural correlates for cognitive adaptability. Conduct experimental studies to establish neural correlates of behavioral metrics for cognitive adaptability.

Summary of Accomplishments

In conjunction with our collaborators at the University of Notre Dame and University of Memphis, we first created a suite integrating numerous widely accepted individual difference measures assessing subjects in a wide range of cognitive traits.

Next, we developed software for a drawing/tracing task environment. The software provides a wide range of stimulus/feedback conditions to place various cognitive demands on experimental subjects. Options include rotation of the drawing, imposition of a time limit, drawing from memory, and a scoring function with parameters that trade off reward emphasis between speed and accuracy. We implemented task computers with drawing tablets which were installed at the universities for data collection.

With approval from Sandia and University Institutional Review Boards, this project has collected 1–2 hours of drawing performance data from each of over 200 human subjects. Each subject performed the drawing/tracing task on between 12 and 17 conditions (drawing task settings). In total, we have collected nearly 50,000 individual drawings. Preliminary analysis has revealed insights between strategy shift and standard measures of intelligence and creativity.

Each of the collaborations has been extremely productive, contributing to the experiment design, amount of data collected, and data analysis. Soon the collaborative work will include authoring and submitting academic publications.

Finally, FY 2009 accomplishments include initial preparations for the planned FY 2010 study which consists of the three primary components: the National Aeronautics and Space Administration (NASA) multiattribute task battery (MATB), computer vision hardware/software to monitor the state of this environment, and eye tracking hardware/software to capture data for a model of selective visual attention on this task. We have procured and installed MATB, conducted significant computer vision software integration, and are currently evaluating various eye tracking solutions.

Significance

Sandia's current AKC capabilities have already demonstrated value in several DOE and DOD applications including physical security, tactics training, and intelligence applications. However, the limiting factor for AKC in these applications is predictive accuracy of individual models in varied contexts and the inability to characterize the accuracy of these predictions. Cognitive adaptability is a confound for current models that disregard it; this research will fill that gap.

High-Throughput, Cell-Free Protein Production and Characterization

139461
Year 1 of 1
Principal Investigator: E. Ackerman

Project Purpose

Relatively little is known about intra- and extracellular gradients of pH, ionic strength, and electrical potential. Yet these gradients exist in cells and exert synergistic effects on many (inter- and intra-) cellular interactions, e.g., proton pumps drive ATP (adenosine triphophate) synthesis in mitochondrial membranes, electrical stimuli control nerve cell interactions, and calcium waves propagate in and around cells. Are the effects of these electrical gradients limited only to a specific cellular process, or does nature exploit these gradients for unrelated purposes? In prior work led by the PI, Eric Ackerman, while at Pacific Northwest National Laboratory (PNNL), it was shown that applying electrical potential during cell-free translation of a secreted protein was necessary for proper protein folding. The purpose of this project is to build on this exciting result and provide fundamental insights into cellular function as well as illuminate new aspects of translation and protein folding.

A crude power supply provided varying potential during translation reactions of organophosphorous hydrolase (OPH), a protein yielding grams/liter with *E. coli*, nearly all of which is present in inclusion bodies and hence inactive. One of the tremendous advantages to the cell-free approach is that screening multiple translation conditions is feasible. Activity assays are often easier because the extracts are cleaner than lysed cells. New approaches that produce active, "difficult" proteins would be valuable, especially if the advance resulted from a fundamentally new approach, such as including an electrical potential during translation. With the tremendous capabilities at Sandia, it should be possible to build a sophisticated platform to screen wide ranges of electrical potentials during translation and more precisely map the effects of potential gradients on protein folding and activity.

Summary of Accomplishments

In preparation for the protein expression tasks on the project, the team installed and made operational a high-throughput, cell-free, protein production robot, and a large-scale cell-free robot. These robots were exercised in a series of preliminary experiments to produce a test protein, green fluorescent protein (GFP). These preliminary experiments successfully demonstrated the high-throughput, cell-free production of GFP. Lab renovations required to conduct later phase experiments were not completed by the end of FY 2009 which prevented the achievement of all R&D goals within the timeframe of the project.

Significance

Harnessing proteins for missions in energy generation, remediation and security cannot be accomplished until we can readily make active versions of the proteins. Other agencies such as the Defense Threat Reduction Agency (DTRA), the National Institutes of Health (NIH), and the Defense Advanced Research Projects Agency (DARPA) have similar needs to utilize proteins and suffer from the same bottleneck when essential proteins cannot be made, or if the proteins quickly lose activity. The proposed work may provide a generally applicable, new method to overcome the problem of making difficult proteins in active form.

Feasibility of Neuromorphic Computing to Emulate Error-Conflict Based Decision Making

139587
Year 1 of 1
Principal Investigator: D. W. Branch

Project Purpose

A key aspect of decision-making is determining when errors or conflicts exist in information and knowing whether to continue or terminate an action. Understanding the error-conflict processing is crucial in order to emulate higher brain functions in hardware and software systems. Specific brain regions, most notably the anterior cingulate cortex (ACC) are known to respond to the presence of conflicts in information by assigning a value to an action. Essentially, this conflict signal triggers strategic adjustments in cognitive control, which serve to prevent further conflict. The most probable mechanism is that the ACC reports and discriminates different types of feedback, both positive and negative, that relate to different adaptations. Unique cells called spindle neurons that are primarily found in the ACC (layer Vb) are known to be responsible for cognitive dissonance (disambiguation between alternatives). Thus, the ACC, through a specific set of cells, likely plays a central role in the ability of humans to make difficult decisions and solve challenging problems in the midst of conflicting information. In addition to dealing with cognitive dissonance, decision-making in high-consequence scenarios also relies on the integration of multiple sets of information (sensory, reward, emotion, etc.). Thus a second area of interest for this proposal lies in the corticostriatal networks that serve as an integration region for multiple cognitive inputs. In order to engineer neurological decision-making processes in silicon devices, we will determine the key cells, inputs, and outputs of conflict/error detection in the ACC region. The second goal is to understand *in vitro* models of corticostriatal networks and the impact of physical deficits on decision-making, specifically in stressful scenarios with conflicting streams of data from multiple inputs. We will elucidate the mechanisms of cognitive data integration in order to implement a future corticostriatal-like network in silicon devices.

Summary of Accomplishments

All the existing models of the ACC were found to be neural network implementations. The major differences in the models were the type of the signals used to represent perceived conflict. The well-established models are based on the conflict-control loop theory of the ACC that suggests trial history impacts level of conflict. More recent models argue that the conflict models fail to account for learned behavior whereas the conflict-model proponents argue that there is a lack of experimental data to support error-likelihood models. Despite these differences in the ACC models, there is a sufficient understanding of the ACC to model the primary conflict-control behavior. To implement the ACC as a neuromorphic system would require training sets similar to those used in neural networks in the form of congruent, incongruent, neutral, and go/no go type tasks. We expect the primary challenges for success would be translating the neural network equivalents into the neuromorphic chip, either as differing neuron types or altering synapse functionality. A clear benefit of the neuromorphic approach is that a more-physical representation of the ACC could be created. Clearly, the flexibility or analogous plasticity inherent to neuromorphic chips would be an ideal media to model the behavior of the ACC.

Significance

Relating to DOE's scientific discovery and innovation thrust, our goal is to discover the key mechanisms of neurological computation and use them to solve problems that are beyond the capability of current digital methods. Such a breakthrough will provide approaches to reveal possible weaknesses that are otherwise overlooked in vast data sets for achieving superior national security. This will position Sandia and DOE as key leaders in national initiatives advancing neurotechnologies.

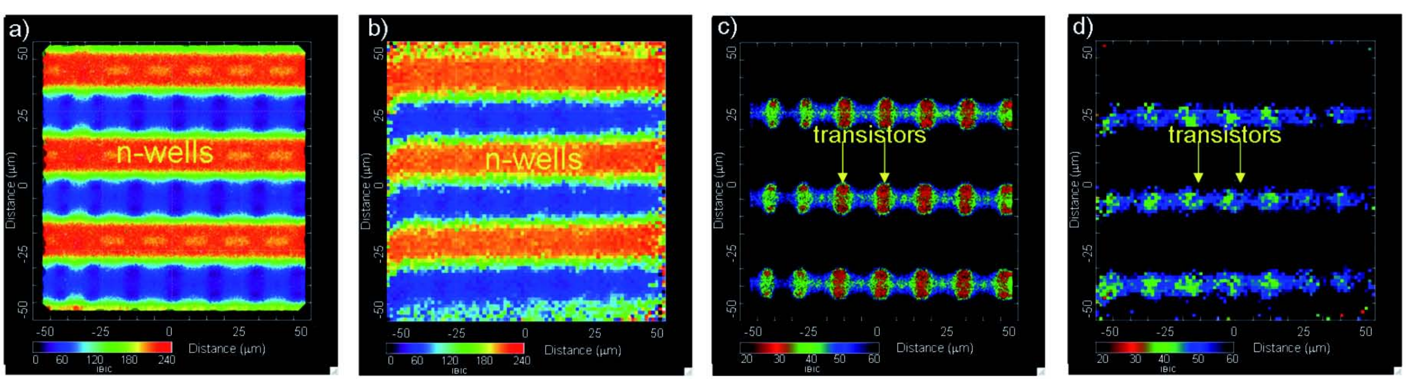
SCIENCE OF EXTREME ENVIRONMENTS INVESTMENT AREA

The Science of Extreme Environments (SEE) investment area seeks to create new knowledge that enables revolutionary advances in the areas of high energy density physics, radiation sciences, pulsed power, and fusion energy for national security needs. A synergistic combination of experiments and theory provides insights into the nature of electronics under exposure to x-rays, gamma rays, neutrons, and other charged particles, and enables the production of high power density x-rays from impressive pulsed power systems. Theoretical computational studies reveal the nature of the complex plasmas formed and aid in such pursuits as the production of high power microwaves for missile defense. Pursued through a thoughtful combination of experiment and modeling, this IA clarifies scientific understanding about environmental conditions rarely encountered in everyday experience (save for example, rare situations such as lightning), but which are nevertheless commonplace in several Sandia national security mission areas.

A Radiation Microscope for SEE Testing Using >10 GeV Ions

Project 105966

Radiation effects microcopy (REM) is utilized by federal agencies such as NASA and DTRA and by certain corporations to diagnose problems in integrated circuits (ICs) caused by ionizing radiation, and to pinpoint unanticipated radiation-intolerant regions in ICs. For this purpose, REM utilizes focused high-energy heavy-ion beams generated by cyclotrons. As technologies increase chip layering, this diagnostic tool will require energies in the GeV range in order to penetrate to the components being assessed. In this project, an alternative to focusing a high energy ion beam is being pursued, namely the use of an ion photon emission microscope (IPEM) to detect the impact point of individual ions and correlate this position with a luminescent photon emission from the target device. This requires optimization of the IPEM luminescent film, and subsequent development of a portable, tabletop IPEM system that can be transported to any cyclotron facility to diagnose newer ICs whose diagnoses would not otherwise be possible. In addition to proving the concept and examining different luminescent materials, the project team has installed a functional IPEM on Sandia's tandem Van de Graaff accelerator, and on a cyclotron at Lawrence Berkeley National Laboratory (LBNL).

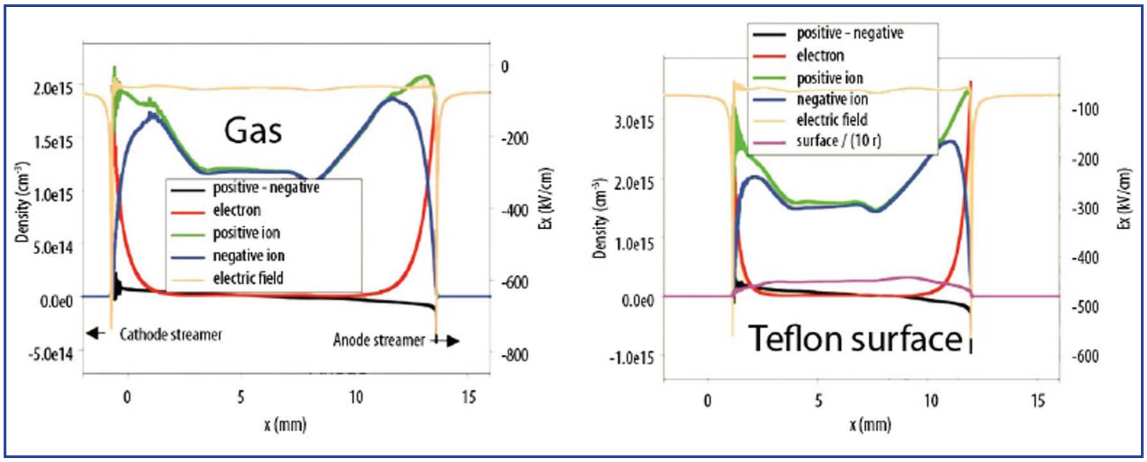


IPEM images illustrating penetration of the technique to reveal deeper-layer structure.

Understanding Surface Breakdown in Electronegative Gases

Project 105987

An electrical "short" or breakdown can occur within high-power gas, pulsed-power switches. As seen in the figures below, this project compared the differences between surface ionization waves in a gas and those along a Teflon surface to try to understand the breakdown process. Surface flashover along an insulator — the phenomenon primarily responsible for the shortened lifetime of high-power gas switches — is being experimentally investigated and modeled to try to reduce the impact of such lightning-like breakdowns and resulting pulsed power system failures.



Comparison of surface ionization waves in a gas (left) and along a Teflon® surface (right).

SCIENCE OF EXTREME ENVIRONMENTS INVESTMENT AREA

A Radiation Microscope for SEE Testing Using >10 GeV Ions

105966
Year 3 of 3
Principal Investigator: G. Vizkelethy

Project Purpose

Radiation effects microscopy (REM) using focused high-energy heavy ion beams has been used successfully to diagnose problems caused by ionizing radiation in Sandia-made integrated circuits, such as the Permafrost application specific integrated circuit (ASIC). It also helped understand the basic physics of interactions of radiation with devices that has led to improved modeling, and to guide the design of radiation-hard parts. REM can pinpoint unanticipated radiation intolerant regions in integrated circuits (ICs). The Sandia REM facility is used by several other agencies (the National Aeronautics and Space Administration [NASA], the Defense Threat Reduction Agency [DTRA], etc.) and major US companies (e.g., Medtronic defibrillators) to diagnose radiation caused problems in their devices. As the ICs are becoming more complex and evolved, the metal and insulating overlayers are approaching the penetration depth of the ions used at Sandia for REM. Furthermore, the increased use of flip-chip technology (the device is on the back side of the chip) increases the distance that the ions must penetrate to several hundred micrometers. To penetrate this much material, energies in the GeV range are required. These energies are available at a few cyclotron facilities in the US. The problem is that it is extremely hard to focus these ion beams due to their long penetration depth and high magnetic rigidity. There is no nuclear microbeam in the world that operates at these high energies. Our approach is that instead of focusing the ion beam we will use the ion photon emission microscope (IPEM) to detect the impact point of individual ions and correlate this position with a single event effect (SEE) from the device. This project involves upfront research required to optimize the IPEM luminescent film, and then develop a portable IPEM system that can be taken to any of these cyclotron facilities to diagnose newer ICs whose diagnoses would not be possible at the current facilities.

Summary of Accomplishments

We invented a new technique, ion photon emission microscopy (IPEM), that allows radiation effects microscopy (REM) without using a focused ion beam. We investigated several luminescent materials as potential IPEM films (used on top of devices to produce photons) and studied their responses. We found that the best candidates are GaN films and InGaN/GaN multiple quantum well (MQW) structures. We characterized several films, determined their efficiency, lateral resolution, and decay times. We used the “time-to-first-photon” and “time-between-photons” techniques to determine the lifetime. The theory for the above methods, which can be more widely used, was developed to provide theoretical support to this project. We found that the n-type GaN with low doping has the highest light yield, but has a relatively long decay time. MQW samples had somewhat lower light yield and their lifetime varied over a wide range, depending on the actual MQW structure. We designed, built, and installed an IPEM on the Sandia tandem accelerator. We tested and characterized the tandem-based IPEM and compared its performance to the nuclear microbeam. A new version of the IPEM used in air at the Lawrence Berkeley National Laboratory (LBNL) 88” cyclotron was designed, built, and installed. When this new cyclotron IPEM was tested, unexpected problems due to the GeV ion beam’s interaction with air were discovered. Mitigation techniques were developed and will be applied.

Significance

Sandia's mission includes providing radiation-hard electronics for the military and the space industry. It is important to be able to pinpoint sensitive components in these ICs and modify their design to make them more radiation hard. Without this new development Sandia could lose its ability to diagnose and rectify problems caused by radiation effects in the next generation of microelectronics because the ever-increasing thickness of IC overlayers will exceed the penetration depth of our ions.

High Power Density X-Ray Sources

105970
Year 3 of 3
Principal Investigator: R. A. Vesey

Project Purpose

High energy density physics applications (e.g., inertial confinement fusion, [ICF]) require both high x-ray energy and power density. Wire array radiation sources are energy rich and efficient, but the typical array sizes limit the power density. For example, wire arrays have generated x-ray power of 130 TW with a length and radius of ~1.0 cm. The development of advanced, compact sources seeks to significantly increase the achieved power density.

Summary of Accomplishments

Two-dimensional radiation-magnetohydrodynamics (2D-RMHD) simulations have been developed and matured to model advanced source dynamics and hohlraum physics, and have been quantitatively benchmarked against available data. These simulations suggested several feasible experimental measurements that further constrain our models and enable more rapid optimization of these sources for programmatic applications. Detailed experimental designs were developed, including target fabrication specifications and diagnostic requirements, for an initial Z campaign. The goals of this initial series were to re-establish and mature a new x-ray source platform on Z, measure the secondary hohlraum re-emission temperature history (over several shots), and for the first time, correlate the source plasma dynamics with the secondary hohlraum temperature evolution. This shot series was completed with nearly 100% data return, and the data are being used to further our understanding of our new advanced x-ray sources.

Significance

High power density hohlraums are a breakthrough and could reduce the cost of pulsed power fusion (inertial confinement fusion [ICF]) ignition by a factor of three. This work is relevant to DOE strategic needs in nuclear weapons stewardship (allows weapons physics experiments for secondaries and primaries, and weapons effects), energy security (decreases the cost of future z-pinch inertial fusion energy sources), and improves the capacity of existing facilities for world-class scientific research (allows access to new regimes).

Automated Monte Carlo Biasing for Photon-Generated Electrons Near Surfaces

105971
Year 3 of 3
Principal Investigator: B. C. Franke

Project Purpose

Our goal is to produce an automated technique for the biasing of Monte Carlo coupled electron-photon calculations, even for problems where electrons have high importance only near surfaces. We plan to accomplish this by implementing a weight windows method that can accurately represent the adjoint importance map for an arbitrary problem. The primary challenge is obtaining accurate importance maps in problems where electron ranges are 4 or 5 orders of magnitude smaller than the system geometry. This requires an adaptive, efficient data structure. The combination of tree data structures and functional expansion techniques offers the best solution. Tree structures can be used to partition space. A functional expansion can represent the importance map within each partition. Allowing both the tree and expansion to adaptively refine is similar to hp-adaptivity in finite element methods. For our problems, the adaptation must be based on particle fluxes calculated in adjoint Monte Carlo simulations.

The greatest impact of this project will be for problems that require accurate determination of electron flux. These types of problems are abundant in radiation hardness assessments of electronics for nuclear survivability. Two examples are cavity system-generated electromagnetic pulse (SGEMP) and dose enhancement in microelectronics, both of which can contribute to the electrical response of a component under radiation. Cavity SGEMP requires detailed resolution of electron surface emission in space, energy, and angle. Dose enhancement, a phenomenon arising from variation of the electron flux at material interfaces, can occur at many locations inside an electronic component. The method could also expedite satellite shielding analyses involving deep penetration of radiation. Such calculations are crucial for designing radiation-hardened military satellites (both DOD and DOE).

Summary of Accomplishments

We demonstrated an approach to automatically biasing coupled electron-photon Monte Carlo transport calculations. This approach builds on adjoint Monte Carlo calculations, adaptive data structures, and weight-windows biasing. For a realistic test problem, we achieved an order-of-magnitude improvement in computational efficiency compared against manual-biasing methods. This represents a four or five order-of-magnitude gain compared against unbiased calculations.

A variety of adaptivity algorithms for Monte Carlo tallies were developed and demonstrated as part of this project. Several h-adaptivity algorithms were found to be successful. Our p-adaptivity and hp-adaptivity algorithms were ultimately deemed unsuitable for arriving at effective weight window settings. However, the error metrics developed for p-adaptive refinement could be employed to improve the robustness of h-adaptive methods. Also, adaptive functional-expansion tallies have been used in demonstrating adaptive importance sampling algorithms and could prove beneficial in automating Monte Carlo calculations for other applications.

Significance

This project was designed to improve predictive capabilities for assessing the radiation hardness of electronics in both nuclear and space environments. These system survivability issues are mainly of interest to Defense

Programs. The automatic acceleration technique is expected to enable the Monte Carlo transport method to be applied to problems that are difficult or impossible to solve with current radiation transport methods.

Refereed Communications

B.C. Franke and R.P. Kensek, “Adaptive Three-Dimensional Monte Carlo Functional-Expansion Tallies,” to be published in *Nuclear Science and Engineering*.

Ferroelectric Opening Switches for Large-Scale Pulsed Power Drivers

105972
Year 3 of 3
Principal Investigator: K. W. Reed

Project Purpose

Studies indicate that high-gain fusion will require petawatt-class pulse forming systems using voltage driven technology (VDT) based on capacitive energy storage and closing switch technology. Using present technology, these systems would require several tens to hundreds of thousands of high-voltage closing switches housed in a open top tank exceeding 100 meters in diameter. Commercial fusion drivers would likely require several times this power, be highly complex, and extremely costly.

Current driven technology (CDT) using magnetic energy storage and opening switches may allow storage and feed inductances to be better matched to the load inductance, significantly reducing the peak operating voltage requirements and improving energy transfer efficiency. CDT can potentially be far more compact than VDT drivers due to lower operating voltages, higher energy densities in the storage inductor, and high coupling efficiency to the load. These advantages have been well articulated by many researchers, however, development of viable opening switch technology has eluded discovery for decades.

This proposal seeks to leverage Sandia's material science and pulsed power expertise to develop, demonstrate, and optimize a solid-state ferroelectric opening switch for large-scale, high-power applications. We will engage Sandia's significant expertise in ferroelectrics to synthesize and optimize materials for opening switches suitable for pulsed power applications. Furthermore, we will develop concepts and techniques for scaling the effective area of the ferromagnetics to allow operation in the multi-megampere (MA) regime.

Summary of Accomplishments

Theory predicts that materials with narrow squared-off P-E (polarization versus electric field) loop will yield optimum opening switch performance. We began by testing lithium niobate and lithium tantalate because their P-E loops closely approximate this ideal. These materials are single crystal or flaw free, promising to exhibit very high electrical strengths. During the course of our work, we discovered that single crystals exhibit two basic limitations. First, they are very brittle and delicate. Our efforts to make good contact with the metalized electrodes often resulted in breakage. Electrodes were developed with a membrane face that could be inflated in order to get a good contact without stress concentrations. With a good contact, we found that we could not get the ferroelectric to conduct displacement current, even if we applied an electric field many times the coercive field. Within a grain, polarizations are in the same direction which is the high energy state. If one dipole flips due to an electric field, it will convert potential energy to kinetic, bounce off the bottom of the potential well and return to its original polarization. Thus, a domain cannot nucleate in the middle of a grain due to low losses and the shape of the potential well there. At a grain edge, the potential well gets distorted and losses increase, allowing domains to nucleate there.

Significance

High-voltage switches are a key, limiting component in all pulsed power systems. New switching technology would support applications across our stockpile stewardship mission, including pulsed power driven z-pinch sources for inertial confinement fusion (ICF) and radiation effects, generation of dynamic materials properties, and pulsed radiography sources. Inductive energy storage and opening switch technology could lead to highly compact pulsed power systems for directed energy applications within the DOD.

Equation of State and Transport Property Measurements of Warm Dense Matter

105975
Year 3 of 3
Principal Investigator: M. D. Knudson

Project Purpose

Location of the liquid-vapor critical point (c.p.) is one of the key features of equation of state models used in simulating high energy density physics and pulsed power experiments. For example, material behavior in the location of the vapor dome is critical in determining how and when coronal plasmas form in expanding wires. Transport properties, such as conductivity and opacity, can vary an order of magnitude depending on whether the state of the material is inside or outside of the vapor dome. Due to the difficulty in experimentally producing states near the vapor dome, for all but a few materials, such as cesium and mercury, the uncertainty in the location of the c.p. is on the order of 100%. These states of interest can be produced on Z through high-velocity shock and release experiments. For example, it is estimated that release adiabats from ~10 Mbar in aluminum would skirt the vapor dome allowing estimates of the c.p. to be made. This is within the reach of Z experiments (flyer plate velocity of ~30 km/s). Recent high-fidelity equation of state (EOS) models and hydrocode simulations suggest that the dynamic two-phase flow behavior observed in initial scoping experiments can be reproduced, providing a link between theory and experiment. Experimental identification of the c.p. in aluminum would represent the first measurement of its kind in a dynamic experiment. Furthermore, once the c.p. has been experimentally determined, it should be possible to probe the electrical conductivity, opacity, reflectivity, etc. of the material near the vapor dome, using a variety of diagnostics. We propose a combined experimental and theoretical investigation with the initial emphasis on aluminum. If successful we would move on to materials which are of greater interest to the pulsed power and Z-pinch community, e.g., tungsten, tantalum, etc.

Summary of Accomplishments

While we do not fully understand the experimental results obtained through this project, we believe that we have experimental evidence that will enable determination of the critical adiabat that skirts the liquid-vapor critical point upon release. Shock and release experiments were performed from initial Hugoniot states ranging between 475 and 1000 GPa. The shocked aluminum was allowed to release into one atmosphere of helium gas, which acted as a tamper. The resulting data suggests a marked change in the qualitative behavior for release from a Hugoniot state of ~700–800 GPa. This coincides nicely with the predictions from quantum molecular dynamics (QMD) simulations. Obviously, more work needs to be done to better understand the experimental results. However, the potential identification of the critical adiabat is intriguing. In addition to the experimental results, the EOS of aluminum has been investigated using QMD methods. In particular, to better model the behavior of expanded aluminum, QMD was used to investigate the effect of finite electronic temperature in the aluminum-aluminum dimer potential. These calculations indicate the appearance of repulsion in the potential as the atoms begin to ionize. A new global aluminum model has been developed a using new approach to EOS modeling in the expanded regime using these temperature dependent pair potentials. An immediate benefit of this approach is that it is much easier to produce liquid-vapor critical points in the EOS that are more in line with the QMD calculations.

Significance

This work is quite relevant to the inertial confinement fusion (ICF) program at Sandia. Success of this project will provide data and insight into material behavior in the warm dense matter (WDM) regime that is directly relevant to the high energy density physics and plasma physics programs. In particular, transport properties in this regime have significant consequences on our ability to accurately simulate the types of experiments performed in support of ICF at Sandia. Furthermore, understanding the WDM regime has also been identified as a key aspect of the Boost initiative.

Low Impedance Z-Pinch Drivers Without Post-Hole Convolute Current Adders

105976
Year 3 of 3
Principal Investigator: D. B. Seidel

Project Purpose

Z-pinch radiation source drivers such as Z and ZR must supply very high currents at moderate (by pulsed power standards) voltage. This in turn requires very low inductance feeds. Presently this is accomplished by adding several higher impedance drivers in parallel using post-hole convolute current adder. Unfortunately, current addition results in localized magnetic nulls that extend from the cathode to the anode. Since the cathode surfaces emit electrons at the space-charge limit, the nulls result in electron losses. These losses are in addition to those due to magnetically insulated flow over most of the transmission lines, and, more importantly, these losses at magnetic nulls are lost over small areas of the anode resulting in electrode damage and conducting gases that cause major current losses and further damage. It is possible to replace the current adder (convolute) with an auto-transformer that will allow driver power to be combined in series with voltage adders, and then to be converted to lower voltage and higher current in the auto-transformer. In contrast to common transformers, this transformer consists of coils whose individual turns are in parallel rather than series. These coils would be similar to the coils found in a number of other pulsed power devices such as some ion diodes and triggered plasma opening switches. There are several potential benefits to using an auto-transformer approach. Such a system would have no magnetic nulls to cause current losses. Moreover, the current multiplication ratio can easily be varied, resulting in a more versatile driver. There are also potential benefits in the way the wire loads would be installed that should increase the shot rate. The critical issues that must be addressed are achieving sufficient coupling between the primary and secondary circuits, managing electron flow, and building a primary coil with adequate mechanical strength.

Summary of Accomplishments

We have made a study of transformer inductance and efficiency in order to understand the important parameters to be considered when designing coils and how they affect the performance of an overall transformer system. Building upon this work, we have developed accurate circuit models for transformer-based systems, allowing the comparison of such a system with Z-like currents and power to the existing convolute system currently fielded on Z. In addition, these tools have provided a basis for the design of a prototype experiment performed on the Tesla accelerator. This also allowed us to quickly evaluate several potential transformer configurations, including auto-transformers, symmetric double auto-transformers, and parallel-fed transformers.

We have developed a two-dimensional coil model and implemented it in the Quicksilver electromagnetic particle-in-cell (PIC) simulation code. This model provides a 2D approximation for this inherently 3D device that has proven to be extremely accurate. This model includes extensive capability to treat the interaction of the coils with charged particles (typically electrons). This model has been applied to the analysis of Z-like transformer-based systems, as well as the prototype transformer experiments performed on Tesla.

Hardware for the Tesla prototype experiment was designed, engineered, fabricated, and then successfully fielded. In addition to the transformer itself, this included components needed to adapt to the Tesla driver, diagnostics, and other miscellaneous items. The coils for the Tesla experiment were intentionally designed to push the mechanical limit, and ultimately proved to perform acceptably. The hardware was designed to allow the independent adjustment of the inter-coil separations in the transformer from 5 to 17.5 mm. Twenty-two high-voltage shots were taken in ten different configurations.

Significance

We have demonstrated that transformers can provide effective current multiplication for pulsed-power drivers and acceptable coupling efficiency can be obtained with reasonable designs. Electron losses can be significant; however, with further effort, this technology could lead to improvements in the performance, cost, and reliability of high-power, low-impedance pulsed drivers for Z-pinches and other low-impedance applications, with potential impact in such areas as high energy density (HED) sciences, inertial confinement fusion, weapon effects, and weapon science.

Expansion of QMD Materials Modeling to Surface Phenomena of Importance to Electrical Breakdown in Pulsed Power Systems

105979
Year 3 of 3
Principal Investigator: T. K. Mattsson

Project Purpose

The ability to quickly understand and deal with issues on ZR, or to virtually design a future ZX accelerator, requires a physics-based capability to simulate all key pulsed power components. Highly important for gas switches and transmission lines are surface phenomena: thermionic emission, photoemission, field emission, and ion-surface dynamics. These are complex processes even at normal conditions, when coupled to the dynamic environment in pulsed power components, the current state of the art of understanding is not at the level of science based predictive modeling. Modeling efforts at the macroscopic level (finite element based hydrodynamic simulations) require detailed information of these processes to yield more reliable results. This project was focused on describing the physics of surfaces of materials of interest in pulsed-power components. We have calculated the temperature dependence of work functions for metals from first principles using density functional theory (DFT) as well as investigated the effect of initial oxidation and alloying. By using the (Green's function–based) GW method, we have gone beyond DFT to calculate work functions for aluminum. The GW work required baselining the GW results for different systems, since GW lacks a description of total energy. Lastly, we investigated the more macroscopic physics of how a surface and bulk material respond to a very high current under a short time, representative for current loads in pulsed-power components, with emphasis on materials modeling. These simulations were made using two hydrodynamic codes, ALEGRA and MACH2, in order to focus on the materials models themselves.

Summary of Accomplishments

The project had three major parts: calculation of work functions with increasing complexity, simulations of surface emission, and finally, the surface-and near-bulk effect of high current density, including a pilot manufacturing of a graded density conductor.

First-principles simulations of work function was a central part of the project from start to finish, initial results were presented at the 2008 March meeting of the American Physical Society in New Orleans, Louisiana, and a manuscript submitted to *Physical Review B* describing how we developed and applied quasiparticle self-consistent GW (QSGW) method to the problem.

A part of the project was devoted to fundamental work in density functional theory (DFT); we benchmarked a new exchange-correlation functional (AM05) for its overall performance for solid state systems and published the results in *Journal of Chemical Physics* (2008). We also compared AM05 to a more recently developed functional, the comparison was published in *Physical Review Letters* (2008).

Electron scattering was calculated fully within DFT, the electron loss function was calculated using dielectric functions from DFT/Kubo-Greenwood. Furthermore, a Monte Carlo scattering code was written to simulate electron transport in the surface region.

In the high-current effects part of the project, the focus of the third year, we performed simulations of the high-current response of different materials, as well as a graded density conductor. We also made a pilot study of manufacturing a graded density high-current conductor. The conductor is a Ta core, graded to pure Cu within skin depth of a 100-ns pulse.

Significance

Advanced modeling of materials is an important part of the science and technology base of the laboratory. The proposed project will extend our current capability of predictive simulations in the pulsed-power area, maintaining the highest scientific standards. With an improved modeling of surface electron emission, we would be capable of theoretically evaluating suggested materials at an early stage.

Understanding Surface Breakdown in Electronegative Gases

105987
Year 3 of 3
Principal Investigator: L. K. Warne

Project Purpose

Previous theoretical work on breakdown in atmospheric nitrogen across a surface indicated that discharges would not be significantly impacted by the surface interactions. Experiments at Texas Tech University (TTU), while appearing to confirm these initial predictions, surprisingly showed that variations in gas species (for example electronegativity) showed marked differences in discharge path (some tracking the surface and some lifting off). Reasons have been postulated for this behavior that involve not only the gas properties but also the insulator properties. The direction the discharge takes in the vicinity of a surface, and what influences this choice, is thus not understood.

Gas switches rely on high density electronegative gases and insulator barriers, which are often weak links in the lifetime of the components. When attempting to diagnose and remedy problems associated with the insulators, a better understanding of what is taking place near the surface would be helpful in aiding experiments and design efforts.

We propose in this project to develop models and understanding for how discharges interact with surfaces in dense electronegative gases. In dense gases, streamer and leader phenomena are the primary breakdown mechanisms. In this project we need to explain how these different regimes of the filamentary breakdown channel are influenced and directed by interactions with the surface. The scope of the project was limited to the fast ionization processes associated with ionization wave propagation (streamers). The goal is to explain the dominant players involved in the interactions from a fundamental point of view. All future pulsed power machines that rely on gas breakdown would benefit from this understanding.

Summary of Accomplishments

Kinetic calculations were performed for particle multiplication rates in an avalanche near an insulating surface. These calculations included, electric field modifications from image charges in the dielectric half space of the insulator gas elastic and inelastic collisions, including molecular excitation, ionization, and electron attachment processes, gas photoabsorption and photoionization processes, electron collisions with surface, surface photoemission, and electric field modifications from surface electric charging. It was found that critical field levels for avalanche growth were not significantly affected by the presence of the uncharged surface. The rate equations derived from these simulations were then used in the ionization wave (streamer) fluid models.

A fluid model was constructed for streamer propagation in gases and on surfaces, which solves the continuity and particle rate equations with the electric field based on both disc and ring models for the gas and strip models for the surface. In addition, radial expansion of the streamer channel was explored with and without surfaces in an effort to make the model less dependent on initial choices of this parameter. Careful examination of the field levels required to maintain streamers (sustaining fields) were carried out with and without the surface in both air and SF_6. The models reproduced known sustaining field levels in air and indicated that sustaining fields in SF_6 are reduced relative to the critical value. Surface interactions did not change these values significantly.

An experimental setup was designed and constructed to allow electrical, photographic, and other diagnostics to be implemented during surface discharges in various gases. Plane-to-plane discharge levels were measured to detect differences in critical field levels with and without a surface. No significant difference in levels was observed, however velocities were affected. Experiments on streamer sustaining fields were conducted with rod-to-plane gaps and were in reasonable agreement with model predictions.

Significance

High-power gas breakdown switches are critical components in the ZR upgrade of the Z machine and are planned to have roles in future larger power drivers. An understanding of the basic physics of these components is critical to improve the reliability of these components at the higher levels contemplated for future machines. Reliability and extended lifetimes of these switches for repetitive applications, such as needed for future energy production, are essential.

Unlike the situation in a vacuum, the effects of insulating surfaces on discharge levels in dense gases has been an area of some controversy. This study, although limited to fast ionization processes, has attempted to quantitatively account for surface effects and relate their properties to discharge levels. As far as we know, this was the first time that coordinated modeling and experimental efforts were applied to surface breakdown in dense gases.

Surface breakdown issues are also important considerations in safety studies of high consequence operations. Follow-on projects in this area will not only continue looking at fast ionization processes but will also examine thermalization phases of the discharge issue in gases and on surfaces. These future projects will include both experimental and theoretical investigations.

Creation of a First Principles Simulation of Weapons Generated Electromagnetic Pulse

107441
Year 3 of 3
Principal Investigator: R. B. Campbell

Project Purpose

There is a significant national security need to simulate weapon generated electromagnetic pulse (WGEMP). Because yield compositions and timescales could potentially change from the norm as a result of new concepts, it is important to be able to predict the properties of the transient field environment. There are two areas of interest that could be pursued with a physics-based simulation of WGEMP: 1) To assess civilian and military asset vulnerabilities, the prediction of transient field threat (particularly peak fields and rise time) as a function of next-generation device characteristics and 2) To analyze device characteristics based on EM intelligence data. Present capability in area 1 relies mostly on semi-empirical models not applicable to new concepts, and in area 2 the capability is nonexistent. The knowledge derived from this work could also provide valuable information to help define the hardening mission of the MESA project to meet new national security threats.

The physical sizes and a wide range of spatial scales in a relevant problem will require innovative numerical algorithms to capture the relevant time and spatial structure in a tractable simulation. We are considering both low-yield surface bursts on either water or land and higher-yield, high-altitude events. The particle in cell code LSP (large scale plasma) has been designed to solve multispatial and multitime scales in other physical problems. Particular emphasis will be placed on the development of an adequate air chemistry database. Validation of the resulting simulation tool will be accomplished with data comparison with various electron beam/x-ray facilities and eventually the Z-Beamlet/Petawatt facility.

The benefits of the proposed R&D will be to contribute to an area (WGEMP) that has had limited scientific study over many years and has very important national security implications.

Summary of Accomplishments

We developed a first cut of a fundamental physics based computational tool to simulate weapons generated electromagnetic pulse (EMP). We applied this capability to high altitude electromagnetic pulse (HEMP) problems. The team studied models appropriate for both a high altitude and surface burst EMP. We developed several new algorithms which treat the thermalization of Compton and cascade electrons in a more consistent fashion than was available previously. We improved upon the air chemistry to more accurately account for kinetic effects. We developed analytic methods to couple the source region (kinetic particle-in-cell [PIC]) with the free space EM solution. We developed an impedance boundary condition for the air/ground interface for use with surface bursts, with the eventual goal to simulate the presence of on ground structures. We developed a new EM propagation algorithm for the source region that has very good parallel efficiency, stability, and is free from dispersion. Finally, we validated the kinetic thermalization model through experimental measurements of electrical response of gas filled cells subjected to ionizing x-rays.

Significance

This project has a unique combination of elements relevant to Sandia missions by addressing threat assessment and asset protection from EMP achieved through the development of advanced computations. The work would add important capability to initiatives around the Laboratories (intelligence, Microsystems and Engineering Sciences Applications [MESA], Microelectronics Development Laboratory [MDL]) as well as enhance the already important EM and radiation hardening programs. We have received funding for follow-on work from internal Sandia customers.

Electromagnetic Launch Science and Technology

117776
Year 2 of 2
Principal Investigator: C. J. Garasi

Project Purpose

Game-changing firepower can be obtained on next-generation all-electric military ships and vehicles by leveraging electromagnetic (EM) technology for projectile launch. EM launch both reduces the threats and danger associated with carrying propellant or explosive ordnance, and develops the necessary long-range firepower to support troops on land and sea (range > 200 nautical miles) at significantly reduced projectile cost. To date, EM launch systems can only be found in the laboratory where significant technical obstacles must be overcome to mature the technology into a tactical system. For example, extreme environments either generated or encountered (e.g., electromagnetic, sliding electrical contact, and aero-thermo-mechanical) that degrade the bore of the launcher or the projectile during transit to target present formidable obstacles. Advances in physical understanding of the extreme environments created are required through material and physics models, high-fidelity simulation, diagnostics, and experimentation to overcome these obstacles. We propose to leverage unique Sandia tools and experiments to attack the S&T challenges, to advance EM launch technology from the laboratory into the hands of the warfighter. Our research plan involves the evolution of state-of-the-art nuclear weapons code technologies beyond their current scope of applicability to begin addressing multiscale issues associated with the extreme environments associated with rail guns and coil guns. The proposed work is high risk due to the complex multiphysics multiscale phenomena that need to be simulated and understood in order to have impact. If successful, new simulation tools to attack the S&T challenges will be produced.

Summary of Accomplishments

We made significant accomplishments in the areas of: 1) materials science, testing, and processing, 2) EM launch modeling and simulation, and 3) analysis, design, and optimization. In the first areas, novel material screening techniques were investigated using thermal spray torches, ion beam exposures, and lessons learned from an intense corrosive environment, and a novel technique for making refractory rail coatings. In area two, the extended finite element method was pursued in the shock-physics code ALEGRA, as well as substantial improvements to couple advanced circuit modeling to the code to handle multiple, timed capacitor bank firings for EM launch. Also, a novel rail damage model was created. In the third area, optimization activities included two-dimensional rail shape, three-dimensional fast solution of magnetic advective-diffusive effect, and lastly, the ability to couple physics-based codes with technology management to make intelligent decisions in regards to power optimization and design.

Significance

This project will provide a modeling and simulation capability that can address critical gaps in present day high-speed electromagnetic weapons system programs. Sandia will benefit from an enhanced ability to model re-entry systems for current stockpile systems and the reliable replacement warhead. Complex interface physics and materials are highly synergistic with our pulsed power and inertial confinement fusion programs.

Measuring High-Pressure Strength on Pulsed Power Machines

117856
Year 2 of 3
Principal Investigator: C. S. Alexander

Project Purpose

The strength of materials at high pressures and strain rates is a critical aspect of modeling material behavior for DOE weapons applications as well as design of internal confinement fusion (ICF) capsules for ignition at the National Ignition Facility (NIF). Strength is defined as the ability of a material to sustain deviatoric (shear) stresses. It has proven extremely difficult to measure material strength under high-pressure dynamic loading because the governing equations for wave propagation provide no information about stresses in directions normal to the direction of wave propagation. Traditional wave profile techniques to measure strength are limited to ~2 Mbar pressures. This project will develop new techniques that extend this limit significantly. Laser techniques have demonstrated that Rayleigh-Taylor (RT) instability growth is governed by strength properties and offer the only existing capability to measure strength above 3 Mbar. However, sample size is limited to a few microns, thus prohibiting observation of real material effects, such as grain size and internal defects. In addition, the interpretation of RT instability data requires the use of computer simulations, which limits the accuracy of the results to that of the models used. This project has identified a novel method of inducing and measuring shear motion (normal to the direction of wave propagation) behind an applied pressure wave, which will allow a direct measure of material strength without relying on computational models. This approach, if successful, will represent a quantum leap forward in our ability to measure strength at high pressure. We are nearly ready to design and field a demonstration experiment, based on our new technique, to measure shear strength at approximately 6 Mbar, twice the current limitation.

Summary of Accomplishments

Thus far in FY 2009, designs have been finalized for the magnetically induced shear (MIS) experimental platform. Testing has begun on the magnetic pulse generator (MPG) system required to field these experiments. Parts for the initial round of experiments were fabricated and assembled. Integration of the MPG and the Veloce accelerator has begun with further testing ongoing.

The VISAR (velocity interferometer system for any reflector) system used to measure both longitudinal and transverse velocities simultaneously was designed and tested using Y-cut quartz as a combined longitudinal and shear wave generator. Based on the test results, several adjustments have been made to optimize performance and give the greatest likelihood of success when conducting MIS experiments. Further testing is ongoing utilizing the final MIS experimental configuration.

Significance

This project will address the need to measure high-pressure strength of plutonium and other relevant materials in support of Campaign 2 where strength measurement is currently the number two priority. In addition, this project will provide data for the development of predictive models in the advanced simulation and computing (ASC) program and inertial confinement fusion (ICF) capsule design work. This will be accomplished while maintaining realistic sample sizes relevant to real-world applications.

Advanced Magnetized HED Physics Modeling

117859
Year 2 of 2
Principal Investigator: H. L. Hanshaw

Project Purpose

Secondary DT neutrons may be detected in Z experiments, but when current flow and a strong magnetic field encloses a deuterium plasma, areal density cannot be evaluated without accounting for magnetized plasma effects. For a 20 MA load current carried at 1 mm, a triton born from DD fusion sees a Larmor radius of near zero in the fuel bulk, but of a fraction of a micron near the current carrying boundary. Significantly more tritons will react while slowing down than in the non-magnetized case, leading to a larger secondary DT yield. Magnetized high energy density (MHED) physics conditions like the above burn product transport example are understood phenomenologically, but not quantitatively. Designing and analyzing experiments efficiently on Z will require quantitative analysis as much as possible. For the above example, the question arises: can areal density be inferred from neutron yields, and what other diagnostic assessments are necessary in combination with the yields? In addition to affecting burn, magnetization may also significantly affect electromagnetic and thermal transport across field lines, but detailed accounting of these effects is not done by existing code models. We will develop a unique capability to quantitatively study secondary neutron yield as a function of geometry, areal density, and magnetic field strength. We will also study the effects of field containment on charged particle and magnetothermal transport, and the subsequent effect on yield. This modeling capability will be used to design more-efficient experiments on Z, and we ultimately hope that this will help defining requirements for establishing HED conditions for ignition.

Summary of Accomplishments

We have researched the theory behind extended magnetized high density (MHD) and magnetized transport effects, relevant to the warm dense matter regime of imploding liners and the dense plasmas of fusion fuel. With this theoretical groundwork, we have designed and implemented many of the numerical models needed for simulating advanced magnetized effects in Z fusion targets. Once the baseline MHD package in Kull is complete, we will begin integrating the advanced physics in priority order to do integrated testing. These priorities are expected to change as we learn more about the models and physics, and as we learn how to incorporate these effects into Z experiment designs. Specific achievements include the following:

Theory work on extended MHD physics and algorithms.

- Partial implementation of an MHD discretization in Kull meeting requirements for addition of extended terms
- Implementation of tensorial magnetic and thermal diffusion in Kull
- Electromagnetic field discretization added to charged particle Monte Carlo transport
- Limited testing of magnetized effects on fusion targets using standalone Monte Carlo simulations of charged particles

Significance

Quantitative modeling of Z experiments, accounting accurately for magnetized plasma effects, will contribute to stockpile stewardship in multiple ways. Increased quantitative understanding of Z physics and diagnostic outputs like secondary yield will enable more efficient design of experiments and improved facility utilization. In addition, building quantitative modeling tools contributes to DOE's Science goals. Multiple publications should result from this work.

Demonstration of Fast Pulsed Neutron Capability for Device and Board Testing

117860
Year 2 of 3
Principal Investigator: V. Harper-Slaboszewicz

Project Purpose

The early time response and recovery of weapon system electronics to intense neutron pulses is a crucial issue for weapons effects. Fast burst reactors have been the facilities of choice to evaluate this response, but SPR (Sandia Pulsed Reactor) III is no longer available and the future availability of the White Sands Fast Burst Reactor is questionable. The best current facility for evaluation of these effects at very early times is LANSCE (Los Alamos Neutron Science Center). It provides 1–2 $\times 10^{12}$ n/cm^2, 1 MeV (Si) equivalent in a 150-ns pulse over ~8 cm^2 at the experiment position. Other neutron test facilities provide long continuous exposures or much lower fluences that do not access the response regime of interest.

Accelerator-based neutron sources consisting of proton and deuteron beams impacting tritium, lithium, or beryllium targets have been used in a variety of applications. However, they have not been coupled with high-power pulsed power drivers to produce large, fast neutron bursts. This project proposes to couple these sources to the Hermes III accelerator to provide a small area (~10 cm^2), high fluence (~2 $\times 10^{14}$ neutrons), fast neutron burst for electronic device and board testing which provides an improvement in capability compared to LANSCE for this application.

The performance of the ion source is key to the success of this project. The required ion efficiency has been observed in earlier experiments, but modern modeling tools have not been applied to this source. Coupled models of the accelerator and the diode have been developed. Initial experiments suggest reasonable agreement between the modeled and observed behavior.

This project will demonstrate the ability to produce useful levels of pulsed neutron fluence to evaluate weapon component reliability in nuclear environments in a non-reactor facility with easy access for diagnostics.

Summary of Accomplishments

Ion diode experiments with improved diagnostics were performed.

Problems with the initial ion diagnostic, a Rogowski coil at the input to a gas cell, were identified and alternate diagnostics, in particular Faraday cups in conjunction with a witness plate, were identified and implemented.

The ion spatial distribution from the ion diode was characterized and found to differ from the anticipated distribution. Instead of a converging, focusing beam, the protons were found to be diverging. This necessitated a change in approach, requiring a smaller ion source with a higher source ion density and a diagnostic/neutron generation region closer to the ion source to obtain the required neutron source density.

The modified diode was fabricated and fielded, with an order of magnitude improvement in measured ion density. Further refinement of this approach is in progress to achieve the ion density required for a useful neutron source. This refinement is based on power flow modeling and additional diagnostics.

The time dependence of the ion energy is a key issue for the performance of this diode. Initial modeling suggested that the ion energy distribution is highly peaked near the peak diode voltage. More-recent experiments have characterized the ion energy distribution, which is considerably broader than suggested by the initial modeling.

Significance

Evaluation of the reliability of components that will be used in weapon and satellite hostile environments is a key element of nuclear weapons stewardship. With the closing of SPR III, there is now a significant gap in the ability to evaluate neutron effects on weapon system electronics. The technology demonstrated in this effort would allow evaluation of the neutron response of new technologies to provide enhanced reliability or capability in nuclear weapon systems.

The accomplishments so far provide a basis for coupled modeling of accelerator and diode performance. In addition, a number of experimental techniques have been applied in the accelerator environment to characterize the ions produced. A different type of ion source, the hydrogen-loaded titanium film with palladium oxidation barrier, has been applied to a high impedance pinch reflex diode for the first time. The tools provide a basis for characterizing the performance of an ion source for neutron production.

Evaluate Radial Wire Arrays for ICF and RES

117862
Year 2 of 3
Principal Investigator: D. Ampleford

Project Purpose

Wire array z-pinches are a powerful x-ray source being evaluated as potential drivers for inertial confinement fusion (ICF). Current pulsed power generators are unable to drive the large (~25 mm diameter) hohlraums associated with cylindrical arrays to ignition temperatures. Pulsed power must develop more compact x-ray sources (to drive laser-scale hohlraums) to create conditions of interest for high energy density physics and weapons science. Likewise, for radiation effects science (RES), there is an ongoing desire to develop new sources which can deliver higher photon energy, with higher yield to be prepared for future demands.

Experiments on MAGPIE (1 MA, 250 ns) suggest that radial wire arrays can provide high x-ray powers in a compact volume. This could be an alternate compact hohlraum driver allowing a factor of 5–7 increase in energy density. Attractive features of a radial wire array configuration are the achievable energy densities, low load inductance and a switch-like operation resulting from a large magnetic field gradient along the wire compatible with longer rise time generators, each significantly reducing the cost of any future generator. Radial wire arrays also provide a natural geometry for two sided illumination of a secondary hohlraum for ICF while maintaining low inductance with a single power feed. Some risks associated with this approach include uncertainty in the scaling of energy density to higher currents and coupling to hohlraums. At the 1-MA level, Al radial wire arrays emit in the multi-keV regime at similar levels to cylindrical wire arrays. On multi-MA generators potentially higher photon energies and/or yields could be achieved with appropriate access for test objects. Additionally, the basic science of magnetically driven jet dynamics has applications to laboratory astrophysics and could serve as a testbed for the validation of radiation-hydro/MHD codes.

Radial wire arrays will be explored at higher peak currents.

Summary of Accomplishments

We designed radial wire array hardware to perform experiments on the 7-MA Saturn generator. Experiments have demonstrated higher power densities with radial wire arrays (> 2 TW/cm^2 on a possible hohlraum wall) than had previously been produced using cylindrical wire arrays on Saturn in its long pulse mode. To assist in the design of these experiments, the Gorgon 3D resistive MHD code was first benchmarked against existing radial wire array data from the 1-MA MAGPIE pulsed-power machine. A detailed transmission line circuit representation of the Saturn generator was then developed so this code could be used to self-consistently model Saturn experiments. Experiments also studied the capability to perform astrophysically relevant experiments on the periodic formation of magnetically driven astrophysically relevant jets.

Tungsten radial array experiments were completed using Saturn short pulse mode, imploding arrays on both 6-mm and 12-mm diameter cathodes. These shots demonstrated significant gains in power densities with the potential to achieve 90 eV hohlraum temperatures compared to 70 eV obtainable from radial arrays imploded in long pulse mode. This was already a significant improvement over the 55 eV temperatures that could be reached using comparable cylindrical wire arrays. These gains resulted from maintaining comparable powers to long-pulse experiments on a 12-mm cathode, while significantly shrinking the source size by use of a 6-mm cathode. Further shots were also performed investigating the effect of switching the anode and cathode to study the impact of electrode effects on the implosion. MHD simulations were further validated against Saturn experiments demonstrating the factors that are likely to be limiting the power produced by these arrays.

Significance

The demonstration of a compact source using radial wire arrays allows the development of hotter compact hohlraums than currently available with pulsed power devices. Such a capability is relevant to strategic needs in nuclear weapons stewardship (may enhance x-ray load yields for weapons physics and effects experiments), energy security (could decrease the cost of future z-pinch driven inertial fusion energy sources), and improves the capacity of existing facilities for world-class scientific research (improving the output to allow access to new regimes in pulsed-power driven experiments).

Scaling of X-Pinch X-Ray Sources from 1 MA to 6 MA

117863
Year 2 of 3
Principal Investigator: D. B. Sinars

Project Purpose

In an exploding-wire z-pinch, a high current is passed through a single wire strung across the electrodes of a pulsed power generator. As the wire explodes and becomes plasma, the increasing self-magnetic field causes the plasma to implode radially and several bright, x-ray emitting micropinches form at random locations along the wire. An x-pinch is produced by using multiple wires mounted so that they cross and touch at one point. Micropinches form reliably only at the cross point and not in the legs. Experiments at Cornell University have demonstrated that Mo x-pinch-produced micropinches at 200 kA are 0.8–1.5 microns in diameter, have temperatures of about 1 keV, and have densities >10% of solid density, making them warm-dense objects of considerable interest. A recent publication[1] modeling those experiments suggested that if 1-micron micropinches continued to form at higher currents, then an 80 GW Mo source at 10 times solid density can be achieved using a 1-MA drive current and a 3.4-TW source at 250-times solid density at 10 MA. Recent tungsten x-pinch experiments at 1 MA measured sources as small as 11 microns, and it remains unknown what source sizes are possible at 6 MA. We propose to, 1) test the scaling of and requirements for x-pinch sources at 6 MA on SATURN; 2) use these experiments to understand and optimize the production of pulsed-power driven micropinches; and 3) utilize these sources as a platform for basic physics studies (e.g., measuring magnetic fields). We will collaborate with university researchers to execute and analyze the experiments. We will also extend the published calculations using integrated high-resolution simulations with our best equation-of-state, conductivity, and opacity models.

Summary of Accomplishments

In FY 2008 we did two shot series on SATURN that determined the optimum mass/length, size, and geometric configuration. The best results were obtained with solid, machined x-pinch loads. Our third shot series (March 2009) followed up on the success of the solid-machined x-pinches by testing different alloy materials to explore the effects of opacity on the production of small x-ray spots and also to offer the potential of making spectroscopic measurements of the plasma parameters. The alloys tested were W72/Cu28, Ni80/Cr20, and Cu55/Ni44/Mn1, all of which contained Cu or Ni. This series was also the first one to test several advanced diagnostics, including an in-chamber pinhole camera to measure the x-ray spot size, an in-chamber time-integrated convex spectrometer to collect survey spectra, and a filtered x-ray streak camera to measure the time duration of >1 keV x-ray bursts produced by the x-pinches. The alloy x-pinches gave comparable or higher x-ray powers as compared to the previous best results. X-ray streak camera data obtained on the final shot of the series showed that multiple x-ray bursts < 500 ps in duration were produced, and the same shot made an x-ray spot size of < 10 micron diameter. Spectrometer data during the series showed that we made Cu and Ni K-shell radiation, so that at some point during the pinching process we are making very hot plasmas (> 3 keV electron temperatures). The fourth series (August 2009) obtained better quality data with the new advanced diagnostics, which is being analyzed. We also successfully fielded the streaked x-ray spectrometer for the first time, which will be the primary diagnostic in FY 2010.

Significance

This work would advance the theoretical and experimental understanding of plasma science and provide the nation's science community access to world-class research facilities. These goals are consistent with those stated in the 2003 DOE Strategic Plan. Through the anticipated collaborations with universities, our anticipated journal publications, and conference presentations, we also hope it will provide opportunities to recruit outstanding graduate students to Sandia. We believe we have sufficient data at this time for at least one prestigious peer-reviewed journal article and more detailed follow-on articles in other journals.

1. Chittenden et al., *Phys. Rev. Lett.* 98, 025003 (2007)

Phase Conjugate Interferometer for Time-Resolved Measurement of Material Morphology

117864
Year 2 of 2
Principal Investigator: S. C. Jones

Project Purpose

Materials subjected to dynamic compression or rapid energy deposition may have inhomogeneous response due to induced phase transformation, chemical reaction, or plastic deformation. In particular, optical inhomogeneities in the first two cases result from nucleation and growth phenomena that occur at rates dependent on the magnitude of the driving stimulus. Observations of these phenomena are most usually made on a point basis, e.g., VISAR (velocity interferometer system for any reflector), or by time-resolved imaging. Most often, the inhomogeneous response of a material or material surface causes light to be scattered, and therefore, imaging techniques are limited by, and essentially record, the loss of light from a beam. This project is intended to provide a new tool for observing and recording two-dimensional, time-resolved information that measures the differential change in the inhomogeneities of a transparent material or opaque material surface. The time scales over which these changes are to be measured are from subnanosecond to some tens of nanoseconds, thus providing highly time-resolved measurements of material morphology occurring as response to extreme environment stimuli. The approach involves the use of real-time optical phase conjugation as a methodology for performing, in essence, time-resolved holographic interferometry, providing interferometrically derived, and therefore, quantitative, two-dimensional imagery of the material response. Should this R&D be successful, Sandia will have a new tool to quantitatively measure material response, in both space and time, to an extreme environmental stimulus. The scale of the structural information should be in the mesoscopic range. The ability to measure the described responses will be of interest and use to several Sandia and DOE programs.

Summary of Accomplishments

The FY 2009 effort was intended to demonstrate the feasibility of using an optical phase conjugate interferometer to changes in material morphology under high dynamic stress conditions. This work has demonstrated that the degenerate four wave mixing (DFWM) technique for optical phase conjugation will be able to provide the necessary temporal and spatial resolution to achieve the intended application: time-resolved, two-dimensional imaging of changes in materials under loading conditions, such as phase transitions and surface deformation.

The interferometric arrangement provides excellent optical images of time-varying phase aberrations. Time interval for detecting changes variable on nanosecond scale was demonstrated at a 5.2 ns interferometer delay.

Phase conjugate material (PCM) that was selected was shown to have proper time response (< 1 ns) required for this project to be successful.

The optimum DFWM pumping configuration (split or retroreflected) was confirmed, but is not a huge determinant of the phase conjugate reflectivity. Therefore, the pumping method that is simplest to implement in a given dynamic experiment should be chosen without concern for minor differences in phase conjugate reflectivity.

The highest project risk, degeneracy-breaking, was shown to be non-problematic to at least a 100 MHz frequency shift. This was considered a risk because of Doppler shifting of probe beam frequency in dynamic experiments relative to the un-shifted pump beam frequency.

Interferometer arrangement was shown to provide excellent measurement of material differential change over a nominal 5 ns time interval.

Significance

Should this R&D be successful, Sandia and DOE will have a new tool to quantitatively measure material response, in both space and time, to extreme environmental stimuli. Measurement scales are in the mesoscopic spatial regime and nanosecond time resolution. Extreme environment stimuli include impact, ionizing- and laser-radiation. Applicable materials include solid opaque objects as well as transparent materials. Objectives include material response model validation.

Physics of Intense, High Energy Radiation Effects

117866
Year 2 of 3
Principal Investigator: H. P. Hjalmarson

Project Purpose

Intense, high energy irradiation of materials is an important activity at Sandia but the information obtained has usually been empirical. In this project, we propose to use physics-based simulations linked to experiments using Sandia and other facilities to explore the phenomena. To be more specific, we will focus on the effects of short pulses of high-dose-rate ionizing radiation on materials such as insulators and semiconductors. The radiation creates high-energy electrons and holes; subsequently, these hot electrons and holes tend to recombine or produce fast transient electrical current. The recombination can create excitons, and these excitons can cause material damage. Furthermore, the localized heating caused by the cooling of the hot carriers will also cause material damage. The expected phenomena will be similar to those encountered in electrical breakdown and laser ablation. The physics will be approached using a blend of continuum and atomistic methods. Continuum methods for such problems will be applied to understand the electrical effects and lattice damage effects at long times after the pulse. These continuum calculations will use information obtained from molecular dynamics (MD) and time-dependent density-functional theory (TDDFT) calculations focused on transient materials changes during the cooling process. These calculations will be applied to high-dose-rate simulations of radiation-induced conductivity (RIC) in silicon dioxide and other materials, and later to radiation-induced discharge of capacitors and RIC in foam insulators.

Summary of Accomplishments

This project has become focused on the effects of transient, high-dose-rate ionizing radiation on the dielectric function of a material. This conceptual focus was developed in the second year to unify the continuum and atomistic calculations, and it also provides linkage to RIC experiments.

A fundamental radiation effect is the radiation-induced conductivity (RIC) caused by the radiation-created electrons and holes in the insulating material.

These calculations have been applied to a prototypical structure, a simple metal-insulator-metal structure. The good agreement of the calculations with data for a vitreous silica sample lends strong support to the assumed role of defects.

In general, the transient radiation applied to the prototypical structure produces a transient current that generates an electromagnetic pulse (EMP). The combined effect caused by the initial current and the response current called system generated EMP (SGEMP). These continuum calculations have been used to compute the SGEMP response from the prototypical structure. These calculations reveal that electrons, holes and sample defects are all necessary to understand the physics of SGEMP.

A series of molecular dynamics (MD) calculations have focused on transient radiation effects. These results have been obtained by using two temperature modeling (TTM) capability that has been added to the MD code LAMMPS. This TTM capability was used in a series of Lennard-Jones calculations where the various physical parameters were systematically varied to demonstrate their effect on the structure and behavior in the bulk and at interfaces. The results showed how hot electrons can cause damage near interfaces.

Development of a capability for time-dependent density-functional theory (TDDFT) calculations began at the end of the first year of this project. This capability is being implemented in an existing DFT code, Quest. These calculations will produce information about the dielectric function by computing the transient optical absorption.

Significance

Sandia has large experimental facilities that expose materials to high energy radiation for nuclear weapons programs. However, there is little predictive simulation capability focused on understanding the known effects or discovering new effects. Success with this project may enable new national security capabilities at Sandia.

Refereed Communications

C.L. Phillips and P.S. Crozie, “An Energy-Conserving Two-Temperature Model of Radiation Damage in Single-Component and Binary Lennard-Jones Crystals,” *Journal of Chemical Physics*, vol. 131, p. 074701, 2009.

R.L. Pease, P. Adell, B. Rax, X.J. Chen, H. Barnaby, K. Holbert, and H.P. Hjalmarson, “The Effects of Hydrogen on the Enhanced Low Dose Rate Sensitivity (ELDRS) of Bipolar Linear Circuits,” *IEEE Transactions on Nuclear Science*, vol. 55, pp. 3169-3173, 2008.

H.P. Hjalmarson, R.L. Pease, and R.A.B. Devine, “Calculations of Radiation Dose-Rate Sensitivity of Bipolar Transistors,” *IEEE Transactions on Nuclear Science*, vol. 55, pp. 3009-3115, 2008.

R.A.B. Devine, H.P. Hjalmarson, H.N. Alshareef, and M. Quevedo-Lopez, “Negative Bias Temperature Instability and Relaxation in HfSiON Gate Stack Field Effect Devices,” *Applied Physics Letters*, vol. 92, p. 153512, 2008.

Advanced Tactical HPM System via NLTL and LWA

130802
Year 1 of 3
Principal Investigator: J. J. Borchardt

Project Purpose

The DOD has urgent requirements for tactical high power microwave (HPM) systems that disrupt or damage electronic systems in operational scenarios. Current HPM systems suffer from the bulk and weight of source ancillary systems and bulky antennas with extremely large visual and aerodynamic cross sections.

The purpose of this project is to develop and integrate two novel HPM components: the nonlinear transmission line (NLTL) radiofrequency (RF) source and the leaky wave antenna (LWA). NLTL is a novel RF source that converts electrical pulses directly into tunable, narrow-band, high repetition-rate RF pulses. No relativistic electron beam, cathode, vacuum, magnetic field, or x-ray shielding is required. LWAs simultaneously offer high gain, low profile, and electronic steering, thereby making any tactical HPM platform faster, more maneuverable, and more survivable.

The anticipated benefit of this research is increased tactical utility of future HPM weapon systems by (1) significant increase in power on target per unit system size/weight; and (2) significant reduction in HPM antenna platform integration constraints. This work is high risk because significant basic research on scaling NLTL and LWA powers together to the gigawatt regime remains undone (e.g., modeling and materials research). While the rewards of success of this research are great, the technological barriers are commensurate. As such, LDRD funding is appropriate for the high level of risk associated with this project.

Summary of Accomplishments

The FY 2009 primary focus was to implement 1D-periodic structures in the Sandia RF code, Eiger to support design of leaky wave structures, and this has had considerable success. Software for the evaluation of the layered media dyadic Green's function for a 1D array of point sources has been implemented for a complex periodic wave number. This software accommodates currents that are both transverse and normal to the layered media interfaces. This has been carried out in a manner that lets the user specify the choice of branch cuts and integration paths needed to capture the bound surface wave modes, the improper leaky wave modes corresponding to bound mode leakage, and space wave leakage. The Ewald methods used to accelerate the convergence of the Green's functions have also been generalized to allow for complex periodic wave numbers. A secant-based root finding algorithm is used to search the complex plane to find the complex propagation constants associated with each of these modes. Our test cases illustrate that speedup (based on both singularity extraction and interpolation of our 1D- periodic layered media dyadic Green's function) proposed in next year's work is essential for design and simulation of periodic leaky wave antennas. We are also investigating an efficient balanced parallel method for computing the impedance matrices.

For FY 2009 NLTL development, we developed a code to predict performance of magnetic NLTLs. This code agrees well with results published in the open literature, and we have used it to predict the performance of our first magnetic NLTL prototype device. This was a low-power and low-frequency device, however, it proved useful for its ease of construction and testing. Continuing FY 2010 work will scale our magnetic NLTL device to higher frequencies and higher powers and explore dielectric NLTL technologies.

Significance

DOD needs for non-lethal/counter-materiel weapons to enhance US capability in conventional and irregular warfare are well established. The 2006 Quadrennial Defense Review identifies non-lethal technologies as a needed capability to combat both terrorism and WMD threats.

The FY 2009 leaky wave software development effort has resulted in a unique and world-class capability for analyzing leaky wave structures. In particular, the Sandia RF code Eiger can now calculate leaky wave dispersion relations for nonplanar structures that include both metal and dielectric elements. This capability is of interest to the general S&T community. With regard to Sandia's national security mission, this capability is a unique design tool with applications not only in the field of high-power microwaves, but for other low-profile/conformal antenna applications as well, including communications and radars. The NLTL effort, while still maturing, has applications in high-power/compact radar pulse generation in addition to the intended application of high-power microwave pulse generation.

Confinement of High-Temperature Laser-Produced Deuterium Plasmas Using Pulsed Magnetic Fields

130804
Year 1 of 3
Principal Investigator: K. W. Struve

Project Purpose

The purpose of this project is to produce a high-density (10^{19}/cm^3) deuterium plasma that generates a large fusion neutron flux (10^9/pulse) and to enhance that flux by 10^3 with a strong (100–200 T) externally applied magnetic field. The neutrons have application for materials studies and for dense plasma diagnostics, and measurement of plasma diffusion across the magnetic field provides critical information on high-density fusion-plasma transport properties. Recent experiments have shown that interactions of intense ultra-fast lasers with targets of small atomic clusters with hundreds to thousands of atoms can produce very high ion temperature plasmas. This phenomenon has been exploited to produce DD fusion neutrons in a gas of exploding deuterium clusters. Because ion temperatures exceeding 10 keV are achievable, it is possible to produce high fusion yields even with laser pulses of a few joules to a few hundred joules. The fusion yield in these experiments is limited by the fast disassembly time (< 100 ps) of the small, hot laser-produced deuterium plasma. Enhancement of fusion neutron yield might be achieved if plasma confinement could be improved with an external magnetic field. At the densities of these plasmas (10^{19}/cm^3), magnetic fields approaching 100 T are needed to achieve magnetic confinement. The magnetic field will be produced in a magnetic mirror configuration with small coils (5 to 15 mm diameter) driven by a 120 kJ capacitor-bank pulser with currents up to 2 MA. Collaborators at the University of Texas, who have experience with cluster plasma formation and experiments, will provide expertise for the laser-plasma experiments and theory.

Summary of Accomplishments

The first year goals of the project were to design, build, and test a driver, and produce magnetic fields up to 50 T in air. Although we have made considerable progress and are building hardware, we will not complete the 50 T test until early in the second year.

Major changes were made to the original design concept. Originally we planned for a bank of eight parallel 100-kV capacitors (120 kJ) switched by one or two rail-gap switches, as done previously in a similar device at the Humboldt University in Berlin. But for safety reasons, we switched approaches. In the parallel capacitor bank approach an internal short in one capacitor could cause all energy to dissipate locally and cause an explosion. We therefore switched to the approach of the Single-Turn Facility at the National High Magnetic Field Laboratory at Los Alamos National Laboratory (LANL), where each capacitor is independently switched, and output of each capacitor is carried by multiple coaxial cables to a parallel-plate, dielectrically insulated transmission line that connects to the magnetic field coil. Although that machine produces fields up to 300 T, it is not portable (i.e., cannot be placed in front of a laser), and has no provision for driving coils in a vacuum chamber.

A major breakthrough in the design, after considering both strip line and multiple-cable vacuum feed through options, was to focus on a Z-Machine-like vacuum insulator and vacuum chamber configuration. This design uses a small diameter (approximately 1 m) conical magnetically insulated transmission line (MITL) to drive a single-turn coil. Eight or ten capacitor and switch units connected by multiple coaxial cables drive the MITL. A 60-cm diameter prototype is now being built that is driven by two capacitors to produce up to 500 kA and magnetic fields up to 50 T in air or vacuum.

Significance

As part of this project, new experimental techniques will be developed to measure the properties of fusion-relevant plasmas in the presence of strong magnetic fields. These new experimental techniques may lead to a detailed understanding of how strong magnetic fields affect the fundamental transport properties of high-energy-density plasmas. This is relevant to advancing pulsed-power magnetized-target-fusion concepts for inertial confinement fusion.

High-Efficiency High-Energy K-Alpha Source for the Critically Required Maximum Illumination of X-Ray Imaging Optics on Z Using Z-Petawatt-Driven Laser-Breakout-Afterburner-Accelerated Ultra-Relativistic Electrons

130805
Year 1 of 3
Principal Investigator: G. R. Bennett

Project Purpose

Upon its completion, the Z-Petawatt laser (ZPW) will provide a high-energy, ultrashort-duration x-ray source in order to illuminate an x-ray optic that is imaging a Z-accelerator-driven experiment. Crucial to the highest possible success of outstanding x-ray imaging performance is the attainment of significantly higher conversion efficiencies epsilon of laser light into K-alpha-1 x-rays (say, 25 keV) than is presently possible with conventional direct-flat-foil irradiation. We believe that we may have conceived of, or discovered, a short-pulse laser-driven, two-stage K-alpha target concept that may significantly enhance epsilon on ZPW, and any other similar-class short-pulse laser. Through experimentation, guided by computational physics and theory, we aim to demonstrate, or not, the possible significant advantage of this two-stage break-out-afterburner (TS-BOA) x-ray source. Experiments are presently being performed on the ZPW Testbed laser system (ZPW-T) in its present state, but a so-called double-plasma-mirror / polarization-rotator system (DPM/PR) is being added in order to sufficiently reduce the laser pre-pulse and turn linearly polarized light into circular. The former will help keep the first stage of the TS-BOA target intact, as absolutely required, prior the main ZPW-T pulse. The DPM/PR system will not enhance the ZPW-T energy or power. A significantly brighter x-ray source (say, 25 keV) is only one of four key requirements for optimum x-ray imaging on facilities such as Z and the National Ignition Facility (NIF). For instance, one also requires (a) a high spatial-resolution imaging optic (b) a multi-megapixel-digital x-ray camera; and (c) advanced image processing techniques. Items (a) and (b) are already being addressed at Sandia, and item (c) will involve acquiring existing image processing codes from the National Aeronautics and Space Administration (NASA). Developing a successful TS-BOA x-ray source will be very demanding and risky, but (if successful) a huge advantage for Z science.

Summary of Accomplishments

During the first year of this project, the key technical accomplishments and results are as follows:

1. Acquired, installed, modified, and used the LSP particle-in-cell code on massively-parallel systems (Red Storm and Unity) to simulate laser-driven radiation production, for both the direct-flat-foil irradiation and BOA-driven (break-out-afterburner) cases.
2. Preliminary hydrodynamics simulations (Hydra code) indicate that a $< 4 \times 10^{12}$ W/cm^2 irradiance level will keep nm-sized targets from melting and significantly expanding (>100%) on the 10s of ps timescale, therefore given a goal of 10^{21} W/cm^2 irradiance, a contrast of $< 4 \times 10^{-9}$ is required. As such, the acquisition of a double-plasma-mirror (PM) system is essential.
3. BOA simulations successfully benchmarked to original results published by Los Alamos National Laboratory. Preliminary simulations of laser-driven BOA relativistic ion beam and electron cloud impact on high-energy K-alpha-creating targets successfully create time-dependent K-alpha signals. The goal is to devise an efficient high-energy K-alpha source (of a size to be determined) by exploiting favorable particle beam energy deposition physics as compared to direct-flat-foil laser irradiation.

4. Acquired and modified a suitable electron spectrometer.
5. In situ-like plasma mirrors to reduce the ZPW-T contrast (ZPW-testbed, the sub-PW precursor to ZPW), have undergone some initial testing.
6. The optical design of a sophisticated, expensive DPM system (item 2) is complete, and part of the hardware has been delivered. In addition to sufficiently reducing the ZPW-T pre-pulse, this system will also turn linearly polarized light to circular; see item 8.
7. High-quality 35-54 nm thin carbon foils have been acquired and ZPW-T experiments are underway.
8. A detailed purely analytical 1D model of the relativistic pondermotive longitudinal electric field is under development. Notably, and cautiously, there may be a further epsilon enhancement with circularly polarized light compared to linear.
9. A calibrated x-ray detector, a single-photon counting charged coupled device (CCD), is being developed for ZPW-T.

Significance

Although this project is motivated towards the creation, development, demonstration, and understanding of a possibly very bright 25.2713-keV (Sn K-alpha-1 transition) x-ray source, it is noted that if the concept is successful at this energy, then it should also be applicable to other high-energy K-alpha-1 lines too. While the project is indeed motivated by the desire to maximize the quality of Z science using ZPW, it is clear that the x-ray source, if successful, could benefit other inertial confinement fusion (ICF) facilities too.

Modeling Ramp Compression Experiments Using Large-Scale Molecular Dynamics Simulation

130807
Year 1 of 3
Principal Investigator: A. P. Thompson

Project Purpose

Sandia leads the world in characterizing materials in off-Hugoniot regions of phase space using experimental ramp wave loading. However, leadership in dynamic material response also requires state-of-the-art theory and modeling. Molecular dynamics simulation (MD) is an invaluable tool for studying problems sensitive to atom-scale physics such as structural transitions, nonequilibrium dynamics, and elastic-plastic deformation. There are, however, significant difficulties in utilizing MD for extreme environments. First, current atomic potentials are based on ambient material properties and are inadequate for multi-megabar and high-temperature regimes. Second, ramp loading on Z, shock-induced transitions, and melting occur over time scales too long to be simulated with today's methods, which are systematically limited to timescales of 0.1–1 nanoseconds. By generalizing recent innovative methods developed for shock loading, we propose to extend MD timescales by three orders of magnitude or more, enabling us to model ramp compression and other longer timescale phenomena. Further, we will develop new interatomic potentials specifically for extreme environments. Our primary application will be to recent flyer-plate experiments on Z that have shown a gradual drop in wave speed near melt in beryllium. This response is not captured by continuum models. A second application will be to shock melting experiments in silicon being conducted at the University of Texas. Finally, we will address strength and phase transformation behavior under ramp loading. The techniques we develop will allow us to contribute significantly to the understanding of shock and quasi-isentropic physics relevant to weapons and inertial-confinement fusion applications, as well as to substantially expand understanding of several current critical areas of material behavior.

Summary of Accomplishments

Below, we describe accomplishments in four areas.

- Beryllium potential: Two existing modified embedded atom method (MEAM) potentials for beryllium were implemented in LAMMPS, Sandia's molecular dynamics simulation package. Both potentials were found to be inadequate, even at ambient conditions. Working with Mike Baskes, inventor of MEAM, we have developed an improved potential that reproduces observed low pressure crystal properties, including elastic constants, pressure-volume 300 K isotherm, and melting point.
- Shock MD methods: The Hugoniostat and continuous Hugoniot methods have been implemented in LAMMPS. These methods have been used to simulate shock-loading conditions in germanium and polymer materials. A collaboration with the experimental group at the University of Texas has been initiated to provide validation data.
- Ramp MD methods: The direct method for simulating ramp-loading conditions has been implemented in LAMMPS. This method has been used to confirm a scaling relationship for isentropic-loading conditions that may allow us to extrapolate fast ramps to much longer rise times.
- Extraction of continuum information: A module has been created in LAMMPS for calculating spatially and temporally varying fields of continuum mechanics quantities including density, temperature and stress. This module has been used to provide on-the-fly continuum properties in shock-loading simulations of aluminum.

Significance

The techniques we develop will allow us to contribute significantly to the understanding of very high pressure material response to shock waves, rarefaction waves, and quasi-isentropic loading behavior relevant to weapons and inertial confinement fusion (ICF) applications. Using these techniques to model dynamic response of beryllium is particularly relevant to the Campaign 2 strategic goals.

Refereed Communications

J.M.D. Lane and A.P. Thompson, "Molecular Dynamics Simulation of Shock-Induced Phase Transition in Germanium," to be published in the American Physical Society, Shock Compression in Condensed Matter (APS SCCM) Conference Proceedings (2009).

A.P. Thompson, J.M.D. Lane, M.P. Desjarlais, and M.I. Baskes, "Molecular Dynamics Simulation of Dynamic Response of Beryllium," to be published in the APS SCCM Conference Proceedings (2009).

New Density Functional Theory Approaches for Enabling Prediction of Chemical and Physical Properties of Heavy Elements

130808
Year 1 of 3
Principal Investigator: A. E. Mattsson

Project Purpose

Improving plutonium EOS (equation of state) and strength models through is a high NNSA priority. Generating high quality EOS and strength data, primarily through Z experiments, is a key aspect of Sandia's dynamic materials program. We propose improving our ability to theoretically predict plutonium properties.

The microscopic behavior of materials is important for the fundamental understanding of their macroscopic properties. Improving our ability to computationally investigate chemical and physical properties of actinide/lanthanide (f-electron) materials serves the dual purpose of advancing our knowledge and provide insights useful for other, present and future, mission areas, for example providing an enhanced science base for technologies needed for nuclear fuels and fusion reactors.

Density functional theory (DFT) is the preferred computational method for exploring material properties and Sandia scientists are at the forefront of DFT-based EOS construction. However, present DFT techniques are not adequate for f-electron materials. We propose to remedy the two major deficiencies preventing DFT calculations from providing accurate properties of actinides/lanthanides: Inaccurate functionals, and inappropriate relativistic treatment.

Sandia has unique opportunities to develop differentiating computational tools for f-electron materials. The RSPt code from Los Alamos National Laboratory (LANL), already used at Sandia, is specifically designed to handle f-electron systems. However, relativistic effects need to be taken into account non-perturbatively in f-electron systems. We will investigate and add this important physics to RSPt. Available functionals are not accurate enough to capture the complex interactions in f-electron systems. We will develop a new functional appropriate for f-electron systems using Mattsson's promising subsystem-functional scheme.

Solving those fundamental problems will enable quantitative prediction of the behavior of actinide and lanthanide materials under normal and extreme conditions, for the benefit of the entire NW complex.

Summary of Accomplishments

The code development has been contracted to Dr. Andrew Pineda, University of New Mexico (UNM), who has previously worked on RSPt. A theoretically exact Kohn-Sham formulation of the Dirac equation exists and the 4-current plays the role of the density in non-relativistic DFT. However, no 4-current exchange-correlation functionals exist. To allow use of existing functionals we have chosen an approximate formulation in terms of spin-densities. Spin-independent systems are still treated exactly. We will investigate how this approximation can influence our results and prepare the code for possible future inclusion of functionals based on the 4-current. Contrary to other schemes for functional development, the subsystem functional scheme is well suited for such an endeavor. We are also including a thorough documentation effort in order to facilitate future improvements.

For the functional development part, we identified that transition metal oxides, in particular CuO, can be used as good test cases for a postdoctoral research associate. We will perform testing on other systems. A contract is set up with Dr. Cyrus Umrigar, Cornell University, to perform quantum Monte Carlo simulations to extract needed exchange-correlation energies for model systems, for example the fully spin-polarized planar surfaces. These calculations provide additional value in that results from intermediate steps can be used to construct a "confinement-error correction-scheme" for post-processing similar to the successful "surface-intrinsic-error correction" we developed before AM05 (a total of 6 highly cited articles resulted from that work). Such a tool will be valuable for understanding and correcting results with existing functional while we develop a new functional.

An extension of AM05 into a spin density functional has been completed.

Significance

Improving plutonium EOS and strength models is a high NNSA priority. Improving DFT's ability to theoretically predict plutonium properties will broaden the scope of Sandia contributions. Improved ability to computationally investigate chemical and physical properties of actinides and lanthanides will also provide an enhanced science base for technologies needed for, e.g., nuclear fuels and fusion reactors.

Refereed Communications

A.E. Mattsson, and R. Armiento, "Implementing and Testing the AM05 Spin Density Functional," *Physical Review B*, vol. 79, p. 155101, 2009.

Study of Radiative Blast Waves Generated on the Z-Beamlet Laser

130809
Year 1 of 3
Principal Investigator: A. Edens

Project Purpose

This work is motivated by a desire to probe various hydrodynamic theories and simulations forwarded in the astrophysical literature that predict the growth of instabilities on shock fronts in strongly radiating blast waves. These instabilities are thought to give rise to much of the spectacular structure observed around supernovae remnants and may play an important role in star formation. We propose a collaborative study with the University of Texas to study these instabilities, particularly the Vishniac instability.

In particular, there are three aspects of these blast wave instabilities that we may be able to measure for the first time. The first observation we hope to make is an unambiguous measurement of the growth rate of the Vishniac instability. We have seen evidence of growth in previous experiments, but the data has been clouded by small sample sizes and difficulties in diagnosing the blast wave conditions. Use of a high-speed charge coupled device (CCD) camera and streaked spectroscopic diagnostic will allow us to overcome these difficulties. In addition, the spectroscopic diagnostic will give us a direct indication of the blast wave's properties at the shock front, a resource that has not previously been available.

Finally, the astrophysical theories predict that the instability should cause an oscillating perturbation on the blast wave surface, but this oscillation has never been observed experimentally. Previous data taken on the Z-Beamlet laser (ZBL) suggests that we can reach conditions necessary to observe a perturbation oscillation using the new high-speed CCD camera.

All of this work leverages the high energy capability of the Z-Beamlet laser pulses. The >1 kJ laser pulse energy achievable with this system can only be reached by a few laser systems and is necessary to ensure the long lifetime blast waves necessary for this work.

Summary of Accomplishments

Significant progress has been made on the laser modifications necessary for multiframe imaging. These modifications have been designed are in the progress of being implemented. In addition, candidates for the spectral detector have been located, and work to get them ready for use has begun. These new capabilities will be available in time for the second shot run of the project, which may end up being delayed due to a construction project in the ZBL facility.

The first shot run for the project occurred in May 2009. During this run we successfully re-implemented the experimental setup used in prior work. A number of images of blast waves in mixed gases were recorded. The probe laser used in these experiments was fired for the first time following its change of buildings and operators, and several obstacles associated with this move were overcome.

Significance

This project will create well-diagnosed radiative hydrodynamic systems that can be used to benchmark the radiation hydrodynamics capabilities of various codes used in our NNSA stockpile stewardship work. The systematic variation of both the physical and radiative aspects of the experiments provide a particularly robust and varied set of problems that should prove useful for verification and validation efforts.

Characterization of Deuterium Ion Beam Operation on RHEPP-1 for Future Neutron Generation Applications

139463
Year 1 of 1
Principal Investigator: T. J. Renk

Project Purpose

There has been recent interest in using ion beam-generated neutrons for various applications, including detection of special nuclear material (SNM) at ports of entry, and as an alternative to fission reactors for manufacture of radioisotopes. In the first case, the target material irradiated by the ion beam can be ablated or otherwise dispersed. In the second, the target material is also the transmuted end material, so it must be conserved. In both kinds of applications, there are a host of issues for matching the pulsed ion beam source to the final product: 1) determination of relevant reactions that generate neutrons or transmuted material; 2) characterizing beam operation of a desired ion species to induce the reaction(s) (beam purity, energy current density, etc.); and 3) characterizing beam interaction with target material. Many promising reactions involve deuterium ions as the source ion. It has been difficult in the past to generate deuterium beams with high purity to investigate such reactions. The Repetitive High Energy Pulsed Power - 1 (RHEPP-1) facility at Sandia holds promise for generation of pure deuterium beams, once deuterium gas is procured and formed into a beam. Unlike more common proton beams, deuterium reactions have lower thresholds, and so can be explored at the 200–800 keV level generated by RHEPP-1. For instance, D-T yields peak at 100 keV, D-D yields are lower but increasing in this interval, and D-lithium reactions are also accessible. We propose to explore the level of useful neutrons that can be generated with < 1 MeV deuterium, using the same diagnostics as used on the current Hermes LDRD project (117860), but with much better beam characterization possible on RHEPP-1.

Summary of Accomplishments

We addressed three operational questions that determine if RHEPP-1 can be routinely used to generate neutron pulses: 1) can deuterium ion beams be efficiently generated, 2) is the neutron yield high enough to be measured with our diagnostic tools, and 3) can we avoid making long-lived activation that could compromise RHEPP operational status by restricting access to the facility? We first determined from time-of-flight (TOF) measurements that, as we expected, injection of deuterium gas resulted in the formation of a pure deuterium beam, the first such pure intense deuteron beam ever produced. Then, with the use of neutron activation “peppershakers” and Be detector also used in the Hermes LDRD Project 117860, we measured copious amounts of neutrons, well above any detection threshold. The local deuteron fluence measured by the peppershakers matched the fluences seen on Faraday cup current monitors located in proximity to the peppershakers, leading to internally consistent beam current measurements. The Be detector indicated up to 3×10^{10} neutrons/pulse into 4pi when CD2 target material was intercepted by the deuteron beam. This compares to ~ 5×10^{9} neutron fluence predicted prior to our measurements. This is a very interesting level of neutron generation for future applications. Furthermore, all of the intense neutron activity seen was short-lived, so that within 2 hours of beam experiment termination, the experiment area of RHEPP was safe to enter. Since RHEPP uses an advanced MAP ion diode that does not need renewing every shot, we were able to form an indefinite number of beam shots before necessary radiological hold times were required, an invaluable experimental aid in accumulating neutron data rapidly.

Significance

This project addresses Theme 2 (Nuclear Security) and Theme 3 (Scientific Discovery and Innovation) of the 2006 DOE Strategic Plan. It will contribute to the development of a neutron-based screening tool for use at Ports of Entry, aiding in reducing the possibility of adversaries’ smuggling of nuclear materials into the US. This will also be of aid to the Department of Homeland Security mission. Future scaling to higher voltages for medical isotope production addresses a DOE Office of Science mission.

Transmutation Claims

140639
Year 1 of 1
Principal Investigator: C. D. Mowry

Project Purpose

The Ukrainian group under Dr. S. V. Adamenko at the Proton 21 Electrodynamics Laboratory claims to have demonstrated a method to use the focused shock wave from a converging intense electron beam to transmute elements-- including cobalt-60 into nonradioactive elements. Their apparatus produced less than 0.6 KJ of electrons at <0.5 MeV kinetic energy in 30 ns. Their explanation of a high pressure electron-nuclear ensemble producing transmutations is not convincing; however, the yields (50 miligrams per GJ), morphology (clumps of transmuted mass), and the resulting isotopes (both increasing and decreasing atomic number and atomic mass) are difficult to attribute to more conventional physical processes such as neutron production from deuterium accelerated in the space charge of the electron beam. The sophistication (comparable to Sandia) and cost (millions of dollars of investment) of their analytical tools, the > 50 FTE size of their staff on the project, the greater than five-year duration of their effort, the independent verification of their material analyses (multiple locations), and their recent efforts to commercialize the technique indicate that this may be more than another cold-fusion-like claim. The purpose of this project is to discover whether our analytical tools can detect unusual isotopes or elements in a 30-year-old Sandia target irradiated with an intense electron beam (~30 KJ of ~1.8 MeV electrons in 40 ns) compared to the unexposed control surface. Sandia has many of the same techniques and equivalent instrumentation as those published by the Ukrainian group. Additionally, our purpose is to determine if Sandia has the ability to detect any evidence of transmutation should a sample from the Ukrainian group become available and to demonstrate feasibility of our diagnosing targets if we use the Sphinx accelerator to duplicate their experimental configuration.

Summary of Accomplishments

We discovered several elemental composition differences between the irradiated front surface and the control back surface of the Sandia target, both in surface and bulk composition. These differences were detected by multiple techniques including surface elemental mapping by scanning electron microscopy (SEM) and inductively coupled plasma mass spectrometry. Unfortunately most of these differences could be explained by the presence in the original test of a brass (of unknown composition) component that became ablated and deposited onto the aluminum. The uncertainty presented by the brass prevented attribution of the remaining differences. The isotope ratios of these additional elements, however, matched natural abundance within instrumental uncertainty. The results in summary therefore did not detect any potential transmutation products in the Sandia sample. The measurements and lessons learned demonstrate adequate capabilities and procedures to direct future tests and provide high-reliability measurements following those tests. We demonstrated the benefits of having experts in multiple fields (chemistry, metallurgy, physics) involved in data interpretation, and the benefits of a serial analysis plan which saved time and money. Operator expertise prevented potential instances of data misinterpretation (such as the knowledge of measurement bias), and the use of complementary techniques prevented knowledge gaps that might be misleading. These factors all provide a framework that is described in our documented analysis plan that provides a reference for any future attempts at validating the Ukraine work.

Significance

While Ukraine-like transmutation was not detected in the Sandia sample, this result neither validates nor invalidates their work, because there were differences in the starting material and experimental conditions.

Validation of Ukraine results thus remains of interest. If the Ukrainian work can be validated and developed into a large-scale process, the transmutation of radioactive elements into nonradioactive ones at an energy investment of only J/gram could help DOE dispose of high-level waste. It could also potentially mitigate the long-term storage of nuclear waste from weapon processing and commercial power generation, thus having a significant positive impact on DOE and civilian needs.

The results demonstrate Sandia capabilities and provide a level of credibility that may be used for and leveraged into a collaboration with the Ukraine group for future testing and/or independent analysis of their samples.

DEFENSE SYSTEMS AND ASSESSMENTS INVESTMENT AREA

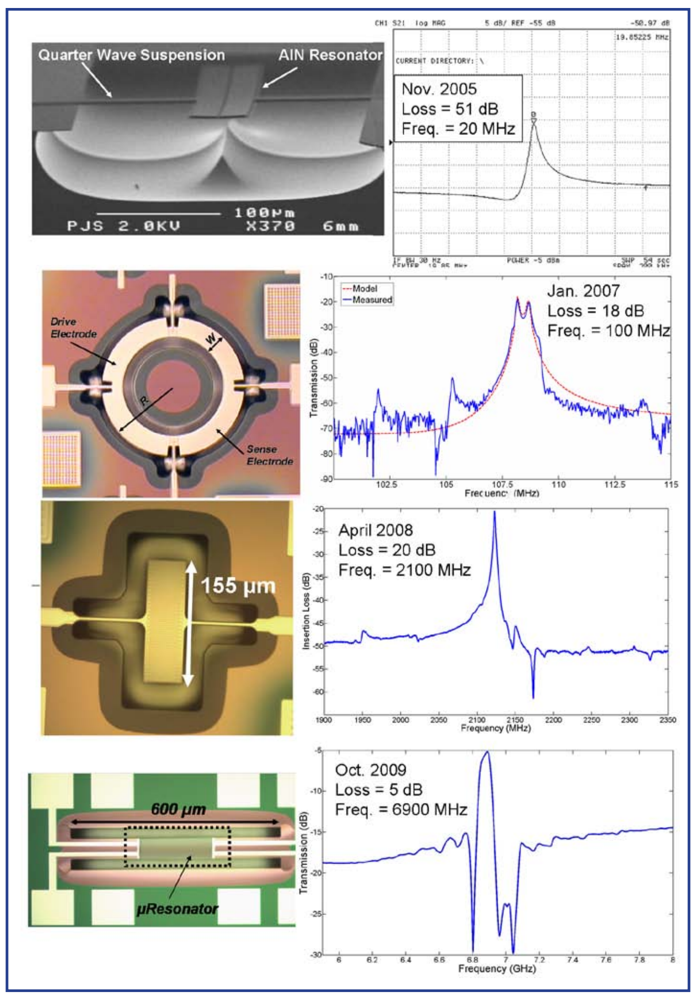
This investment area (IA) funds both fundamental and applied research into science and technology that is or can be rendered applicable to national defense — from software to assist the human intelligence analyst by filtering and more-coherently organizing intelligence streams, to virtual training scenarios for analysts and warfighters, to a variety of improved detection-science and -technology solutions for chemical and biological threats to populations, and even to improved robotic agents to mitigate risks to soldiers and civilians in dangerous scenarios. Through these and other initiatives, projects in this IA contribute to national defense and homeland security — and therefore help diminish the global threat of terrorism.

A Zero Power, Motion Sensitive MEMS Wake-Up Circuit

Project 130698

Most laptop computers will automatically go into sleep mode when their cover is closed, and automatically awaken when reopened or when any key is pressed. Such electronic-circuit wake-up devices are important in many applications, and this project has designed and fabricated a miniature microelectromechanical system (MEMS) device that would respond with a wake-up signal to specific vibrational events, while consuming less that 100 nanowatts of power.

This is especially important to remote sensors, such as tagging, tracking, and locating (TTL) devices, which ideally, should remain “asleep,” that is, in standby mode with zero power consumption, until a chosen event awakens them. Currently, such wake-up events consume significant power, thus shortening the lifetime of these devices. Hence, a wake-up signal consuming near-zero power would substantially increase lifetime. This project makes use of a piezoelectric transducer responsive to acceleration or vibration. By designing the circuitry to respond only to certain frequencies of vibration, complex vibration profiles can be processed without power consumption, unless a threshold is reached, in which case, the “awaken” signal is sent, with zero power consumption until that point. Sensors can be designed to respond to different vibrational frequencies then combined into an array. A mass-prefabrication process has been designed with the assistance of 3D finite element modeling.



Advances in MEMS device fabrication and performance over the 3 years of this project.

Overcoming Jitter Effects for Remote Staring Sensors

Project 117739

Remote staring radiometric sensors are a key element of our national security information-gathering capability, carrying out broad-area surveillance at a relatively low resolution. The goal of these sensors is to record significant scene changes that might impact security measures and responses at deployed locations; therefore accurate analysis of scene changes over time is a critical component of such deployment. This project has engaged in improving the accuracy of that data analysis, specifically as it is influenced by what are known as jitter effects that can easily confuse such analysis, particularly in high-jitter environments. This is critical, given that such jitter effects can readily led to false alarms provoking unnecessary and potentially counterproductive responses. This project has developed data-processing algorithms to facilitate accurate data extraction from such jitter-influenced sensors, algorithms that must run in the real-time, 10–30 Hz frame rates of such sensors.

An example of a local scene utilized to assess the robustness of the algorithms developed in this project. Change elements (motor vehicles) are boxed.

DEFENSE SYSTEMS AND ASSESSMENTS INVESTMENT AREA

Radiation Hardened Components for Space Qualified Point-of-Load Power Conversion

105726
Year 3 of 3
Principal Investigator: J. B. Witcher

Project Purpose

This project proposes the development of essential components for a new approach to space-qualified power distribution using point-of-load (POL) power conversion. The POL approach targets the next generation of low-voltage, high-performance digital components. These digital components find use where higher levels of integration, smaller size, and lower power consumption for a given performance are necessary. In short, these digital components are the future of space data processing and will find use in future remote sensing applications. Low-voltage, high-performance digital components have power requirements that are difficult to achieve with today's satellite power systems. Moreover, the currents associated with these low voltages can be tens of amperes, resulting in large cables and connectors and high distribution power losses. Thus the centralized power architecture incorporated in systems flying today is impractical for the low-voltage, high-current components of future satellites. Compared to the centralized power architecture, the distributed POL power system will reduce distribution power losses, increase overall system efficiency, and reduce the size and weight of cables, backplanes and connectors. The POL approach will improve regulation, which will be crucial as voltage tolerances requirements continue to shrink.

Summary of Accomplishments

In the final year of this project, we continued to build on the progress of the development of a radiation-hardened power n-type metal-oxide-semiconductor (NMOS) field-effect transistor (N-FET) and the development of a high-voltage complementary metal oxide semiconductor on silicon on insulator (HV-CMOS SOI) technology. Also, additional progress was made toward development of a POL controller application-specific integrated circuit (ASIC).

Power N-FET accomplishments:

- Increased 1st and 2nd metal layer thicknesses in power FET processing flow (RS764) to further reduce device on-resistance.
- Increased gate-oxide thickness on 3rd iteration power FET designs to increase single-event gate rupture (SEGR) rating.
- Successfully conducted 3rd iteration power FET device single-event burnout (SEB) modeling and simulations.
- Partnered with University of Central Florida (UCF) to develop an experimental array of 3rd iteration power FET devices.
- Completed 3rd iteration power FET lot (RS764) fabrication and wafer level evaluation testing.
- Conducted wafer-level total dose rad-testing on RS764 devices.

- Packaged 3rd iteration devices (RS764) and conducted single-event effects radiation testing at the Texas A&M University cyclotron. The 3rd iteration N-FETs had significantly better SEB and SEGR performance compared to the 2nd iteration designs tested the previous year.

HV-CMOS SOI accomplishments:

- Completed joint fabrication (silicon-on-insulator process) of HV PMOS and HV NMOS devices.
- Conducted wafer-level evaluation tests on both HV p-type metal-oxide-semiconductor (PMOS) and HV NMOS devices.
- Started work on increasing the SEGR rating for the high voltage SOI devices.

We did not have enough time or funding to complete the joint processing of low-voltage and high-voltage devices (dual gate technology).

We had designed and fabricated error amplifier and voltage reference cells for the upcoming POL controller ASIC in the previous year. We completed the designs for the 3-phase oscillator and pulse-width modulation (PWM) comparator.

Significance

There will be dramatic increases in the required computing performance of Sandia's future remote sensing satellite payloads. Distributed power systems and point-of-load power conversion will be essential to meet the requirements of the improved digital processing components with their higher levels of integration and lower operating voltages.

Results from evaluations of the radiation-hardened power FETs and high-voltage CMOS devices encourage us that we will be able to successfully produce the components needed to implement efficient low-voltage, high-current point-of-load power converters.

This work supports the remote sensing and verification and proliferation assessment missions. The components developed for this project could be used in distributed power systems which target the high-performance digital components anticipated for current and future satellite systems.

Thermal Microphotonic Focal Plane Array (TM-FPA) for High-Sensitivity Room Temperature Infrared Imaging

105729
Year 3 of 3
Principal Investigator: M. Watts

Project Purpose

This project proposed to design and demonstrate an entirely new room temperature infrared imaging technique, which we have termed the thermal microphotonic focal plane array (TM-FPA). Based on its massive scale factor, and few fundamental noise sources the TM-FPA technique has the potential to be the most sensitive uncooled thermal imager. At the conclusion of FY 2007, we demonstrated functionality of thermal microphotonic detection in the visible with an internal noise performance (NEP = $7x10^{-11}$ W/(√Hz) within a factor of ~3 of the best uncooled bolometers demonstrated to date. For FY 2008 and FY 2009, our primary objectives were to drive down the noise floor of single-pixel sensors, integrate infrared absorbing elements, develop a process for scaling to arrays and demonstrate a scalable readout technique. We have now built a vacuum chamber for improving thermal isolation, developed a scalable fabrication process, demonstrated our scalable radio-frequency (RF) readout technique, and demonstrated long-wave infrared detection at 10.6 microns. Further, we expected, by the end of FY 2009 to demonstrate internal room-temperature noise performance not previously achieved by thermal detectors, including the most advanced microbolometers while also demonstrating a small detector array. The TM-FPA technique utilizes the highly sensitive thermooptic effect in integrated optic silicon microring-resonators coupled to infrared absorbing elements to detect minute changes in the microring-resonator temperature caused by the absorbed infrared radiation. Initial calculations indicate that the technique's massive scale factor (~25,000× larger than bolometers), passive operation, and absence of metal thermal paths, should enable near background limited performance (BLIP) in a room temperature infrared imaging system. In addition, the TM-FPA approach utilizes microelectromechanical system (MEMS)-style complementary metal oxide semiconductor (CMOS)-compatible processing — fabrication techniques that have been well developed in Sandia's Microsystems and Engineering Sciences Applications (MESA) complex, and offer the potential for direct integration with CMOS circuitry.

Summary of Accomplishments

1. Demonstrated a detector noise equivalent power NEP < 1 pW/√Hz, to our knowledge a new record for an uncooled thermal detector.
2. With a NEP < 1 pW/√Hz, we demonstrated a pixel thermal time constant of ~2 ms, enabling applicability to 240 Hz frame-rate applications.
3. Demonstrated a viable readout technique, with the required sensitivity, to enable scaling to very large pixel count arrays.
4. Demonstrated the ability to achieve low-loss coupling to passively aligned silicon V-grooves.
5. Patent claims were accepted on the filed US patent application.

Significance

This project demonstrated a substantial improvement in sensitivity over all existing room-temperature infrared imagers, can be passively remoted, and uses substantially less power than approaches requiring cryogenic cooling. The TM-FPA should significantly impact the persistent global awareness / remote sensing and nonproliferation mission. Further, developing the TM-FPA will require substantial use of the MESA facility, providing a strong tie to the scientific discovery and innovation mission.

Tuned Microcavity Magnetometer / Quantum Computation Device

105730
Year 3 of 3
Principal Investigator: M. Okandan

Project Purpose

High-sensitivity magnetic field detection is a critical capability in many applications. Highest resolution magnetic field sensors to date have been superconducting quantum interference devices (SQUIDs) and SERF (spin exchange relaxation free) magnetometers. Operation of SQUIDs requires liquid He temperatures and vacuum, which makes miniaturization very hard, if not impossible. SERF magnetometers rely on detection of the precession of unpaired electron spins in the presence of a magnetic field and are readily miniaturized. We are developing a novel micromachined tunable cavity for miniaturization of this high-sensitivity magnetometer. The tremendous enhancement in fidelity-to-size ratio of such a device constitutes a fundamental scientific breakthrough. This, in addition to dramatic reductions in power consumption and cost will enable new applications. An interesting parallel application and feasibility study in quantum computing is also envisioned for this device. For quantum computation using ions, the same tuned cavity structure is very appealing since it allows extremely precise modulation of the local environment (for the trapped ions) and provides the possibility of coupling the quantum behavior to a mesoscale component. The cavity also has integrated elements (gratings, reflector) for optical coupling and interrogation. Even though the proposed structure is more complicated and larger than the current electrode arrays that are being used for trapping ions, it provides a much larger suite of possible interactions to be modulated and probed for exploiting quantum behavior.

Summary of Accomplishments

We have designed and assembled a high-sensitivity (<picotesla/√Hz) miniaturized atomic magnetometer which does not require cryogenic cooling. Further miniaturization of this device and measurement technique is also possible. We have considered integration of polarization detectors, fiber based beam delivery for lower volume and evacuation of the measurement chamber for achieving further improvement of sensitivity levels and reduction of noise in the system.

While the ultimate sensitivity level achieved by macroscale atomic magnetometers (<femtotesla/√Hz) was not observed (or expected) in this miniaturized device, we have demonstrated the initial feasibility of this approach and have pathways available for approaching the theoretical limits of sensitivity that are possible. For many of the applications that require a fieldable system, the demonstrated sensitivity level is more than adequate (approximately an order of magnitude lower than other approaches).

Significance

High-sensitivity magnetic field measurements and mapping with this reduced volume sensor will enable many strategic applications such as underground structure mapping and remote sensing. If successful, the quantum computation version of the device will allow more diverse options for exploration of quantum computation.

MESA ASML Scanner Based Reticle Field-Stitch Capability Enabling Wafer Scale Integration with Direct Impact on Megapixel Focal Plane Array Synthesis

105732
Year 3 of 3
Principal Investigator: J. L. Rodriguez

Project Purpose

Next-generation remote sensing and verification applications require large area megapixel focal plane arrays (FPAs) — key components for numerous Sandia programs in the areas of nonproliferation (Nuclear Detonation Detection System [NUDET]), surveillance, and remote sensing systems with embedded readout electronics and with more than 64 million pixels (8K × 8K at 5-µm pitch). Because of their large size, these FPAs and other large application specific integrated circuits (ASICs) cannot be built by traditional integrated circuit (IC) manufacturing methods (the size exceeds the photolithography tool exposure field) — reticle stitching is required.

We propose to develop an ASML scanner based reticle stitching process, design and integration technologies to enable megapixel FPAs, high gate count structured programmable ASICs (ViArray), and many other future microsystems applications. Work from this project will enable construction of large FPAs such as those proposed in the "Monolithically Integrated, Backside-Illuminated Photo Diode Array" LDRD project. Other examples where this project will have direct impact is in large silicon motherboards as used in the "Hypertemporal FPA Grand Challenge" LDRD project (95211), the ultrafast x-ray imager for Z-machine as well as future nuclear weapons (NW) programs. These NW programs will require large, reconfigurable ASICs. Currently, the ViArray structured ASIC is planned as a quick turn part for many programs. However, the complexity of the parts required for programs may require a ViArray that is larger than we can produce without reticle stitching.

Success in this project will advance microelectronics design, integration, fabrication techniques and failure analysis in support of Sandia's critical missions.

Summary of Accomplishments

A reticle stitching capability has been established for use in the MESA complex.

The ASML scanner photolithography tool printing and registration limits were established.

An on-grid methodology was proven in simplifying the reticle stitching process and reducing logistic errors associated with entering subfield placement coordinates in the lithography job files.

Reticle stitching design and layout rules were defined and integrated as part of the CMOS7 design rules. Seamless submicron stitched lines were demonstrated.

Out of the box yield enhancement strategies were evaluated in order to be able to yield the large silicon chips. These approaches included thinner metals, more uniform dummy pattern fill in the designs, and greatly reduced test structures.

As final proofs, a 20 mm by 18 mm 4-megabyte static random access memory (RAM) using the full up four level metal CMOS7 process and a 70 mm by 70 mm silicon wafer motherboard (using backend processing) were fabricated. Two full lots for each were run. The 4 megabyte wafer probe functional yields were shown to be 17% and 27% for the first and second lots, demonstrating yield learning. The yield on the first wafer scale silicon motherboard lot was 16%. The second lot is still in test. A defect density number of 0.46 per centimeter squared was demonstrated, showing that large dense circuits can be fabricated using the newly established reticle stitching capability.

Significance

This capability will support DOE's Defense Strategic Goal. It is envisioned that this work will lead to enhanced visible and infrared sensors, which could be deployed in future nuclear detection systems. In addition, sensors using this technology could be applied to overhead nonimaging radiometry projects. Reticle stitching would also enable the development of system on chip NW products as well.

Ultrathin Packaging of Electronic Assemblies

105736
Year 3 of 3
Principal Investigator: J. A. Payne

Project Purpose

Fully packaged and environmentally sealed active electronic systems thinner than 1000 µm with complex performance characteristics have not historically been within reach of Sandia. The third and final year of this project proved such thin assemblies are possible and have significant utility.

The first two years of the project have focused on two activities: thinning COTS (commercial off the shelf) plastic packaged parts and designing a thin interconnect system to integrate those parts in early FY 2008. Thinning has been successful using a technique that removes both bottom and top material followed by a process that allows the part to be assembled in a classic reflow oven. This nondestructive technique has yielded parts about 500 µm thin. Thinning to less than 500 µm has also progressed using a technique that completely removes the lead-frame on the bottom of the COTS part and the wire bonds on the top of the part. The resultant parts are 200 µm thick with a thin layer of encapsulant plastic remaining above the active region of the die. FY 2009 activities integrated 200 µm class components into complete assemblies with significant interest from potential customers as a result.

Summary of Accomplishments

Complete field tests of thin microsystems were performed in FY 2009. These tests demonstrated sufficient reliability to generate technical interest within and outside of Sandia. The complete thin microsystem proved special techniques for the construction of minimized circuit boards which have historically posed significant challenges in TCE (thermal coefficient of expansion) management and compatibility with wire bonds. Additional thinning techniques were created that add to the body of knowledge developed in the first two years of the program. Techniques were also validated that allow surface preparation of electronic circuits for interconnect. Packaging advances were made which allow the microsystem to be environmentally protected.

Significance

Ultrathin electronic assemblies with high performance sensing/communication capabilities offer diverse tactical capabilities to the national security (NS) missions of DOE, DOD, DHS, etc. Advanced NS hardware, information collection, specific task-oriented sensing, and tactical reconnaissance represent mission functions enabled by this project. Discussions with potential sponsors have elicited responses indicating extremely useful applications of such a technology.

Graph-Based Informatics for Nonproliferation and Counterterrorism

105737
Year 3 of 3
Principal Investigator: B. N. Wylie

Project Purpose

Graph algorithms are a key component in a wide variety of analysis activities. This project addresses the critical need of making these graph algorithms accessible to Sandia analysts in a manner that is both intuitive and effective. Specifically we have designed and implemented a flexible toolkit for doing graph analysis, informatics, and visualization that provides Sandia with novel analysis capability for nonproliferation and counterterrorism. This work is being conducted in close collaboration with analysts at Sandia, and their applications are driving the technical development. These collaborations have been the foundation for efforts to build a deeper partnership between the analysis and high performance computing organizations at Sandia.

Summary of Accomplishments

This project started as an effort to combine graph algorithms and visualization into a functional toolkit. As the project progressed, it became the genesis for a much larger and broader effort that is now called the Titan Informatics Toolkit. The authors believe the work conducted in this project will have a significant long term impact to both the Sandia analysis capabilities and to the global informatics community.

The following publications and tutorials were a direct outcome of the work funded by this project.

B. Wylie and J. Baumes, "A Unified Toolkit for Information and Scientific Visualization," *Visual Data Analytics*, January 2009.

B. Wylie, J. Baumes, and T. Shead, "Titan Informatics Toolkit," IEEE Visualization Tutorial, Columbus, OH, 2008.

B. Wylie, J. Baumes, and T. Shead, "GSpace: A Linear Time Graph Layout," *Visualization and Data Analysis*, Proceedings SPIE Vol. 6809, January 2008.

A. Cedilnik, J. Baumes, L. Ibanez, S. Megason, and B. Wylie, "Integration of Information and Volume Visualization for Analysis of Cell Lineage and Gene Expression during Embryogenesis," Proceedings SPIE Vol. 6809, January 2008.

Significance

The continually evolving threats to national security require continued advance in analysis capabilities. We are creating a novel capability that will allow analysts to explore and analyze large, complex datasets to recognize and characterize emerging threats. This collaboration between Sandia's high performance computing and analysis organizations will facilitate bringing additional new capabilities to bear on national security problems.

All of the graph algorithms and visualization techniques developed as part of this LDRD have been deployed into an open source informatics toolkit called Titan (www.sandia.gov/Titan). The toolkit is quite flexible and can be combined in various ways for different problem domains, including large-scale network packet monitoring and deep unstructured text analysis. Our expectation is that the, already popular, open source toolkit will have a lifetime in excess of ten years, and that Sandia will be developing and using the toolkit during that lifetime.

We believe the open source toolkit will have significant external impact as well. The Titan toolkit already has users/developers from around the world: Indiana University, Harvard, California Institute of Technology, Leeds University and University of Utah all have known users or developers. We also believe that the toolkit's open standards and application programming interfaces (APIs) will attract organizations dissatisfied with proprietary and inflexible commercial offerings.

Advanced Line of Sight Stabilization Experiment

105738
Year 3 of 3
Principal Investigator: J. T. Spooner

Project Purpose

Line of sight (LOS) stabilization of an optical system is generally needed whenever sensor data is obtained by integrating optical energy from the imaging system field of view over a period of time. Since this is the approach taken when using film, charge-coupled device (CCD) or complementary metal oxide semiconductor (CMOS) imagers, we find LOS stabilization is required to some degree in most optical systems. Sandia's advanced satellite payloads place very stringent requirements upon the LOS stabilization approach. These requirements are pushing our ability to use traditional gimbal-based pointing systems because of the disturbances from bearing friction and cables that are inherent with gimbal-based approaches. Within this project Sandia will evaluate the use of modern beam-steering and other nontraditional configuration alternatives to an all gimbal approach for LOS stabilization.

Within this project, special attention is being given to pursuing approaches that are compatible with the needs of future programs in both the airborne and satellite arenas. We are considering designs that allow for very precise jitter control and large field of regard coverage while enabling the system to be packaged in a small volume. This is a nontrivial pursuit that will require a dramatic change from the traditional gimbal-based approach including noncontact actuators and sensors, flexure-based mechanisms, and reactionless designs (minimized reaction disturbances transmitted back into the system). The end goal of this project is to evaluate the capabilities of a new pointing approach through a hardware demonstration.

Summary of Accomplishments

Within this project we designed a seven-axis pointing platform that can be used to precisely steer the line of sight within airborne or space based optical systems. The approach took advantage of traditional bearing techniques to create a large field of regard while also using a flexure based fine pointing mechanism to allow for precise pointing. A reactionless design was used that keeps the high-frequency torques of the gimbal system from being transmitted to the vehicle, which is particularly important in some space-based applications.

The system was also built and tested within this study to evaluate ease of manufacturability and performance. It was demonstrated that a very high level of performance is achievable with the approach taken. In addition the time required to achieve this level of performance was reduced from what has typically been needed when using tradition bearing-based gimbals. The performance achieved in this study was limited by the sensor noise associated with the components used and not the underlying approach.

Significance

The harsh vibration environment and stiction associated with bearing assemblies in airborne radar applications often make jitter control a nontrivial problem. The approaches demonstrated in this project provide a jitter suppression solution for a number of airborne and space-based applications. Improved line of sight stabilization for ground-based applications and narrow-beam airborne optical systems will also benefit. By demonstrating the viability of more advanced stabilization approaches, this project will better position Sandia for advanced future programs.

Scannerless Range Imaging for Autonomous Rendezvous and Capture

105739
Year 3 of 3
Principal Investigator: R. O. Nellums

Project Purpose

Many US applications require 3D sensing for autonomous rendezvous and capture. In flight integration of Sandia's 3D technology has proven to be very useful for the National Aeronautics and Space Administration's (NASA's) Space Shuttle program. Relative to other technologies, the Sandia sensor has demonstrated electronic stabilization, minimum size and power, and superior resolution. However, performance must be extended to be successful in the rendezvous and capture application to enable on-board pose estimation of typical specular spacecraft surfaces, and to enable location and ranging at larger standoffs. This investment will ensure Sandia's ability to meet present and emerging national needs for robust space operations as humankind continues to explore space.

Spacecraft are typically wrapped in aluminized mylar or similar specular material, resulting in bright glints which proportionally suppress the diffuse return and prevent accurate pose estimation. This work has enhanced sensitivity to weak diffuse return relative to bright specular return.

Anticipated future missions will require a compact and efficient light source at larger standoff for early detection and location of objects, whereas Sandia LADAR (laser detection and ranging) has only been demonstrated at long range using large and inefficient light sources. This work investigated efficient, compact, radiation-tolerant light sources, capable of extending the range of the Sandia LADAR.

Autonomy requires on-board pose estimation. This work investigated algorithms that tolerate glint and function over a wide dynamic range.

Summary of Accomplishments

All of our LADAR systems to date have relied upon image-intensifier technology to provide optical gain modulation at frequencies up to 140 MHz, prior to focal-plane imaging. During this project, we demonstrated electro-optical modulation at these frequencies. These modulators extended our capability to image specular targets.

Our approach to efficient and reliable illumination in space is a pulsed laser-diode modulated at up to 140 MHz during each pulse. Our most powerful, space qualified laser to date was 20 watts, with a bandwidth of 6 nanometers. During this project, we demonstrated 1000 watt operation with a bandwidth of less than 1 nanometer, greatly extending our range capability.

Computer-aided registration of 3D data sets represents a problem of particular interest for the autonomous rendezvous and docking problem. Work by others has ignored potential errors due to multiple reflections from the surface. Our sensor is particularly prone to this type of error and a solution was vital to this potential application. During this project, we developed an error-tolerant method for registering 3D data sets, that takes advantage of the unique performance of our LADAR systems, such as high resolution and high data-rate, while permitting a relatively large number of anomalous errors due to multiple reflections.

Significance

This project advances Sandia/DOE-developed technology for current and future US space applications. In particular, our objective is to improve the reliability of space exploration operations. Issues addressed in this project also apply to DOE program objectives.

Managing Thermal Emission: Subwavelength Diffractive Optics Technology in Support of SOF

105742
Year 3 of 3
Principal Investigator: S. A. Kemme

Project Purpose

In this project, we will design, fabricate, and demonstrate a passive emissivity control coating that could be applied in a variety of military assets including ground based assets, unmanned aerial vehicles (UAVs), and unmanned ground vehicles (UGVs) to control the emissivity of surfaces. Additionally, this technology could be utilized for thermal control of microsystems where thermal transfer due to radiation must be controlled to develop low power sensing systems for unattended sensor systems and persistent intelligence.

Any material radiates energy, which is a function of its temperature, and so can be called a thermal source. A thermal source is typically viewed as noise to be eliminated; but this emission is difficult to manage, because it is incoherent and quasi-isotropic with radiation exiting the surface at every angle. If the thermal radiation was instead coherent, then the angular emission could be directed into desirable lobes, as in antenna patterns.

This new proposed technology enables thermal emission pattern management by structuring of the surface on a subwavelength scale. This structuring may be in either the lateral or depth dimension. An air/metal interface allows photon/plasmon coupling, which has been shown to preferentially emit at certain wavelengths.

This project addresses the Defense Systems and Assessments call for the following: 1) advanced technology solutions to the special operations forces (SOF) platforms/weapon systems/operators with enhanced protection and armor; 2) to identify, influence, and insert relevant technology with emphasis on UAVs, UGVs, persistent intelligence, and denied area access; and 3) to capitalize on emerging and leap-ahead technology.

Summary of Accomplishments

We designed, fabricated and tested devices that change the typical spectral and angular emissions (Lambertian in angle and broad spectrally) of an object emitting in the mid-wave infrared (MWIR) and long wave infrared (LWIR). The emissions are changed to look like antenna patterns with a restricted wavelength band. Devices were also fabricated that lend themselves to practical fabrication and applications.

The successful performance of all the devices was measured with indirect methods using an hemispherical directional reflectometer to measure their directional absorption; and direct methods like the variable-angle directional emissometer that measures their directional emissions, and by using a commercially available LWIR camera.

Significance

DOE and DOD clearly would benefit from a passive thermal emission management surface demonstration that could apply to military assets. Additionally, this technology could be utilized for thermal control of microsystems where thermal transfer due to radiation must be controlled to develop low power sensing systems for unattended sensor systems and persistent intelligence.

Enhanced Inverse SAR

105743
Year 3 of 3
Principal Investigator: D. L. Bickel

Project Purpose

Inverse synthetic aperture radar (ISAR) is the technique of coherently processing a set of radar pulse echo data to image a target object which has unknown motion. Conventional synthetic aperture radar (SAR) assumes a stationary target whereas ISAR assumes unknown angular motion, and perhaps unknown translational motion as well.

In order to focus the image, ISAR attempts to compensate for the unknown target motion. This leads to inferring the target motion using the radar sensor. ISAR must focus the target using data-driven algorithms. Due to the limited number of degrees-of-freedom in the data, this is a difficult problem.

Ultimately, it is the relative motion between radar and target that must be compensated to properly focus an image, whether for SAR or for ISAR. Relatively small radar motion errors in SAR data are typically compensated using well-known data-driven (autofocus) techniques. Recently, this capability has been extended by Sandia to mitigate larger problematic errors in high-performance fine resolution SAR images. It is postulated that the even larger unknown relative motion between radar and ISAR targets can be similarly compensated using derivatives and enhancements to the latest autofocus techniques developed by Sandia.

Sandia is concurrently developing advanced moving target indicator (MTI) radar systems with multiple phase centers that show potential for measuring additional aspects of target motion. Using these measurements to aid the autofocus techniques will be investigated.

Summary of Accomplishments

A few methods for tackling the imaging of a moving object with a radar system were investigated over the life of this project. In particular, we focused on special waveform coding techniques and on data-driven techniques. The in depth analysis of the special waveforms showed some promise, but also revealed limitations. The limitations may constrain the geometries and scene types for which this technique works.

The data-driven techniques also showed preliminary promise, but were performed on a limited set of real data. We will require more investigation with a diversity of data sets to investigate the limitations of this technique.

Significance

Sandia's national security customers are relying more heavily upon monitoring objects that are moving, along with being able to distinguish between specific types of traffic. DOE proliferation-detection customers need to monitor both ship-borne and land-based movements, as do DOD and Homeland Security customer applications.

Heterogeneous Microsystem Integration as Applied to the Practicality of a Small-Caliber Guided Bullet

105744
Year 3 of 3
Principal Investigator: J. F. Jones

Project Purpose

US military doctrine has changed to widespread application of guided weaponry. Currently, these systems are sophisticated, large, and expensive. According to a 1999 DARPA study, there is a desire to develop a small-caliber, inexpensive guided bullet for ground forces. The basic problem is that it is generally accepted that a bullet cannot be guided and that even if it were possible, it would be prohibitively expensive and impossible to manufacture. Consequently, the US military is investing in improved fire control for sniper weapons to give warfighters improved small arms accuracy. Improved fire control will reduce shooter error but will not overcome inherent inaccuracy or the problem of moving targets.

The generally accepted belief that a guided bullet is not feasible or practical is not valid due to a combination of poor assumptions and evolving technology. Our guided bullet idea is quite simple, which is to laser designate a target and fire a guided bullet from a conventional rifle. The rifle will be a smooth bore and not impart a spin to the bullet. In addition, the center of gravity of the bullet would be moved forward by packaging dense material in the forward section and the guidance package in the rear of the projectile; thereby, obtaining aerodynamic stability without spin. The small scale and absence of spin stabilization significantly improves the response of the bullet to guidance (acceleration) commands allowing a relatively simple, primitive method of navigation, guidance, and control without the need for an inertial measuring unit.

The goal of the R&D was to explore the viability of an inexpensive small-caliber guided bullet and demonstrate feasibility through a combination of analysis and experimentation. Toward this end, this project proved highly successful.

Summary of Accomplishments

From this work we were able to demonstrate that, although challenges remain, an inexpensive small-caliber guided bullet appears possible. Further, that an experimental test flight phase could be conducted at modest cost because COTS (commercial off the shelf) electrical and electronic components are able to survive the launch environment.

Significance

This research is focused on permitting ground troops to efficiently inflict damage on desired targets with minimal collateral damage. The technology would be of immediate benefit to troops involved in counter insurgency operations and to various special forces operations within the DOD. In addition, this technology could be of interest to DOE site security and to law enforcement SWAT teams, FBI hostage rescue team members, etc.

Autonomous Intelligent Assembly Systems

105746
Year 3 of 3
Principal Investigator: R. J. Anderson

Project Purpose

The Iraq war has proven the value of mobile robot systems in high-consequence environments for the DOD, but those systems rely heavily on human operator commands and are used almost exclusively for surveillance and reconnaissance. The potential for autonomous, robotic manipulators in high-consequence environments, however, dwarfs any current utilization of robots. The US Army would like the ability to perform robotic assembly in "green zone" construction, the Navy needs robot systems for weapons loading, fueling, emergency repair, and general transport, and the National Aeronautics and Space Administration (NASA) needs autonomous robots for a planned 2018 lunar base mission. Although pedestal robots have been able to perform part docking and welding for years in a controlled factory environment, there are issues that have prevented similar success in an unstructured outdoor environment. First, factory environments are static. Humans do not coexist with robots, and parts and infrastructure remain in fixed locations. Work-cell awareness is not required, and the robots are programmed off-line.

Our goal has been to develop and demonstrate technologies to make this vision a reality. Technology development has moved forward on multiple fronts: Improved perception algorithms for unstructured environments, flexible planning commands for distributed command and control, distributed broadcast communications, integration of advanced 3D range imagers, and demonstrations of voice directed behaviors. Algorithms of merit include new approaches to visual tracking using both polygon snakes and color grid patterns, and the application of marching cubes to 3D range data. Our target demonstration of an autonomous brick stacking robot system consisting of two robots working in an unstructured outdoor environment, however, proved too difficult to achieve under time and budget constraints.

Summary of Accomplishments

In this project, we set out to demonstrate that autonomous mobile robots could perform an assembly task in unstructured environments. We selected a target task, the act of building a brick wall using specially made bricks that included grasp points and markings, and planned to navigate to the work site using cone markers. With this task in mind we set out to determine which technology was needed to achieve success.

In the first year we explored scanner and vision approaches. We developed a robust communication framework, and implemented a precise Kalman filter based navigation scheme on a mobile robot platform. Our vision approach using conventional vision techniques was able to find cones and approach them, but without suitable accuracy or robustness to justify continuing this path. The Canesta scanner based investigation was also disappointing, since the sensor data fitting algorithms failed to produce the desired target registration and recognition.

In the second year, we developed a far more robust approach to finding and tracking known colored features called polygon snakes. This algorithm was able to maintain state information between image frames and gave us the required accuracy needed to move towards assembly. A patent is being pursued for the algorithm. A command and control framework was also developed that would enable complex behaviors from an abstract command class.

The vision based approaches were adequate for finding and recording the locations of known marked objects, but were still not adequate for allowing robot motion in unknown uncluttered environments. In the third year a new sensor, the MESA RangeImager became available and was integrated into the Umbra software environment. The sensor is promising, but ultimately requires far more data processing before it can be used for rapid determination of known objects and uncluttered motion paths.

Significance

Rapid response robotics technology plays a critical role in national security. Whether it is radiation sources, chemical munitions, improvised explosive devices, or remote ordnance, mobile robotic systems can respond to a number of potentially lethal environments without risk to human life.

This project has developed technologies that increase the level of autonomy of mobile robot systems by utilizing advanced sensing, modeling and planning. Improvements in distributed communications and commands scripting have already positively impacted other programs. Autonomous behavior scripting from this project has been used for automating robot surveying and camera calibration. The communications framework we developed is also supporting multiple robot projects. The software base is also being used to support visual targeting for external military customers.

The dream of complete autonomy for mobile robots performing assembly tasks, however, remains elusive, and the missing component is perception. We focused heavily from the outset on perception, and advanced the state of the art in perception with new algorithms for vision tracking and 3D scanning. The polygon snake algorithm provides rapid real-time identification and tracking of known objects, and the color grid blob tracking provides highly flexible and robust feature points for zoom camera systems. We investigated two commercial scanning systems: the Canesta and MESA imagers, and were able to acquire real-time data from both. These efforts, however, did not go far enough for mobile ground based robot systems to safely operate without operator supervision.

Although we have not achieved the target demonstration of autonomous brick stacking robots, we have furthered our technology base, and have developed tools that are impacting multiple projects. A patent for the polygon snake algorithm is pending, and copyright assertion is being pursued for a number of Umbra based software packages including image processing (imageApps) and robot kinematics (kinApps).

MEMS Sensors and Telemetry for Prognostic Health Management

105747
Year 3 of 3
Principal Investigator: M. A. Smith

Project Purpose

With modern advances in sensors, software, and other technologies, many people are recognizing the potential to combine them to perform prognostics and health management (PHM), on critical systems. PHM entails sensing anomalies, diagnosing impending system failures, estimating remaining useful life, and deciding how to manage maintenance and operations (M&O) in such a way to optimize overall system utility against cost. Successful PHM will save billions of dollars in M&O costs to the US economy every year.

The goal of this project is to advance Sandia's capability to do PHM by assembling a suite of sensors, collecting data in real time from a reciprocating internal combustion engine, and developing appropriate algorithms to analyze the data. PHM efforts will promote R&D of sensor hardware and decision algorithms in general as well as further their application in other areas.

Another goal of this project is to leverage the microsystems and sensor technology base at Sandia including microelectromechanical Systems (MEMS). If sensors can be selected and/or designed with a view toward the prospects of miniaturizing the technology, they could be incorporated into low-power, wireless sensor nodes and used to retrofit existing systems such as cars and trucks. Sensor nodes could also be adopted for monitoring the state-of-health of critical infrastructures such as power generators.

Summary of Accomplishments

We demonstrated that all the sensor and analysis hardware of a wireless, low-power MEMS vibration sensor node could fit inside a standard automobile oil filter. Data acquisition and reduction software for the sensor node, wireless communication, and base station were written and successfully tested.

We successfully applied infrared spectroscopy to detect changes in oil constituents over time. During early engine runs, we periodically sampled the oil for off-line analysis with a commercial spectrometer. Using the resulting spectra, we were able to perform chemometric analysis in the form of principal components regression to predict the age of the oil.

We subsequently designed and built an attenuated total reflection (ATR), or evanescent wave, spectrometer to measure infrared spectra in real time on a running engine. We seeded faults in the oil by injecting water and/or propylene glycol. Through on-line data analysis, we could visually track the presence of those species in real time. This technology demonstration enables true, on-line, in-situ monitoring of oil condition.

Other sensors and data acquisition hardware were assembled to measure time-series data consisting of engine vibrations, spark plug activation, crankshaft speed, and various temperatures. We seeded various faults on five identical engines and collected the time series data as they ran to failure.

Finally, we created software to display and analyze the time-series data to diagnose faults and understand the physics of failure. Self-organizing maps were trained on vibration data and used to provide fuzzy classifications of engine conditions. Then we developed an algorithm that combines data from the accelerometers, the spark signal, and the crankshaft encoder to detect and track the growth of damage at particular points in the engine cycle.

Significance

Most PHM research up until now addresses machinery with static or uniformly rotating parts such as gearboxes and turbines. This project has the added challenge of monitoring a rough, sooty, single-piston engine.

The Department of Defense has mandated that CBM+ (condition-based maintenance plus) be incorporated in all new weapon systems and current systems where feasible and beneficial, and this has obvious significance to Sandia's defense work.

This work may lead to application in any area of technology (mechanics, electronics, and perhaps even software) where prescience and management of impending failures could improve efficiency, safety, security, reliability, maintainability, readiness, sustainability, or any other measure of utility.

Finally, this line of research will lead to new fundamental understanding of how physical phenomena can be sensed and the data used to predict and manage impending failures. In a similar vein, it will also lead to improved scientific understanding of the underlying physics and chemistry. For example, we observed a superlinear response in the sensitivity of the custom spectrometer to the amount of water added to the oil. We speculate that the crossover occurs because either, (1) water droplets wet the surface of the ATR crystal, thus enhancing the water concentration in the evanescent wave region, or (2) a cooperative absorption effect is induced by water being in the liquid phase where it experiences greater hydrogen bonding with the surrounding molecules.

Building a Live/Virtual/Constructive Experimental Testbed

105748
Year 3 of 3
Principal Investigator: E. P. Parker

Project Purpose

To meet the evolving needs of DOE security, US warfighters, and homeland security, the DOE, DOD, and DHS need the ability to perform testing, experimentation, and training involving interactions between live (real people and hardware), virtual (real people and simulated hardware), and constructive (simulated people and hardware) entities (LVC). This allows designers to examine complex systems performance throughout their life cycle, especially during design when it is important to discover problems early.

To enable LVC experiments we extended our virtual and constructive simulation tools and incorporated the capabilities into a live system testbed. For an LVC framework to be useful it must be able to incorporate hardware and simulations developed elsewhere. To facilitate incorporating new hardware, we continued to analyze communications between live/virtual robotic and sensor assets and constructive assets, determining how to replicate simulated information exchanges and enable virtual projection or presence between environments (e.g., making virtual elements seem to affect the live environment and vice versa). To facilitate linkages to other simulation packages we explored methods to share objects between simulation packages.

LVC testing enables spiral development so interactions and dependencies can be tested before implementation. Sandia is involved in surety, security, and military projects requiring high degrees of integration between subsystems, including counter–improvised explosive device (IED). efforts. LVC experimentation makes testing and integration of these systems substantially more rigorous and accurate.

Summary of Accomplishments

FY 2007

- Developed and demonstrated live, virtual, and constructive entities interacting in a closely coupled fashion. All assets can access state data for other assets and affect / be affected by other assets.
- Established compatibility with JAUS (joint architecture for unmanned systems) for Gemini unmanned ground vehicles (UGV).
- Developed a unique robotic operational control interface (TA SD10712).
- Incorporated human tracking using vests outfitted with global positioning system (GPS) receivers and radio transmitters with 1 Hz update.
- Incorporated the augmented reality training system as an immersive visualization system.

FY 2008

- Examined methods to reduce compute load for complex simulations
  - Scaled an urban scenario simulation to push single machine compute limits
  - Identified bottlenecks: line of sight look-ups for communications, communications protocol calculations, visualization
  - Extended Modeling Architecture for Technology, Research, and Experimentation (MATREX) federation object models for communications modeling

  - ○ Developed a communications protocol federate
    - ▪ Designed to federate Umbra Comms world and OPNET (Optimized Network Engineering Tools)
    - ▪ Will allow interchangeable communications modeling
  - ○ Developed communications link federate
  - ○ Off-load compute-intensive link calculations
- Implemented methods for reducing LVC compute load
  - ○ Using high level architecture (HLA) federates on separate computers
  - ○ Line of sight polygon lookups
  - ○ Communications protocol calculations
  - ○ Robot models
- Using multithreading on multiple core machines,
- Separated visualization from computation, allowing utilization of multiple cores
- Developed software LVC communications multiplexer (TA SD11297) – module that drops or passes messages to hardware based on information from the LVC control framework.
- Implemented robotic models driven using real wireless communications.

FY 2009

- Examined methods of sharing objects between packages: requires a connection through a federation architecture such as HLA/TENA (test and training enabling architecture), or tools like the Spread toolkit (a socket interface)
- Conducted LVC communications experiments incorporating the LVC testbed into purely constructive communications studies using OPNET Modeler, Joint Communications Simulation System (JCSS), and QualNet®.
- Developed the serial controlled unmanned tactical robot (SCUTR) – a mobile LVC demonstration based on a roboticized vehicle.

Significance

The DOE, DOD and DHS are developing systems for security and warfighting that are highly interdependent. The reliance of their subsystems on data sharing requires that they be tested within the context of realistic operations. LVC testing facilitates integration and testing of proposed and existing assets along with human interactions. LVC capabilities provide understanding early in the development cycle and make testing more rigorous and accurate. LVC testing also supports system assessment.

We envisioned a framework where tightly coupled live, virtual, and constructive assets can access information about other assets and influence other assets, with all components acting as members of a single network. The current state of the art in DOD LVC exercises emphasizes integrating live platforms with simulators, while the constructive assets are dealt with separately. Because our approach is unique (and very difficult to execute), Sandia currently has a lead in developing tightly coupled LVC capabilities.

Refereed Communications

E.P. Parker, N.E. Miner, B.P. Van Leeuwen, and J.B. Rigdon, “Testing Unmanned Autonomous System Communications in a Live/Virtual/Constructive Environment,” *The ITEA Journal*, vol. 30(4), p. 513–522.

Plasmonic Antireflection Coatings (PARC)

105749
Year 3 of 3
Principal Investigator: D. W. Peters

Project Purpose

Current antireflection technology in the infrared is inadequate for many applications that require broad spectral and angular bandwidth. This is particularly true in the 8-12 micron wavelength band (thermal infrared). This band corresponds to an atmospheric window and is of interest for infrared sensing and imaging, an important area for military technologies.

We are adapting a concept from the radio-frequency (RF) community to address this need: frequency selective surfaces (FSSs) are common in radar applications, however scaling to the infrared is nontrivial, involving considerable modeling and fabrication challenges. We are designing, simulating, fabricating, and characterizing infrared FSSs that show broad spectral and angular passbands on commonly used substrates in this wavelength band. We believe there will be significant interest in this technology for infrared sensor windows as the technology can lead to low reflectivity while maintaining a planar surface.

To date, we have designed and fabricated antireflective surfaces in the mid-infrared to thermal infrared. We have designed structures that create low-reflectivity, high-transmission gold surfaces on gallium arsenide. Simulations of designs that use a top coat of silicon nitride show reflectance in simulations below 5% over a broad spectral range (5.5 to 8 microns) and broad angular range (0 to 30 degrees from the normal), with a narrower spectral band having low reflectivity out to 60 degrees. Determining the transmission through these designs required code revisions to EIGER that we have done. These revisions will be useful for future projects. Fabrication methods have been developed also in this project that account for fine features mixed with relatively broad unpatterned areas.

Final year efforts will be focused on fabricating low-reflectivity, high-transmission thermal infrared FSSs.

Summary of Accomplishments

We have designed infrared frequency selective surfaces (FSS) that allow a continuous metal layer to an optical surface with only a small affect on its transmission at the design frequency. We can thus reject electrical noise from entering a system through the optical aperture. These designs functioned over a broad angular range from normal to near-grazing. This represents the first achievement of infrared transmissive frequency selective surfaces in the published literature.

Using the transmissive FSSs as the top layer, we also designed and fabricated infrared antennas that can absorb radiation using only a thin layer of absorbing material. We achieve this by coupling to surface modes on the underside of the FSS patterned metal layer that are then absorbed in the active material underneath the FSS. This advance can lead to infrared detectors with lower dark noise since less active material is required.

We have explored the use of these antennas as a component of a rectifier that could be used for infrared energy harvesting. The surface modes could be coupled into a traveling wave rectifier that could convert the very fast oscillations of infrared radiation.

Significance

This project addresses a national security need for thermal infrared antireflection technology. We address real-world issues such as large spectral and angular bandwidth. This project has also explored improvements to infrared focal plane arrays by designing infrared antennas that can take a broad angular range of infrared radiation and direct it to a thin layer of absorbing detector material through surface modes. Thinner layers of active material lead to lower dark current in FPAs.

Overcoming Jitter Effects for Remote Staring Sensors

117739
Year 2 of 2
Principal Investigator: K. M. Simonson

Project Purpose

The purpose of this project was to develop practical image processing algorithms that incorporate robust spatial measures of image pixel variance. The intended application is the detection and extraction of target signals within images from fast-framing, staring, remote sensors that are subject to high levels of jitter. Such jitter presents a significant challenge when the target signals lie within structured background scenes.

In addition to utilizing spatial variability measures, the algorithms that we have developed apply modern methods of adaptive subspace projection in modeling jitter-induced changes in background intensity. While approaches to background estimation based on subspace projection had been suggested for many years, this project was the first to exploit recent advances in adaptive subspace estimation, enabling real-time performance.

Working with measured data from an operational sensor, the new algorithms have demonstrated a 1-2 order of magnitude reduction in jitter-induced false alarms, while maintaining a high detection rate for challenging target signals.

Summary of Accomplishments

During the two years of this project, research has focused on the development of algorithms for the detection of new transient energy with staring radiometric sensors. Key accomplishments are as follows:

1. Formally documented a mathematical technique for spatial variance estimation in a Department of Energy (DOE) invention disclosure. Filed an application with the US Patent Office.
2. Implemented a new approach to image background subtraction, based on efficient modern methods of adaptive subspace estimation.
3. Assembled a working set of real-world sensor data for algorithm training and evaluation. The set includes many stressing targets in high-jitter environments, along with some easier targets. Some of the background scenes are highly structured, while others are relatively uniform. Events in the working set all have associated ground truth information, which is essential for proper scoring of algorithm performance.
4. Developed a software demonstration system for transient energy detection. The software allows performance evaluation over a range of algorithm variants and parameter settings. Direct comparison between LDRD project-developed algorithms and current "baseline" processing methods is enabled. Outputs include numerical and graphical performance summaries, and associated tools allow visualization of target and clutter signals.
5. Achieved substantial improvement (1–2 orders of magnitude) in the rejection of clutter-induced false alarms, without adversely impacting target detection. While the biggest improvements are seen for structured scenes in a high-jitter environment, our algorithms also out-perform baseline processing when jitter is nominal.

6. Developed an unclassified demonstration system that allows testing of our algorithms on open-source data. Collected numerous new test range videos from a tower-mounted camera, for use in a technical journal article.
7. Completed final SAND report, detailing detection algorithms. Presented algorithm approach and performance figures at a conference held for the appropriate technical community.

Significance

The work has direct applicability to the remote sensing and verification program area, where Sandia is a key player for national systems. The project matured a promising technical approach for one of the key challenges associated with such sensors: the mitigation of jitter-induced artifacts in the processing stream. The technology developed here could be readily transitioned to several existing and planned future remote sensing systems.

Precision Nanobumping Technology for Large Format Focal Plane Arrays

117742
Year 2 of 3
Principal Investigator: S. S. Mani

Project Purpose

Large format focal plane arrays (FPAs) are a key component in numerous remote sensing systems. Mission requirements drive the need for increasing the number of pixels in addition to forcing pixel dimension minimization. This proposal investigates innovative solutions to this problem by leveraging current capabilities as well as exploring new technologies to produce uniform indium nanobumps for use in readout integrated circuitry (ROIC) and photodetector hybridization. Used for conductivity at cryogenic temperatures, indium nanobumps will be grown with controlled pitch, exact geometry, and uniform thicknesses. Combining advanced lithographic techniques and optimized electrodeposition techniques, controlled pitch, exact geometry, and uniform thicknesses will prevent pixels from shorting between neighbors and effectively limiting the pixel pitch. This nanobump fabrication technology allows for pixel assemblies across large format FPAs with areas greater than 3 cm^3. Techniques for indium interconnect separation of the detector array and ROIC (readout integrated circuit) chip will also be investigated. Re-workable interconnect technology will allow for recovery and re-work of a defective part after testing at cryogenic temperatures on proven ROICs before permanent attachment. This critical innovation in photodetector screening will dramatically impact hybrid FPA yields.

Summary of Accomplishments

This year we have demonstrated significant improvements in producing large area areas of indium electroplated bumps for use in large format FPAs. In addition, a collaboration with an external vendor for aligned indium bump hybridization was established. Successful work has also progressed in the area of selective indium removal for detector/ROIC separation.

Improvements in the macro and micro uniformity of the indium electroplating process have been made by utilizing galvanic, periodic, reverse pulsing during the deposition. A series of pulse regimes were tested beginning with a theoretical model. Ultimately, a final pulse was determined based on scanning electron microscopy (SEM) and interferometer analysis. In addition to improvements in the local uniformity of the indium depositions, indium bumps were also successfully electroplated at dimensions less than one micron. Using standard galvanic plating in the current plating bath, indium bumps were plated with diameters as small as 600 nanometers.

A contract with DRS Technologies Inc. was negotiated as a collaborative development effort to improve and advance the current state of the art for indium hybridization to enable larger area focal plane arrays. Indium electroplated bumps from Sandia were delivered to DRS and were successfully aligned and hybridized. Successful boning with pitches of 25 microns and 12 microns were performed. Continued efforts with DRS will lead to determining the minimum pitch, minimum feature size, and minimum aspect ratio for which hybridization is successful.

Leveraging year one strategies for indium interconnect removal; established techniques utilizing particular chemistries are being tested on Sandia electroplated indium bumps hybridized by DRS.

Significance

This work supports remote sensing missions that use FPAs as well as future space missions requiring large area hybridized detectors with small pixel pitches. Missions requiring multicolor pixels will benefit from this effort of reducing the pitch and the feature dimension required for the interconnect between the photodetector and the ROIC.

Advanced Data Processing Module for Future Satellite Projects

117743
Year 2 of 3
Principal Investigator: R. R. Mills

Project Purpose

In today's satellite systems, Sandia has been at the forefront of creating module designs using static random access memory (SRAM)-based field programmable gate array (FPGA) components. However, current Xilinx Virtex-II FPGA designs utilizing triple mode redundancy (TMR) consume large amounts of device resources preventing complex image processing algorithms from being implemented within satellite payloads. Simply increasing the device size on existing modules using the same FPGA family gives a higher gate count, but at the cost of increased power, slower device speeds, increased board layout complexity, and continued architectural limitations. During the first phase of this project, a reconfigurable advanced data processing (ADP) module using newer technology Xilinx Virtex-5 FPGAs was developed. The remaining two years of the project will be used to demonstrate the capability of the module to perform complex image processing algorithms, using embedded processing cores. Several ADP modules will be connected together creating a complex node based network. The new "node" module is hosted on a main board having a similar form factor to a current design thus allowing use of existing test hardware and software for validating and demonstrating the new module. By leveraging existing module and system test hardware, the project focuses on advancing current capabilities by using resources found on these newer FPGA devices. A trade study between using the Virtex 5's PowerPC and various softcore processors will be made to determine the most efficient embedded processing element to use to execute image processing algorithms. The chosen processor will be implemented and tested in the module design providing the platform for the final project phase. During the last project phase, existing Sandia image processing algorithms will be investigated, modified, and tested using the new ADP module.

Summary of Accomplishments

The first year of the project consisted of researching and designing the host and node ADP modules. Technologies chosen for these modules include Xilinx Virtex-5 FPGAs, and Tundra Semiconductor RapidIO switches. The Virtex-5 FPGAs will allow for higher-density designs than current Virtex-II FPGAs currently in use at Sandia for space missions. They will also provide a platform highly similar to the upcoming single-event effect immune reconfigurable FPGA (SIRF) Virtex-5 parts. The Rapid input/output (I/O) switches will allow multiple node modules to be interconnected and will allow for future development of remote FPGA configuration and FPGA self-scrubbing techniques. Layout was begun on the node module.

The second year of the project consisted of completing layout of the node module and completing design of the host module. In addition, the node boards were fabricated and assembly was begun.

Significance

Sandia currently produces technologically advanced space based systems capable of transmitting data to ground stations providing awareness of events occurring at predetermined locations. The advanced data processing module increases this capability by implementing real-time detection at the data collection source. By reducing the latency between when an event is detected and transmitted to the ground station, the ability to quickly determine criticality may be greatly increased.

Miniaturized 3D Magnetic Phasors

117745
Year 2 of 2
Principal Investigator: B. H. Strassner II

Project Purpose

Phased radiators (phasors) are key components in millimeter-wave sensors and arrays. They enable fast beam steering needed for monitoring and tracking multiple targets critical to surveillance and reconnaissance missions. Despite the maturity of modern microwave electronics, low-loss, lightweight, low-cost, high-power, miniaturized phasors remain elusive. No single existing technology, ranging from waveguide to diode or microelectromechanical systems (MEMs)-based components can meet all of these requirements.

We propose to answer this challenge with an innovative, miniaturized 3D magnetically actuated phasor and its associated interconnects. The proposed design utilizes gyromagnetic materials to impart continuous (rather than discrete) phase shift using only milliamperes of current. Besides the engineering difficulty inherent in material modeling, device analysis, and component miniaturization, a key science and technology obstacle lies in making compact broad-band true-time-delay (TTD) devices tunable using dispersive materials. Weight and size reduction can be accomplished by embedding gyromagnetic materials inside a 3D aperture radiator surrounded by inductive coils. The integrated phasor/radiator "plug-and-play" unit enables flexible array architectures for applications requiring unique element spacings and/or conformal mountings. Large-angle steering necessitates tight interelement spacing, constraining the size and routing of feed structures. Novel 3D macro-coax technology with dimensions in millimeters will be used to provide higher power handling capability. In addition, prototyping and technology demonstration at the macroscale provides the foundation for future design and fabrication at the microscale. Phasor integration with macro-coax interconnects provides the fundamental mechanism for precision control of dynamic beams, yielding an array form factor suitable for aerial/space reconnaissance platforms.

Summary of Accomplishments

We have made the following accomplishments:

1. A microwave-frequency measurement apparatus has been manufactured for characterizing ferrite rods within a circular waveguide that contains a longitudinal magnetic field.
2. A 2-to-4 port test kit has been designed and manufactured for differential measurements.
3. A 4 x 4 macro-coax array with SMA input has been fabricated and measured with promising results.
4. A 16 x 16 wire-EDM macro-coax array with SMA input has been fabricated and measured with promising results.
5. A 16 x 16 wire-EDM macro-coax array with WR-51 input has been fabricated and measured with promising results.

Significance

Successful development of a miniaturized phasor and its associated macro-coax interconnects enables beam flexibility and polarization diversity of active microwave sensors. These added functionalities offer the possibility of tracking and identification of multiple targets while simultaneously beaming communications and telemetry. Such sophisticated methods improve and strengthen the nation's homeland security, defense, communication, and surveillance and reconnaissance efforts.

Innovative Solutions for Terrestrial Based Tagging, Tracking, and Locating and Clandestine Data Exfiltration

117746
Year 2 of 2
Principal Investigator: R. C. Ormesher

Project Purpose

Current systems for tracking radio-frequency (RF) sources from airborne platforms do not provide a good solution when a when operating in extreme loss conditions, which are prevalent in real-world operations.

To solve these problems we will make technical advances in

1. receiver sensitivity required to detect severely attenuated signals
2. communications channel-coding methods required to operate in fading situations
3. geolocation algorithms using multiple signal parameter-measurements

During the first year of this project we developed a new terrestrial based receiver, developed several new waveforms, and performed several field tests to characterize the performance of the new waveforms and receiver design. The second year of research will focus on developing angle-of-arrival methods for geolocation in the presents of multipath and mitigating multipath effects on existing time-of-arrival (TOA) measurement techniques.

Summary of Accomplishments

- We developed a set of waveforms that provide characteristics desired for a real-time terrestrial based tracking system. We performed simulations to verify system performance.
- We developed a prototype terrestrial tracking system that provides real-time detection and geolocation of RF tags in severe obstructed and highly attenuated conditions.
- We performed multiple field tests in various difficult non-line-of-sight conditions, collected and analyzed test data, and characterized system performance. Results demonstrated that our non-line-of-sight signal detection, real-time processing, and geolocation goals were met.

Significance

This project significantly advances the state of the art and adds new mission capabilities for tracking, RF sources. It will have immediate impact in the global war on terror. It provides Sandia the potential to support several users, including military, law enforcement, DHS, and the intelligence community who have a need for terrestrial-based or extreme (non-line-of-sight) applications.

Adaptive, Lightweight, Coated Fabrics for Protection from Low-Velocity Fragments and Projectiles

117748
Year 2 of 3
Principal Investigator: J. W. Foulk III

Project Purpose

Fragmentation weapons such as improvised explosive devices (IEDs) are responsible for 60%–70% of troop casualties and the majority of injuries in modern warfare. Most of these injuries occur to the extremities. The threat of fragmentation weapons has grown dramatically with the urbanization of combat, and this has caused the rate of amputation in the Iraq war to double from previous conflicts. Soft-fabric armor offers optimal personnel protection from fragments and other low-velocity projectiles. However, current designs for bullet-resistant vests are too heavy and bulky to extend protection to the extremities. Through novel, multifunctional fiber coatings, we propose to develop lightweight, flexible armor with superior ballistic resistance. The thin coatings impact relative yarn motion and do not compromise breathability and mobility. Customization of the proposed fabrics also offers significant enhancements to current vehicle armor systems and innovative solutions to broader surety applications such as drapable fabrics for blast mitigation and asset protection during transport or storage.

This project will integrate Sandia's unique capabilities and experience in the areas of polymer science and modeling and threat and armor characterization to innovate in synthesis, computational mechanics, characterization, and validation. In contrast to colloidal solutions, we seek to develop multifunctional polyurethane coatings that tailor the yarn-yarn frictional response. The mechanisms of weave deformation, inter-yarn friction, and fiber failure will be addressed through fabric models that resolve each yarn as a continuum. Discovery and characterization of the dominant mechanisms is being explored through targeted mechanical (single yarn, yarn-yarn, fabric-fabric) and instrumented ballistic testing (with digital image correlation). An increased understanding of the multiple, interacting mechanisms operative during impact will enable Sandia to not only design new materials but also treat soft armor as a system.

Summary of Accomplishments

In chemistry, we are pursuing multifunctional fiber coatings to tailor the frictional response. We have applied uniform coatings of two different urethanes with comparable densities but different compliance/elongation. A novel technique to ensure thin uniform coatings is dielectrophoresis. We are collaborating with Sigma Technologies to leverage this technology and initial microscopy indicates that several micron coatings are being applied to ten micron fibers (600 fibers/yarn). Targeted fiber-pullout testing illustrated that a less compliant urethane (with more cross-linking) will immobilize the fabric and degrade the performance. This allowed the team to focus on more compliant urethanes. We have also completed fabric-fabric friction testing and studied wave propagation for a single yarn (via Hopkinson bar). The impact velocity, break angle, and wave velocity of the yarn are precisely determined from the recorded images. In a drive to make ballistic testing more quantitative, we redesigned hardware to limited shot-to-shot velocity errors to ± 3%. The ballistic testing has also moved beyond V50 quantification and we are now examining front-face and rear-face fabric deformation with high-speed video and digital image correlation. Quantifying the deformational mechanisms and understanding the impact of coatings will enable us to tailor the frictional response to improve V50 and minimize the out-of-plane deformation. Along with improvements in fabrication and testing, we are also improving the modeling tools in Sierra mechanics. Our goal is to generalize anisotropy for all elements and thus enable current and future models to be easily implemented with increased accuracy. We are also improving macroscale models to better understand fabric-fabric interactions during the initial impact and prior to yarn failure. Novel mechanical, ballistic, and numerical experiments developed this year enabled the team to iterate on coating methodology and we will continue this iterative process in the last year of the project.

Significance

This project contains elements of both fundamental research and technology development focused towards innovative solutions that can potentially have high impact for DOD, DHS, and DOE. The project strengthens our efforts in ballistic testing and helps develop the computational and experimental tools to study/design/improve fabric armor systems.

Oxygen Insensitive Anode Chemistry to Enable the Spray-Paintable Battery

117749
Year 2 of 2
Principal Investigator: C. A. Apblett

Project Purpose

This project intended to develop a battery composition and structure that could function without the need for a casing to protect the chemistry from the environment; in essence, making a battery that was a series of paints, that could be cast sequentially one on top of the other to build up a functional battery. The original intent was to focus on the anode only, and the original concept was to use proteins as catalysts for a sugar-based anode. The proteins would be selective only to the sugars, enabling operation in the presence of oxygen and water, and could operate without a package. Ionic liquids, essentially ionically conductive oils, would be used as the electrolyte, due to their extremely low vapor pressure. However, no combination of protein and ionic liquid could be found that would produce an oxidation reaction. On the other hand, the ionic liquids were found to have a very low solubility of oxygen and water. With this information, we decided to move away from proteins, and focus instead on running lithium ion chemistries in the ionic liquid exposed to the environment. The lithium in ion form would be protected from oxygen and water by the ionic liquid, and electrochemical intercalation compounds could be chosen that allowed the lithium to exist at two different electrochemical potentials that were compatible with oxygen and water in the anode and cathode.

Summary of Accomplishments

We have demonstrated the function and performance of a battery that is capable of sourcing 1 mA/cm^2 and above at room temperature, and which can do so without the need for a package. The chemistry of the system that was finally developed was using $Li_7Ti_5O_{12}$ for the anode, $FePO_4$ for the cathode, and DMPI-NTf_2 (1,2dimethyl-3-propylimidazdium [DMPI] bis(trifluoromethanesulfonyl)imide [$N(SO_2CF_3)_2$ abbreviated as –NTf_2] solvent with a lithium bis(trifluoromethanesulfonyl)imide ($LiNTf_2$)supporting salt. A polymer separator mixed with ceramic was used as the separator, and all of these materials and chemistries are compatible with spray painting onto a surface. The protein based anode chemistry, while still a promise for the future, was not pursued due to the difficulty in finding a common solvent that would support protein function on the anode, oxygen reduction on the cathode, and be stable enough to not evaporate quickly when exposed to the environment.

Significance

The development of small, thin, high-capacity energy sources has application in homeland security, defense systems and assessments, and missions where conformality of the power source is important. This power source can be thin and conform to the shape of the surface to which it is applied. Unattended sensing and on demand power for leave behind tags could be addressed by a spray paintable battery. Nuclear weapons applications could also benefit from this type of source where design geometry prohibits prepackaged power sources.

Real-Time Individualized Training Vectors for Experiential Learning

117752
Year 2 of 3
Principal Investigator: E. M. Raybourn

Project Purpose

Sandia's experience with deploying operational military game-based training systems has highlighted a growing concern about the efficacy of commercial game-based solutions. Fundamental questions asked by military leaders include the following: "What metrics should we use to measure performance in game-based training?" "How can we quantitatively demonstrate that game-based training enhances cognitive agility?" and "Can training be tailored to the individual warfighter's specific needs so we can do more in less time?" We believe there is utility in applying Sandia knowledge capture techniques (text processing, spatial-temporal behavior, and real-time evaluation feedback) to the ill-defined domain of nonkinetic engagement training. However, these knowledge capture techniques have never been employed in an integrated fashion to fully populate learner models, whether a priori or in real-time, nor have the text processing or spatial-temporal behavior capture approaches ever been used to quantitatively assess experiential learning, especially in an operational setting.

Our three-year goal is to verify whether the knowledge capture technologies together perform more robust real-time in-game diagnostics of cognitive state and quantitative assessments of experiential training than they would singly. Additionally, we seek to identify individualized training strategies and create algorithms that can be used to update, populate, and classify learner models in real-time during training. This project will produce an adaptive military training system for enhanced experiential learning.

Summary of Accomplishments

We accomplished the following in FY 2009:

- We evaluated candidate game platforms in which to instantiate our algorithms. These included DARPA's "RealWorld" virtual training environment, the Ground Truth game environment used by LDRD Project 105872, and the Delta3D game engine used in LDRD Project 93596.
- Delta 3D was selected as the training engine and engineering changes were made to the system to interface with the cognitive foundry.
- The project team has analyzed quantitative and qualitative data collected during the Year 1 multiplayer and single-player studies. The team collected self-report quantitative data, psychometric data, qualitative training performance data, observer/evaluator trainee performance measurement data, recall data, after action review (AAR) debriefings, and 86 hours of video of training environment, and 86 hours of video of facial expressions and upper body movements associated with the training study.
- Transcriptions were completed for over 45 hours of data. A brown bag presentation was given on preliminary results.
- Training objectives and metrics for a tactical site exploitation scenario have been identified and initial progress has been made in the development of individualized vectors.
- The Sandia Titan Informatics Toolkit was chosen to assist with data integration, analysis, and clustering of salient phenomena as well as novice vs. expert behaviors.

- Project study methods were presented in conjunction with a poster presentation at the Army Science Conference December 4-7, 2008. The preliminary quantitative frequency results were presented at the Program Executive Office Simulation, Training and Instrumentation (PEO-STRI) Defense GameTech Conference held March 9-12, 2009.

Significance

Cognitive systems can make a significant innovative training contribution by creating new scientific understanding for assessing learning and accelerating novices' learning toward becoming more expert. Our results could enable transitioning this capability to DOD, DOE, and NNSA. This will enable DOE to enhance action/counter-action predictive simulations, co-evolutionary training, and assistive decision-making, as well as lower costs and increase performance for DOE response to the new design basis threat.

Micro Mobility / Propulsion

117755
Year 2 of 2
Principal Investigator: J. R. Salton

Project Purpose

The purpose of this project is to create a small-scale hopping mobility platform to serve as a sensor emplacement device and/or communications relay in hazardous DOE, homeland security (HS), and DOD environments. Outfitted with miniature radiation detectors, cameras, and radios, these miniature hopping robots could be inserted into otherwise inaccessible areas to monitor and assess potentially hazardous situations. Sandia has unique capabilities in the areas of micro-energetics, hopping robots, and cooperative robot control that enable this development. Sandia has developed hopping robots on a larger scale, which can negotiate obstacles over twenty times their height and have a range of several thousand feet. The hydrocarbon-based fuels used in current hoppers require complex valves, fuel metering manifolds and controls, and comparatively large on-board fuel tanks. This project will create miniature, self-contained micro-explosive propellant cells embedded in a combustion cylinder. An array of these cells will allow multiple nominal height hops or few hops of great height. The array contains eight or more propellant cells for providing consecutive hops. Microelectronic packaging technology enables individually controlled cell combustion without sympathetic ignition of neighboring cells.

Summary of Accomplishments

We designed a proof of concept vehicle using a passive spring that enables a single hop. The vehicle is controlled wirelessly via a hand controller with a graphical user interface (GUI). When cocked, a latch holds the hopping foot in place until a command on the wireless controller is given to release it. In addition, the cylinder, piston and energetic array head to perform the hops has been designed in detail. The design and manufacturing of the microelectromechanical system (MEMS) boards for addressing the individual cells is complete. One of the five wafers manufactured has been diced into boards, which have been validated and are ready to be used for testing. The electronics designed for the proof of concept vehicle have been manufactured and validated. Further, the circuit boards for this vehicle are designed to be used for hop testing on the hop test stand and in the final vehicle once it is fully developed. While the energetic array design has not been empirically validated, all of the parts for the initial design cycle have been manufactured and a test plan developed.

Significance

Small, long-range, and highly mobile robotic vehicles would precipitate a revolution in mission capabilities with potential benefits to key Sandia mission areas including defense, intelligence, and homeland security. Beyond obvious benefits to missions requiring small mobility platforms, this project is well-aligned with nuclear weapons missions related to explosive components. This project also advanced research on miniaturized actuation, wireless video and addressable microenergetics.

Automated Entity Relationship Extraction

117758
Year 2 of 3
Principal Investigator: T. L. Bauer

Project Purpose

Intelligence analysts have identified the critical need for automated methods of processing large volumes of textual data with the goal of extracting the most important information and determining how such information is related. This is a task that analysts cannot do with existing tools. Information that is potentially relevant to aiding analysts in target identification and predictive analysis is generated at a far greater rate than anyone can manually review. Thus the need for automated tools for information extraction and organization is crucial to accurate, efficient, effective analysis of emerging threats to national security. In order to provide such tools, this project will investigate and develop language-independent techniques for automatically identifying relationships between named entities in unstructured text while maintaining data provenance.

This research will create a unique capability to generate entity relationship graphs (ERG) from unstructured text. ERGs are graphs consisting of nodes that are entities (people, places, organizations, etc.) and links between nodes that represent their relationships (works-for, member-of, lives-at, etc.). ERGs have been used effectively to organize and analyze information associated with individuals and groups, how they are related, and how they interact. However, these ERGs are most often constructed manually by expert analysts intimately familiar with the associated entities and documents. The creation and maintenance of such graphs is time consuming and does not scale to the massive amount of data available.

This project will result in tools that will expand existing Sandia text analytic and visualization capabilities by enabling automatic ERG generation across multiple languages. These tools will provide a unique graph-generation capability for intelligence analysts, reducing the amount of time spent on manual document processing, thus providing time for analysis. This will enable analysts to provide more-efficient assessments on national security with a high degree of confidence in their assessments.

Summary of Accomplishments

Accomplishment 1: Core architecture — built the core architecture for running a stochastic, parallelized analysis of text.

Accomplishment 2: Basic Processing Elements — Built text-based processing elements on top of the core architecture

Accomplishment 3: Demonstration — demonstrated basic processing elements functioning inside of the Repast Simphony agent architecture

Invention disclosures:

- Probabilistic Analysis for Information Extraction
- A method for processing text on a blackboard agent system (to be filed)
- Application of minimum description length encoding concepts to agent-based text analysis (to be filed)

Copyrights:

- Blackbeard — a library for agent based information analysis (to be filed)
- Blackbeard-text — a library for agent-based text analysis (to be filed)

Paper:
P.A. Chew, B.W. Bader, and A. Rozovskaya, "Using DEDICOM for Completely Unsupervised Part-of-Speech Tagging," to be published in *Proceedings of the NAACL-09 Workshop on Unsupervised and Minimally Supervised Learning of Lexical Semantics*.

Significance

The results of this research will enable analysts to extract information hidden in massive amounts of data much more rapidly and accurately than is done today. This will help analysts create assessments on national security where the sources of information are verified and validated, which consequently provides a high confidence in their assessments. These capabilities meet critical needs important to intelligence analysts and support the goal of strengthening national security.

Extremely Thin Chemical Sensor Arrays Using Nanohole Arrays

117759
Year 2 of 3
Principal Investigator: I. Brener

Project Purpose

The choices for making sensitive chemical sensors are very limited: for example, most optically based sensors require enough interaction length (centimeters or even meters). Other approaches require less depth but larger areas. Lately, nanohole-arrays have emerged as a plausible platform for chem-bio sensors. These samples are made by fabricating subwavelength holes (~50–200 nm for visible light) with spacings of 200–1300 nm onto very thin metallic layers. Although subwavelength, a disproportionate amount of light can go through these holes through coupling to surface plasmons, in what has been termed “extraordinary optical transmission.” This transmission is exquisitely sensitive to the microscopic surface chemistry in the vicinity of the nanoholes. Furthermore, multistacks of these nanohole-arrays show an even further sensitivity and suppression of unwanted background. By using these nanohole-arrays in transmission mode, with small areas functionalized with specifically designed molecules to ligate desired analytes such as explosives and chemical weapons agents placed directly on top of thin photodiode arrays (<50 μm), we can have a complete solution to chemical sensor arrays.

Summary of Accomplishments

In the second year: a) we developed a robust process to fabricate single-layer nanohole array samples with different hole geometries and theoretically explored double-layer samples which show sharper resonances; b) we designed and synthesized two diazonium compounds designed to sense dimethyl methylphosphonate (DMMP) after a deprotection step and applied them to nanohole array samples; c) we developed the necessary hardware for controlled exposure and calibration; and d) we purchased all the necessary components for a proof of concept of a simple multiplexed sensor.

Significance

These sensors can have multiple applications in national security such as space control, surveillance, nonproliferation and the security of our armed forces.

Flexible Thin Film Battery Development

117761
Year 2 of 2
Principal Investigator: P. G. Clem

Project Purpose

Rechargeable power sources such as batteries are needed for thin, remote-powered sensors and microsystems, but direct integration options to incorporate very thin custom batteries on flexible microsystem platforms have not been fully developed. We are using direct-write fabrication to print thin (submillimeter) lithium ion batteries on flexible substrates, and characterize resulting power capacity and current capacity. Well-characterized materials used for cylindrical cell fabrication have been printed in thin film form, aimed at 50 micron to 500 micron battery thicknesses. A resulting design map of power-current values is being developed, including available commercial options, which would be valuable for design of portable sensors for transmit/receive and other sensor options.

Thin film batteries were fabricated by spray coating and direct write using existing commercial and Sandia battery microparticle and nanoparticle materials to print thin (< 500 micron) and conformal 3D batteries, perform electrolyte filling and sealing, and test battery performance. As an example, a 100 micron thick lithium battery the size of a sheet of paper contains an equivalent volume to a 3.6 volt, 650 mA-h cell phone battery, suggesting a capability adequate for thin film batteries to provide sufficient power for long-term sensing and transmitter/receiver (Tx/Rx) applications.

Direct write provides a potential means of eliminating packaging that limits performance of commercial off-the-shelf (COTS) 100 micron thickness batteries; in addition, custom battery shapes and areas may be fabricated by direct write. A potentially attractive feature of direct write batteries is the capability to prepare custom 3D batteries on space-limited volumes to maximize battery capacity compared to planar-only COTS cells. Finally, use of lead-acid battery chemistry would enable a larger temperature range of operation (–40 to 60 °C) than COTS lithium cells (–10 to 60 °C), at a cost of energy density. These capabilities enable new power options for radio-frequency identification (RFID) and microsystems.

Summary of Accomplishments

In this project, we successfully demonstrated what we believe to be the first fully functional, printable thick film lithium batteries, which enables flexible design of thin power sources for portable electronics. Mature lithium battery technologies ($LiFePO_4$) cathode, Celgard or polyethylene oxide separators, ($LiPF_6$ liquid electrolyte, and carbon anodes) were extended from traditional tape casting deposition and may now be printed using a robotic toolpath syringe dispense or Robocasting™ approach developed at Sandia. Batteries thus printed displayed energy densities of 110 mA-hours/gram, with stable 3.4 volt output. Minimization in packaging volume enables a doubling of energy density compared to commercial off the shelf batteries, as well as an arbitrary printed form factor. A key advance was development of printable encapsulation materials that are compatible with the liquid electrolyte as well as diffusion barriers to oxygen and moisture diffusion.

This work has led to alternate approaches to thin battery fabrication, including investigation of solid state electrolytes for robust, printed portable power sources.

Significance

Compact power sources are critical, differentiating and enabling technologies for personal electronics, RFIDs and remote environmental and structural sensors. The ability to directly integrate high performance batteries on compact packages enables new, monolithically integrated sensor/RFID topologies. These integrated power sources may be coupled with microsystems for compact sensing and communication technologies with applications to environmental sensing, power monitoring, and structural health monitoring. This work has been leveraged into programs where compact and flexible power platforms compared to commercial parts are a significant advantage. For future applications, the ability to develop arbitrary form factors has advantages for integration into defense systems with maximum design flexibility and compactness. Finally, printable power sources may be applied to printed or thin film solar cells to enable distributed energy storage for power supply leveling to overcome power fluctuations inherent due to variable cloud cover.

Integrated Point-of-Use Two-Dimensional Fuel Cell

117762
Year 2 of 3
Principal Investigator: K. R. Zavadil

Project Purpose

Proliferation assessment requires high energy density and long-lived power sources with moderate currents (mA) that can be used as building blocks in platforms for the continuous monitoring of chemical, biological, and radiological agents. Fuel cells are an optimum choice for a power source because high energy densities are possible with liquid fuels and power generation and fuel storage can be decoupled for independent control of energy and power density for customized, application driven power solutions. Fabrication of two-dimensional, mechanically compliant fuels cell is a technical challenge. We propose to capitalize on new developments in nanotechnology, advanced fabrication techniques, and materials science to create a planar direct methanol fuel cell that could be collocated with electronics in a chip format. Massively parallel, directed assembly of a variety of nanomaterials will be used to fabricate multifunctional electrode arrays encapsulated in an ion conducting membrane. Materials will be largely polymer-based, including a methanol reservoir, to provide a mechanically compliant and possibly optically transparent device. Total dimensions of this device will be less than 100 micron in thickness with an area that could reach 600 square centimeters. The fabrication approach is sufficiently flexible to incorporate a wide variety of material types, further expanding the utility and applications of the developed technology pathway. The benefit produced by this proposed research effort will be the creation of a building block power source that is durable, rechargeable, and geometrically functional (i.e., conformal and low dimensional). The envisioned technology path is expected to serve as a model for other applications that require the integration of multifunctional nanomaterials, specifically where catalysis, electronic and ionic conductivity are critical.

Summary of Accomplishments

We have demonstrated an ultrathin prototype direct methanol fuel cell (DMFC) platform based on arrays of carbon fibers that serve as a conductive and structural scaffold for the power source. Electrocatalytic films are deposited onto these fibers using this project's previous accomplishment of developed layer-by-layer chemistries involving conductive polymers. We have demonstrated that functionalized metal nanoparticles can be directly bound to the carbon fiber surface and further incorporated into a porous polyelectrolyte layer. Additionally, selective electrocatalysis of oxygen reduction, in the presence of methanol, has been demonstrated using shape directed synthesis of palladium structures. The significance of having demonstrated selective catalysis is that the prototype power source will be tolerant of some degree of fuel cross-over, expected at the small length scale of a thin power source. We have demonstrated coating of these carbon fiber electrodes with Nafion as a proton conducting electrolyte without loss of electrochemical activity. The structure is encapsulated in cellulose as a fuel, oxidant, and water permeable coating to provide dimensional stability for the electrode pair. This packaged unit will serve as a prototype platform for optimizing the three-phase boundary necessary for achieving the target 1000 Whr/L energy density possible with a DMFC.

These basic concepts have been extended to produce much thinner composite electrodes that can be patterned onto planar substrates. Microcontact printing has been used to print polyelectrolyte patterns onto oxidized silicon surfaces. Functionalized carbon nanotubes are employed similarly to the carbon fibers. Electrical conductivity of the resulting electrode is ensured by using nanotube densities above the percolation threshold. Appropriate functionalization of the silicon surface, carbon nanotubes, and the use of a polyionic polymer allow control of the thickness of the resulting electrode pattern. These structures provide an approach to further dimensional scaling of fuel cell power sources.

Significance

The prototype power source and technology pathway developed over the course of this work will enable device development for a range of surveillance, reconnaissance, remote sensing, and validation technologies for addressing concerns of national security. The technology is expected to impact the missions of homeland security, by addressing countermeasure sensor architectures needs, and DOE's nuclear weapons program, by addressing the need for microscale manufacturing technologies.

Understanding and Developing Countermeasures for Botnets

117764
Year 2 of 3
Principal Investigator: J. Van Randwyk

Project Purpose

Bots and botnets are a more recent form of malware that present myriad threats to our information systems. The purpose of this project is to study bots and botnets and develop tools to better understand them and mitigate their threat(s).

Summary of Accomplishments

We have conducted a deep-dive analysis on one of the more interesting and potentially harmful bots currently "in the wild." The Waledac bot appears to be a follow-on to the notorious Storm bot and has shown some loose connections to the Conficker making it an ideal candidate to study and follow. Getting this bot to a point where we could analyze the assembly code was a significant accomplishment because of the packing and other obfuscation techniques used by the authors.

We built a sandbox capability for running and observing bots without negatively impacting the Internet (i.e., the bot cannot successfully spread or attack out of our sandbox). We are currently observing the Waledac bot and learning more about its behavioral characteristics. The sandbox environment allows us to monitor and receive updates to the bot as it evolves.

We wrote an internal report on the topic of bots and botnets describing why they are a problem and what general mitigations can be applied.

Additionally, we presented the FARM (forensic analysis repository for malware) work at the IEEE International Carnahan Conference on Security Technology. This capability, developed early in this project, has now "spun off" from the LDRD project, and further FARM development continues under funding from internal and external sponsors.

Significance

Our research results can help in securing information systems from Sandia through the rest of the federal government. Additionally, bots/botnets pose a threat to most any computer, meaning that a typical home Internet user is susceptible to having this malicious software on their computer. The economic consequences to our country of such a large base of installed malware could be extremely large. Our work contributes to better understanding and mitigation of this malicious software.

Composite Thermal Protection Systems Incorporating Energy Absorption With Oxidation Resistance

117770
Year 2 of 2
Principal Investigator: A. C. Hall

Project Purpose

Present flight profiles for hypersonic vehicles are severely constrained by the lack of insulation materials that can protect the underlying structures in the very high temperatures and aggressive oxidizing conditions encountered during high-speed atmospheric maneuvers. Available carbon-carbon (C-C) composites have sufficient thermal and mechanical stability for high velocity flights above the atmosphere. However, they are susceptible to oxidation, rendering them useless for long duration hypersonic flights at lower altitudes. We have been investigating inorganic materials that can be infiltrated into the pores of a C-C matrix and that convert to high-temperature, oxidation-stable coatings as they undergo endothermic transitions on heating. Our work plan for year 2 makes use of previously developed multilayer refractory coatings for C-C composites that were adherent, continuous and that survived thermal cycling and heating to $T > 2600$ °C in static air for several minutes. We also propose to investigate materials modifications and a new, more production-compatible method to coat multilayer refractory boride and carbide coatings onto C-C composites. This uses low pressure plasma spray process. We also propose to modify an existing Sandia plasma torch facility to allow more realistic high-temperature test conditions for our materials without having to resort to slow and expensive arc jet tests. Additionally, use of low pressure plasma spray deposition may provide a coating method that is more scalable to large part sizes than our previous methods.

Summary of Accomplishments

We discovered that the low pressure plasma spray system can be used to create a heat flux and atmosphere that are more representative of the arc-jet test that is used to screen thermal protection system (TPS) materials than the furnace testing or solar tower testing that are traditionally used. This same system was evaluated as a more production-compatible method for producing adherent refractory coatings that would protect the C-C coating from oxidation. Although continuous coatings that appear to be adherent were produced, there was limited penetration of the coating into the porous C-C beyond the immediate surface.

Significance

This project will strengthen US national security by addressing the national need for global presence and strike capability with a rocket-boosted, expendable, flight vehicle that reaches its target by executing unpowered glide maneuvers at hypersonic speeds. Lack of TPS capable of long-duration hypersonic flight in the atmosphere has been identified as the main technical barrier to meeting this mission need.

Investigation of Technologies for Hypersonic Payload Release

117773
Year 2 of 2
Principal Investigator: W. P. Wolfe

Project Purpose

Due to significant interest at the Department of Defense (DOD) for developing a weapon system for prompt global strike (PGS), an investigation is proposed to continue researching technologies for payload release at hypersonic speeds. PGS will require cruise flight of the weapon system at hypersonic speeds. Currently, limited research is available considering the flowfield physics and mechanical system technologies required to release payloads in this speed regime. Therefore, the primary objectives for this project are the following. 1. Establish the feasibility of hypersonic payload release. 2. Investigate the maturity of technologies for hypersonic payload release. 3. Develop preliminary designs to demonstrate viability. Successful development of technologies for hypersonic payload release will enable numerous, desired payload applications for PGS.

Desired payload applications for hypersonic release include strike missions, pre-strike sensing systems for targeting, and post-strike damage assessment. Pre-strike sensing systems would include both airborne and ground-based sensing systems. These systems could provide updated target location information to a hypersonic weapon en route to the target. Post-strike airborne and ground-based sensing systems would provide damage assessment after target engagement by the weapon system. A post-strike sensing system could be integrated on the hypersonic weapon system and released prior to target engagement; thus, providing both target defeat and damage assessment on a single weapon system.

The primary challenges for hypersonic payload release are related to the separation event. During separation, the ballistic body must maintain aerodynamic stability, avoid re-contact with the parent vehicle, and provide acceptable rigid-body motion to allow the sensing payloads to navigate throughout separation. First, the feasibility of hypersonic payload release will be demonstrated through conceptual designs. Then, these concepts will be matured through additional mechanical, aerodynamic, and thermal analysis to reduce risk.

Summary of Accomplishments

A study was conducted to investigate the feasibility of store separation from a reentry-like body cruising at hypersonic speeds. Unlike lateral store separation from conventional aircraft, the store is ejected from the base of the reentry vehicle (RV). Since the base flow gradients behind a reentry body are more benign than the shock-induced lateral flow gradients, an aft-deployed store will encounter a less-stressing environment than for lateral deployment. Considering launch perturbations and flowfield gradients, the two-body computational fluid dynamics (CFD) flowfield solutions coupled with trajectory simulations demonstrate that maximum pitch rates and angles of attack for the aft-deployed body are less than 100°/s and 10°, respectively. These flight dynamics are well within limits of commercial off-the-shelf (COTS) inertial measurement units (IMUs), thus allowing the payloads to navigate during the separation event without saturating the sensors. This project demonstrates that aft deployment of a store from the base of an RV is feasible and practical. A generic preliminary design was developed to accommodate any payload within the available volume.

The current concept uses a universal ballistic body that is aerodynamically stable and has sufficient thermal protection to survive the hypersonic flight environment. This body carries the final payload vehicles which are deployed after the ballistic vehicle decelerates to subsonic speeds and descends to lower altitudes, thus releasing the final payloads in relevant flight environments for their design. Preliminary designs were developed for the

RV ejection mechanism, the universal ballistic body, and the mechanism for deploying the final payloads from the ballistic body. Although the current point design concentrates on sensor minidarts as the final payload, the concept and general vehicle design can be tailored for a wide range of payloads.

Significance

This work benefits Sandia's mission by developing hypersonic payload release technologies necessary to strengthen national security and to protect our nation against terrorism. This technology will strengthen US national security by providing a conduit for intelligence gathering. This technology provides a means to rapidly deploy sensing systems and strike payloads to detect, characterize, and destroy mobile terrorist threats and transform our military into a more effective, agile force.

The SEPIA Hybrid Network Analysis Environment

117774
Year 2 of 2
Principal Investigator: T. D. Tarman

Project Purpose

A key aspect of Sandia's significant computer security research program is to understand and protect against threats to networked systems. Security analysts typically utilize real network systems, computer emulations (i.e., virtual machines) and simulation models separately to understand the interplay between threats and safeguards. In contrast, Sandia is investigating new ways to combine these three technologies to provide hybrid "simulated, emulated, and physical investigative analysis" (SEPIA) environments. SEPIA environments extend the existing system-in-the-loop (SITL) interfaces provided by network simulation tools. It lets simulated networks pass network traffic and perform, from the outside, like real networks. We connect both emulated (also referred to as virtualized) and physical (i.e., real) network routers and computers to those simulated networks to provide higher fidelity representations of key network nodes while still leveraging the scalability and cost advantages of simulation tools. The result is to produce large experimental networks of computers and network devices using the SEPIA environment where we can analyze threats and test various protection approaches with the desired fidelity at a reasonable cost.

This project successfully proved the utility of the SEPIA approach and aggressively expanded and improved SEPIA to address larger problems. Additional R&D activities and developments were focused on understanding the approach's limits. We expanded our simulator and emulator libraries, automated the creation of SEPIA networks, and tested the SEPIA approach at larger scale. In terms of impact, our research dramatically improved Sandia's approach to computer network security analysis and created spin-off tools and processes that support this new approach.

Summary of Accomplishments

In FY 2009, the SEPIA team accomplished the following:

- We refined the set of specifications for defining SEPIA experiments, and developed tools for constructing scenarios and experiments. Experiments are defined using the OPNET (optimized network engineering tools) network editor, and exported into extensible markup language (XML) format for post-processing by SEPIA tools.
- We developed initial theories and tools for predicting whether a SEPIA simulation can perform at real-time and can "keep up" with virtual machines and physical devices. We conducted experiments to determine parameters for this model, and ran additional experiments to validate the predictions that this model makes. Good agreement between the model and experiments was observed.
- We expanded the OPNET system in the loop (SITL) capability to implement the exchange of standards-compliant border gateway protocol (BGP) messages between real (or virtualized) routers and routers in the simulation.
- We submitted a paper describing the SEPIA research to the Institute of Electrical and Electronics Engineers Military Communications Conference (IEEE MILCOM) conference for peer review, the paper was accepted, and we submitted the finalized paper.
- We updated the FY 2008 demonstration to incorporate the updated tools and to demonstrate a more interesting scenario.
- We completed our final report.

Significance

This work will benefit Sandia's counterintelligence, homeland security, and work for other programs. Sandia's ongoing and comprehensive effort to assess, detect and deter foreign intelligence and terrorist threats to areas within our purview as well as those of our DOE, DHS and work for others (WFO) customers points to computer network security as a key vulnerability area. This work greatly enhances our ability to understand and deter such cyber threats.

High-Speed Spectral Sensor

117775
Year 2 of 3
Principal Investigator: S. A. Kemme

Project Purpose

This project investigates a multicolor spectrometer and radiometer based upon an active resonant subwavelength grating (RSG). This active RSG component acts as a tunable high-speed optical filter that allows miniaturization and ruggedization not realizable using current sensors that use conventional classical optics. Furthermore, the geometrical characteristics of the device allow for inherently high speed operation.

The differentiating technology — the active RSG device — can be geometrically scaled to access a wide wavelength range and accommodate a set of phenomenologies from initial fireball flash analysis (ultraviolet [UV]-short-wavelength infrared [SWIR]) to debris cloud evolution (out to long-wavelength infrared [LWIR]). Sandia invested considerable effort on a passive RSG three years ago, which resulted in a highly efficient (reflectivity greater than gold), wavelength-specific reflector. In this project, we intend to transform the passive RSG into a high-speed optical filter array and integrate it with high-speed data acquisition hardware for a compact, low-power sensor without moving/scanning elements. In this way we can demonstrate a growth path toward a fly-away instrument, missile, airplane, or other high altitude platform.

Because of the inherently small critical dimensions of the RSG devices, the fabrication of these sensors can prove challenging. However, we leverage the state-of-the-art capabilities of the Sandia microfabrication (MicroFab) facility to realize these subwavelength grating devices. Another challenge involves the high-speed data acquisition required to discriminate the proper spectral information from a rapidly changing scene. In years two and three, we anticipate ramping up this effort to complement focal plane arrays with integrated passive and active RSG components.

Summary of Accomplishments

We have achieved each of the stated FY 2009 goals and milestones for the project. We have designed the signal amplification and data acquisition components and procured parts for these systems. We have fabricated a passive resonant subwavelength grating (RSG) array with a linear detector array configuration. Finally, we have fabricated and tested an active RSG device and are now optimizing this design for higher speed operation.

Specifically, we have demonstrated the device modeling, fabrication, and testing of an active resonant subwavelength grating device. By applying a voltage to interdigitated fingers on a $BaTiO_3$ electrooptic thin film, we were able to modulate the effective refractive index and thus the reflection/transmission spectra of the device. We achieved electric fields upwards of 80 kV/m between the Ti/Au electrodes and observed red-shifting of ~1530 nm RSG transitions by 2 nm at maximum applied voltage. We also observed a nonlinear shift of peak/trough position with respect to voltage. This is possibly related to the quadratic electrooptic effect, which would be expected in a $BaTiO_3$ film.

The system integration and demonstration phase of this project will utilize an active RSG device in a spectrometer configuration. A narrow band laser source will be incident on the RSG filter and any transmitted photons will pass through the filter and excite a photodiode. The bias voltage, and hence the pass band wavelength, of the RSG will be driven by a bias generator circuit. The bias voltage signal will also be collected and used to derive the optical energy (photodiode current) versus pass band wavelength (bias voltage) spectrometer signatures.

Significance

The work described has direct relevance to various missions that seek to reduce the threat of long-range projectiles.

Creating a Model-Based Secure Digital Radio Design Methodology

117777
Year 2 of 2
Principal Investigator: K. D. McDowell

Project Purpose

We seek to create a military global positioning system (GPS) receiver design capability that will be unique in at least two aspects.

The first unique aspect of the receiver will be the ability to retain GPS signal lock while experiencing extremely high dynamics and provide precise carrier-phase measurements. The proposed dynamics are currently unmatched in any available receiver. However, the dynamics are very representative of what would be experienced in various advanced aerospace applications.

The second unique aspect of the design is a National Security Administration (NSA) approved secure state machine on a field programmable gate array (FPGA). The secure state machine will implement the GPS key data processor (KDP). The KDP enables the receiver to receive and decrypt military positioning signals. If successful, Sandia will have the first NSA approved FPGA implementation of a military GPS receiver.

The FPGA implementation of the receiver will not only meet the needs for advanced military aerospace applications, but also afford the flexibility for future precise navigation applications and secure radio designs.

Summary of Accomplishments

We demonstrated a flexible GPS receiver capable of tracking through high dynamic conditions. Our receiver tracked through dynamics 20 *g* higher than a standard military receiver. The flexible design allows the receiver to be modified to address exotic navigation problems that Sandia is often asked to solve.

Also, the investment has created an indigenous expertise in global navigation satellite systems and associated technology. This expertise can be used not only in radio navigation but in the field of general satellite communication.

Significance

A robust model-based digital radio design capability benefits DOE's national security missions by helping sustain the technology backbone needed for both ground-based monitoring and flight test elements. This effort also anticipates future developments for precise and reliable delivery of weapons. The proposed state-machine theory approach to safe and secure digital design has potential for far-reaching applicability.

LEEM Examinations

117778
Year 2 of 3
Principal Investigator: M. L. Anderson

Project Purpose

In this project, the LEEM (low-energy electron microscope) has been used to image application-based integrated circuits in a nondestructive manner. In particular, we are interested in determining if it is possible to extract quantitative dopant information from the LEEM. We will continue to demonstrate the LEEM's applicability to several analysis problems on multiple structures. A significant portion of the work remains in determining optimum sample preparation as well as determining the limitations of image contrast generation.

Summary of Accomplishments

Over the past two years, we have successfully proven that even though the LEEM is generally used for surface science studies, it is also a useful tool for imaging devices. We have designed methods for deprocessing and mounting samples in this ultrahigh vacuum system. We continue to work towards improving sample preparation, defining the source of image contrast, and determining methods of improving signal to noise.

Significance

LEEM would give Sandia an important, new, and widely applicable and differentiating technology for sample imaging. This would be of significant value for Sandia's science and national security mission.

Ultrathin Optics for Low-Profile, Innocuous Imager

117779
Year 2 of 2
Principal Investigator: R. Boye

Project Purpose

The goal of this project is the demonstration of a novel imager with a thickness measured in microns rather than inches. Traditional imaging systems, i.e., cameras, cannot provide both the necessary resolution and form factor required in many applications. Designing an imaging system with an extremely thin form factor (less than 1 mm) immediately presents several technical challenges. For instance, the thickness of the optical lens must be reduced drastically from currently available lenses. Additionally, the image circle is reduced by a factor equal to the reduction in focal length. This translates to fewer detector pixels across the image. To reduce the optical total track will require the use of specialized micro-optics and the required resolution will necessitate the use of a new imaging modality. While a single thin imager will not produce the desired output, several thin imagers can be multiplexed and their low resolution (LR) outputs used together in postprocessing to produce a high resolution (HR) image. The target of this project is to demonstrate the feasibility of producing high-quality images in a form factor approaching 100 microns.

Summary of Accomplishments

The ultimate goal of this project was to demonstrate a thin imager and determine the feasibility of reducing an imager's total thickness to 100 microns. The approach taken was to survey what was available and consider advanced fabrication techniques for lenses. Additionally, the postprocessing required to synthesize usable images from the small, low-resolution images that would be recorded by the imaging array would be demonstrated.

The utility of the iterative back projection (IBP) algorithm was successfully shown with simulated imagery. Techniques for registering individual images were also investigated and the limits on these approaches were quantified. The fabrication of a diamond turned lens demonstrated the ability to increase image size and quality while also decreasing the optical track length. Experimental results also showed increased resolution using the IBP; however, these improvements were somewhat limited due in part to fixed pattern noise and defects in the imaging array (leading to registration errors). The smallest optical total track demonstrated was 400 microns.

Significance

This kind of novel form factor imaging system will allow integration into many systems and applications. It would be a very versatile sensor that would have direct utility for Defense Systems and Assessments, Energy Resources and Nonproliferation, and Homeland Security and Defense missions.

Solving Unique Challenges Associated with Packaging and Materials Interactions for Things Thin

119355
Year 2 of 2
Principal Investigator: C. C. Mitchell

Project Purpose

Packaging and environmental protection of small thin components creates a great challenge that is currently unsolved. The fragility of small items means that the inherent stresses of the materials and techniques used in packaging can significantly damage the thin component, especially if there is a desire for flexibility. Packaging processes also have specific requirements of flexibility, infrared (IR) transparency, radio-frequency (RF) transparency, and opaqueness in the visible light range that present additional challenges. We have chosen three surrogate systems for experimental development of thin packages. They are an integrated sensor system, silver nanoparticle traces and compliant substrates. These three technologies represent thin flexible devices for packaging and will allow the development of thin packaging strategies. Standard encapsulation materials comprised of rigid, semirigid and flexible polymeric substrates have been expanded to include solid sheet stock material that can be laminated by heat and pressure or adhesive means. Paper and paper-like products (both pulp and plastic-based) were also identified as a key area of research. A variety of thin polymeric sheet materials, as well as paper and paper-like materials have been obtained and examined with respect to processing and RF properties. The primary processing method utilized to date has been CO_2 laser etching. A new tool/processing method is necessary to allow the development of packaging schemes for paper and paper-like products that are not amenable to standard machining. Currently there are essentially no integrated flexible packaging schemes for thin devices that meet customer and sensor requirements. This LDRD project is trying to fill this void, at least in part, and equip Sandia with the expertise to be a leader in thin packaging.

Summary of Accomplishments

We obtained a variety of thin polymeric sheet materials, as well as paper and paper-like materials. The bulk of these materials were characterized with respect to CO_2 laser cutting and forming and their RF properties. In this way we started building a database of mechanical, electronic (RF) and processing methods properties to enable future thin package engineering. We also completed some light transmission testing for our paper materials, since it might be desirable to use our thin packaging methods for devices containing thin flexible photovoltaics.

When looking for plastics for thin packages, a variety of materials were considered. However, while a number of novel materials might have been promising, it was decided that the sheet plastic currently most used for encapsulation is polyvinyl chloride (PVC) and that it would be the best test bed for pushing the limits for thin packaging.

A successful thin encapsulation method for forming a printed PVC package was developed. It involved printing on both the top and bottom layers using modified commercial equipment prior to assembly. Heat lamination was used to bond as many layers as possible. Finally, spray adhesives were used to bond the top layer to the internal filled layers without warping.

This project successfully demonstrated both paper packaging and thin plastic packaging methods on mock thin devices.

Significance

Sandia currently plays a strong, leading role in packaging of sensor devices. This project allowed us to gain capabilities that are necessary to remain a leader in this area as devices become smaller and thinner. Current device development is moving into a size arena where packaging capabilities do not exist. Successful demonstration of thin packaging should establish Sandia at the forefront of packaging thin devices required to meet future national security challenges.

A Toolkit for Detecting Technical Surprise

130697
Year 1 of 2
Principal Investigator: M. W. Trahan

Project Purpose

The detection of scientific or technological surprise within a secretive country or institute is very difficult. The ability to detect such surprises would allow analysts to identify capabilities that could be a military or economic threat to our national security. Sandia's current approach utilizing ThreatView has been successful in revealing potential technical surprises. However, ThreatView has limitations.

ThreatView presents data visually, which allows analysts to identify trends, patterns, and relationships that otherwise are very difficult to detect. However, this detection is dependent upon the analyst: some analysts see the patterns; some miss the patterns (false negatives); and still others see patterns that are not real (false positives). Also, ThreatView uses a single algorithm to cluster the data. There is no way to compare its results to an alternative clustering or to measure the quality of the clustering. ThreatView's algorithm is optimized for textual data and is not easily extended to other data sets, which limits its data fusion capabilities. We propose to address these limitations by developing a toolkit, which can be used independently or as an extension to ThreatView.

As datasets become larger, it becomes critical to use algorithms as filters along with the visualization environments. We will create a suite of algorithms to filter the data so that analysts are presented with less, but more relevant, data increasing the chance of detecting a scientific or technological surprise. Also, by using suites of algorithms, we will reduce the number of false positives and false negatives while establishing confidence limits. We will also implement several standard metrics to measure the quality of our results and allow direct comparison of results across multiple algorithms. By using non-text specific algorithms, we will provide a toolkit which can be adapted to provide future data fusion opportunities.

Summary of Accomplishments

This year we have achieved the following:

1. Identified and acquired several textual data sets for training/testing. These data sets include standard data mining data sets, which will be used to validate our algorithms, and technical surprise-specific data sets, which will be used to demonstrate the utility of our algorithms for the detection of technical surprise.
2. Selected a set of standard data mining metrics to measure the performance of our algorithms and ThreatView. These algorithms will allow us to quantitatively compare the performance of competing approaches.
3. Implemented a set of preprocessing algorithms for removal of stop words, stemming, etc.
4. Completed the basic research on the use of SOM (self-organizing maps) in data mining and implemented and tested a SOM.
5. Implemented a set of visualization algorithms for the SOM results.
6. Completed the basic research on the use of GA (genetic algorithms) in data mining and have developed an implementation plan for next year.

Significance

Sandia has an ongoing mission to find, evaluate, and exploit technical surprise. A toolkit to discover evidence of technical surprise in textual data sets will provide opportunities for early investigation, evaluation, and exploitation of potentially disruptive capabilities and technological developments that could threaten our national security.

A Zero Power, Motion Sensitive MEMS Wake-Up Circuit

130698
Year 1 of 2
Principal Investigator: R. H. Olsson

Project Purpose

Eliminating standby power is critical to extending the lifetime and reducing the size of tagging, tracking and locating (TTL) devices. Ideally, a TTL device would remain in standby consuming zero power until an event triggers power-up of the entire device for data logging, processing or transmission. In reality, processing the wake-up event often requires significant power consumption, particularly for complex event signatures, which limits device lifetime and size. We propose a zero power microelectromechanical system (MEMS) circuit capable of waking-up a TTL device upon the detection of simple motion or complex vibration signatures. The proposed wake-up circuit operates based on piezoelectric transduction of mechanical vibration, producing an output current proportional to mechanical displacement. When no acceleration/vibration is present there is zero displacement, zero output current and thus zero power consumption. Under acceleration, a strain induced in a thin film piezoelectric layer produces a current that is passed through a resistor to create a voltage that must be large enough to turn on a transistor. Since the accelerometer displacement/piezoelectric output current can be engineered to respond only to certain vibration frequencies, complex vibration profiles can be programmed into the wake-up circuit and processed in the mechanical domain without consuming power. Major challenges to be overcome in order to realize the proposed TTL wake-up device are covering the frequency range of interest in a single microfabrication process and realizing a large enough voltage signal swing to trigger tag wake-up in an event but consume zero power in standby.

Summary of Accomplishments

We began FY 2009 by exploring different vibration sensor designs and comparing devices in terms of resonant frequency, output charge, size and fabrication complexity. Based on these findings, a fabrication process was developed for mass producing sensor arrays with in-plane displacement under acceleration. To date, we have modeled, designed and partially fabricated an array of 4 MEMS wake-up sensors covering the 500 Hz to 1 kHz vibration frequency range. Utilizing 3D finite element modeling (FEM), we are able to individually control both the resonant frequency and the amplitude of the acceleration response. For the initial mask designs, each device operating at a different frequency was designed to give an identical response to vibration on resonance of 7 V/G with capacitive termination. This voltage swing is large enough to completely turn on (> 10 µA) a transistor when the specified vibration is present while having the transistor hard off (< 10 nA current) when the vibration on resonance is below threshold or the vibration is off resonance. The initial prototypes were designed to displace laterally as this allows for a simplified process flow when compared to vibration normal to the substrate. In these designs, lateral displacement of the proof mass causes strain in the sensor beams. This strain is transduced into a charge using a thin piezoelectric layer of AlN. Using FEM, the resonance frequency and charge output were determined to be independent of device thickness, reducing variations due to manufacturing tolerances and allowing a thickness to be chosen based on reliability and ease of fabrication. We have successfully fabricated and packaged an array of four vibration spectral sensors and will characterize these sensors in October 2009.

Significance

The development of the proposed zero power MEMS wake-up circuit for tagging, tracking and locating (TTL) directly impacts Sandia missions in nonproliferation of weapons of mass destruction (WMD) and homeland security. The successful development of the proposed wake-up circuit can significantly reduce the size and power consumption of this important class of TTL devices.

Advanced Optics for Military Systems

130699
Year 1 of 3
Principal Investigator: B. Bagwell

Project Purpose

Today's fighting forces in Iraq and Afghanistan need continuous, 360° situational awareness and the ability to rapidly zoom in for identification, targeting, and tracking. Urban environments are inherently a mixed-range, rapid transition environment. Troops on the ground must enter and clear a building, dictating short range shots (< 10 m), and then move to an alley-way, roof-top, or open area where distances might exceed 300–500 m. The first scenario requires a 1X reflex sight, the second a higher magnification (typically > 3X). Troops in vehicles must monitor the entire area surrounding them, given that they never know where the next threat might come from. Current imaging systems simply do not provide the 360° situational awareness needed.

In this project, we plan to leverage our previous work in "foveated imaging" and "adaptive optical zoom" to mature the variable magnification and wide field-of-view scanning necessary to address both these situations. We propose to develop and integrate two related systems: 1) an adaptive polymer lens-based (rifle) scope and 2) a 360° microelectromechanical system (MEMS)-based imaging system, to provide both push-button variable magnification and full situational awareness. This approach is high risk and not being addressed by industry. We believe that we can sufficiently mature the adaptive lenses and MEMS mirrors to overcome conventional limitations and develop demonstration systems.

This will serve both DOE and DOD personnel and infrastructure security missions. The ability to scan and zoom within a wide field of view has general applicability to other areas including unmanned ground, air, and space systems.

Summary of Accomplishments

We have thoroughly evaluated adaptive lenses from Holochip, Varioptic, Rhevision, and Boulder Nonlinear Systems (BNS). None of these are acceptable for this application. Aperture size (Varioptic), chromatic/polarization limitations (BNS), and wavefront quality (Holochip and Rhevision) preclude these from being used in a military rifle scope. We documented detailed analysis information in a separate report.

In order to understand the nonlinear behavior of the polymer membrane, we measured the material properties and fit the response to an appropriate constitutive equation. The material is Slygard 184, a commonly used silicone, and we fabricated samples for both tensile and compressive testing at large strains. This material is considered hyperelastic, which means that it can experience very large elastic strains (sometimes in excess of 100%) without failure. The material data was used to fit the stress-strain relationship to a 3rd-order Mooney-Rivlin constitutive equation. This information will be used in the future to assess potential improvements to adaptive lenses.

As a proof of concept, we designed and demonstrated an 8X zoom system using manually actuated adaptive polymer lenses from Holochip. The results from this demonstration are impressive, however, the system was 23-inches long. This length was necessary to minimize the impact of poor wavefront quality. These results are being published.

Although nearly all of the effort during this first year was focused on the rifle scope, we have characterized the Sandia MEMS mirrors and determined that they are not sufficient for the 360° application. Instead, we are designing a preliminary breadboard system that will use a custom fast steering.

Significance

This project serves our national security mission by “providing world-class scientific research capacity and advancing scientific knowledge.” This will serve both DOE and DOD personnel and infrastructure security missions. Within Sandia, this project benefits multiple mission areas, including the special operations thrust and the global awareness thrust (sensor systems and supporting technologies).

High-Performance, Highly Producible Focal Plane Arrays

130700
Year 1 of 3
Principal Investigator: R. R. Kay

Project Purpose

Sandia space programs presently rely on industry to design and fabricate high-performance focal plane arrays (FPAs). Present and future program performance requirements stress state-of-the-art FPA design and production capability to the point where development risk and cost cannot be adequately managed under traditional Sandia-contractor relationships. Furthermore, large system development and delivery programs can no longer tolerate critical path FPA development due to high risk to schedule and cost estimates. R&D investment in next generation FPA development is an essential springboard to establish capability which is within reach of a full system development program.

This project addresses the gap between identification of performance and manufacturability improvements for existing products through design and production of an engineering prototype. Specifically, this proposal outlines an approach to achieve higher yield of the back-to-back (BTB) focal plane arrays, while also addressing performance improvements such as higher frame rate, higher unit cell gain, 2-color, and inclusion of fiber-optic data transfer directly from the FPA to warm signal processing electronics. Programmatically, the relationship between Sandia and the FPA contractor also changes from a customer-supplier relationship to a development partner relationship, with both industry and Sandia contributing to the design, technology development, and production of a prototype unit.

Summary of Accomplishments

Teledyne Imaging Sensors (TIS) was selected as the contractor based on the response to the competitive procurement solicitation. TIS has significant experience in BTB2K of implementing the unit cell, analog-to-digital converter (ADC), and analog readout path analogous to that for high-performance focal plane arrays. The joint design effort was initiated early this year after the contract was placed. The technology and foundry were selected to be CA@5 and Jazz, respectively, based on the intellectual property Teledyne brings to this project from the BTB design effort. Sandia is adding the digital blocks, integrating and validating the entire design. TIS is working on the pixel design while they have provided Sandia with their ADC design. Sandia is using the International Organization for Standardization (ISO) certified process incorporating verification and validation steps to reduce the risk and increase first pass success. The unit cell will be compatible with 2-color, dual bump detector arrays. The design naturally partitions into quarters and will fit within a single reticle field. Single unit cell gain is possible due to the higher operating speed. Sandia and TIS have jointly agreed to the design implementation document. We have received and set up the process design kits from Jazz, and are working with Jazz on design for manufacturability, using lessons learned from the BTB program to reduce risk. Preliminary discussions regarding the assembly process are underway as well.

Significance

The user community is looking to Sandia to provide concepts for next generation systems for a variety of government agencies. Advances in FPA architectures could bring a significant increase in performance, specifically in minimum detectable signal.

Assessing Vulnerabilities of Wireless USB

130701
Year 1 of 2
Principal Investigator: D. J. Wiener

Project Purpose

Wireless USB (universal serial bus) is a new technology that promises to ease and improve connectivity between peripherals and computers. Wireless USB (WUSB) will eventually replace cabled USB as the primary peripheral connection technology. West Technology Research Solutions projects that 84 million wireless USB devices will ship in 2010. As wireless USB replaces cabled USB, these devices will make their way en masse into national laboratories, research institutions, and military facilities.

This research is aimed at conducting a vulnerability assessment of this new, potentially disruptive (from a cyber security standpoint) technology. It will analyze the protocols, security implementation, and source code to evaluate the strengths and weaknesses present in wireless USB implementation. Recommendations for how to use and limit use of wireless USB in secure environments will be presented.

There are only a handful of wireless USB chipset and driver providers, meaning a vulnerability discovered in one implementation could lead to the exploitation of millions of devices. Another concern is that there are currently no intrusion detection systems that could detect an attacker trying to exploit wireless USB devices. These concerns highlight the need for proper analysis in the use of these devices in secure facilities and laboratories.

Summary of Accomplishments

The team has accomplished the following tasks:

- Designed a fuzzing infrastructure for fuzzing WUSB hosts and devices.
- Established a test lab in a wireless screen room for WUSB vulnerability testing.
- Conducted initial protocol analysis using standard and actual device transmission.
- Characterized the security association between two WUSB devices.
- Identified initial vulnerabilities in WUSB protocol and security association process.
- Completed three project reports:
    - Certified wireless (CW-USB) media access control (MAC) layer
    - Security mechanisms of CW-USB
    - Design of wireless USB fuzzing infrastructure

Significance

Protecting classified and sensitive unclassified information is critical to the national security mission of DOE. This research is pertinent to that mission in that it evaluates the security and implementation of a new, potentially disruptive technology that will make its way into most computers and peripheral devices.

Automated AOI Management for Future Sensor Systems

130704
Year 1 of 2
Principal Investigator: K. W. Larson

Project Purpose

A persistent system engineering challenge exists in 24/7 operational satellite systems whose data require sophisticated algorithmic processing for exploitation: the data-rich environment of the sensor is spatially separated from the human-, computer-, and power-rich environment of the ground station. One can idealize several naïve solutions to the problem that are generally infeasible. For example, transmitting all data to the ground involves downlink resources that are very expensive to obtain and maintain, while implementing all data exploitation algorithms on the sensor involves unacceptable trades between probability of detection, false alarm rate, system maintenance, and mission flexibility. Furthermore, mission flexibility is becoming ever more important, and the sets of targets that need to be detected and characterized are becoming more diverse. We think the solution to this problem involves a smarter distribution of data exploitation among satellite resources, ground computation, and human operators. We call this strategy area of interest (AOI) management. The key concept in AOI management is that the downlink carries data whose spatiotemporal resolution is variable across the sensor's field of view, so that resolution of important features is high, and background noise is sparse. This project will discover how AOI management can be implemented within a unified flight and ground architecture. We will evaluate and compare architectures by modeling and simulating net system performance under ranges of objectives, constraints, and configurations. While all current and reasonably foreseeable missions will be considered, special emphasis will be given to tracking dim moving targets (DMT).

Summary of Accomplishments

In 2009 we accomplished significant portions of the necessary evaluation of DMT detection and tracking algorithms and analysis of AOI system concepts. Three significant detection and tracking techniques were considered. First, the scene kinetics mitigation (SKM) method of noise-reduction/correction was invented and its performance analyzed both from first principles and probabilistically with various mixtures of scene and sensor noise. We compared SKM to a conventional noise reduction technique and in doing so demonstrated the importance of treating noise sources with respect to their motion frame of reference. Second, we analyzed the velocity-matched filter (VMF) technique to enhance the signal of moving targets at the time of detection, using a realistic modeling system. Since stock VMF is computationally prohibitive, we use AOIs and model-based cueing to prioritize the parameter space that is searched. Third, we began to investigate Bayesian track before detect algorithms.

Significance

This project responds to national requirements for effective detection and assessment capabilities against diversifying strategic and tactical threats, as well as global and theater situational awareness, and specifically relates to the DOE strategic goal to advance technologies to detect the proliferation of weapons of mass destruction worldwide.

Boundary-Layer Transition on Maneuvering Hypersonic Flight Vehicles

130705
Year 1 of 3
Principal Investigator: D. W. Kuntz

Project Purpose

Boundary-layer transition is the phenomenon which occurs within the boundary-layer of flight vehicles when the flow changes from laminar to turbulent. As this process occurs, flow properties change significantly, most notably the heating rises drastically. Transition on ballistic flight vehicles has traditionally been predicted by correlations based on flight-test experience. New designs of hypersonic maneuvering vehicles will fly long-duration trajectories, and accurately predicting boundary-layer transition would mean less conservatism in thicknesses of thermal protection systems. Current correlation-based approaches are insufficient to address this critical need. Numerical techniques for predicting boundary-layer transition based on stability theory are becoming the state-of-the-art for hypersonic flight. One such tool, STABL, funded by Sandia and the Air Force Office of Scientific Research (AFOSR), was developed to provide this predictive capability. This project is combining STABL calculations with Sandia's flight experience to develop a prediction capability for boundary layer transition of maneuvering hypersonic flight vehicles.

Validation and fine-tuning of the stability approach for predicting boundary layer transition in realistic hypersonic environments is being performed using data from the numerous ballistic vehicles that have been flown by Sandia. During the next two years flight data will be used to develop techniques for applying stability theory to maneuvering vehicles, and the lessons learned will then be used to develop techniques for accurate transition prediction on future flight systems.

An understanding of boundary layer transition on maneuvering hypersonic flight vehicles is critical to the design of next generation atmospheric flight systems, and the successful completion of this project will provide a new level of understanding of this phenomenon.

Summary of Accomplishments

The STABL code has been successfully loaded and normal operation has been confirmed. The flight vehicles to be studied have been determined and prioritized, and, to date, stability computations have been completed for a total of six reference ballistic fight vehicles, some at multiple trajectory points. Mean flow and stability calculations performed for a flight vehicle equipped with a carbon-carbon heatshield with three nosetip geometries have indicated that the N factors (numerical representations of the amplification of the most unstable waves within the boundary layer) obtained at transition are highly dependent on the nosetip geometry used for the simulations. The results of these analyses have been compared to stability analyses for the same flight vehicle performed at CUBRC, Inc. These comparisons have shown that the wall blowing and temperature boundary conditions used for the mean flow analyses have as large of an impact on computed N factors as the nosetip geometry does. As a result of this, all vehicle analyses have been performed using the actual ablated nosetip geometry, surface temperature profiles, and surface blowing profiles computed by legacy material thermal response codes. Although this result was not anticipated, sufficient flexibility is available within the project to incorporate these more complex boundary conditions in the stability calculations of Sandia's suite of hypersonic flight vehicles.

Significance

Development of new, long-range, hypersonic flight systems is currently a critical need. An understanding of transition on hypersonic vehicles is critical to the design of the heatshield for these systems, and this project will provide a new level of understanding of this phenomenon.

Space Object Imaging and Signal Transmission Through Turbulence and Debris

130706
Year 1 of 1
Principal Investigator: S. P. Kearney

Project Purpose

This project conducted and evaluated the results from a field environment test series to characterize the viability of nonlinear optical methods (e.g., Brillouin enhanced four wave mixing laser illuminator combined with stimulated Brillouin scattering optical amplifier) for imaging hypervelocity space objects in the size range of 1 mm to 30 cm. Further, we numerically analyzed the scattered laser light from objects with characteristic dimensions between 1 mm and 10 cm to quantify the degradation of free-space optical communication links as a function of cloud parameters, to evaluate the viability of using these scattering events as a method for performing laser threat warning and other situational awareness functions, and to assess the impact of these scattering events on the proposed nonlinear optical imaging system. A full understanding of this area will allow us to design and build more robust optical communications for satellite-to-satellite and ground-to-satellite links and evaluate performance degradation in various environments, as well as set the stage for the development of state-of-the art ground to space high-resolution imaging capabilities for tracking and imaging objects in low earth orbit (LEO) to geostationary orbit (GEO) altitudes and advanced approaches for mitigating turbulence degradation. Further, some countries have proposed or are experimenting with microsatellites. Because of their size, such satellites are hard to track and catalog and present similar challenges to those of space debris. The developed technologies would also provide the ability to image such objects. Previous national efforts to address this challenge, such as the National Aeronautics and Space Administration (NASA) and United States Air Force (USAF)-sponsored Orion project, identified the lack of these technologies as a barrier to be overcome for debris removal.

Summary of Accomplishments

We determined that existing particle scattering levels should not present an unacceptable degradation to space based communications except in the proximity of dense debris clouds (e.g., after a collision). We demonstrated that Brillouin enhanced four wave mixing (BEFWM) can provide adequate phase conjugation to correct for laser beam propagation and imaging though atmospheric turbulence levels as high as $C_n^2 = 10^{-12}\,m^{-2/3}$. Controlled tests demonstrated that near diffraction level imaging is possible through this strong turbulence and that BEFWM can provide a mechanism to focus a laser through this same strong turbulence producing a focused beam with a Strehl ratio exceeding 0.5

Significance

This project benefits space systems (detector designs, laser threat warning, satellite hazard identification/ mitigation), missile and satellite imaging and tracking, and space debris mitigation efforts. The demonstrated BEFWM technology gives hope that the longstanding challenge of imaging small debris can be overcome, potentially enabling the development and deployment of a reliable method to detect, identify, and deorbit space debris.

Directed Robots for Increased Military Manpower Effectiveness

130707
Year 1 of 3
Principal Investigator: B. R. Rohrer

Project Purpose

There continues to be a trend in all branches of the military toward doing more with fewer people. The proliferation of unmanned aerial, ground, and underwater vehicles attests to this, as do stated goals for increased manpower effectiveness in major programs such as Future Combat Systems (FCS). Fully automated unmanned vehicles (UVs) are appealing, since they require no attention during operation. However, full automation has not yet become practical for most systems, particularly for ground vehicles operating in unmodeled environments. Instead, current designs require almost constant supervision from at least one operator.

In order to increase the effectiveness of UV operators, we propose to develop robots that can be "directed" rather than remote-controlled. They would be instructed and trained by human operators, rather than driven. Over time, as they learn appropriate behaviors and world models, directed robots will increase in autonomy and require less supervision. This approach is analogous to how a human apprentice is trained—not through controlling his actions, but through repeated instruction, demonstration, and feedback.

The technical approach will be modeled closely on psychological and neuroscientific models of human learning. Two Sandia-developed models will be utilized in this effort: the Sandia cognitive framework (SCF), a cognitive psychology-based model of human processes, and BECCA, a psychophysical-based model of learning, motor control, and conceptualization. Together, these models will span the functional space from perceptuo-motor abilities, to high-level motivational and attentional processes. BECCA (brain-emulating cognition and control architecture) will be used to translate raw sensory information into symbolic semantic tags, which will be passed to SCREAM (Sandia cognitive runtime engine with active memory), an implementation of the SCF. SCREAM will process the tags, decide what general action to take and pass the symbolic command back to BECCA, which will then translate that into low-level commands for the robot, appropriate to its current state and environment.

Summary of Accomplishments

Robot hardware:
The proposed work for FY 2009 was limited to implementing BECCA and SCREAM on simulated robots. However, due to the team's enthusiasm and the large benefits of hardware implementation to the project's progress, the move to hardware, the Surveyor SRV-1 robot platform, was completed early this year.

Milestone demo:
Typed command-directed behavior, basic principles:
In this first-principles demonstration, we directed the robots using scripted commands. The robots were directed with specific commands "hide" and "seek." It was used to alternately search for high- and low-contrast visual scenes in a cave-like structure, relaying images wirelessly to the operator outside. Although similar behaviors can be attained without the cognitive infrastructure used here, the autonomous learning demonstrated in this stage is a steppingstone to the more sophisticated behaviors. To simplify training and operation of the system, a graphical user interface (GUI) was developed that allows for intuitive user interaction and exposes the robot's relevant internal states.

SCREAM integration with robot hardware:
Two significant development efforts are underway to allow SCREAM to be fully integrated into the operating robot platform. First, a SCREAM C++ cognitive model object has been wrapped in a Java class for use with the rest of the Java-based directed robots code. Second, in order to allow SCREAM to begin to recognize temporal sequences of concepts, sequential recall capability of episodic memories has been implemented.

Communication of Results:
Four conference papers have been submitted and/or presented to a wide variety of technical audiences. A journal article has been submitted to the journal, *Neurocomputing*. A video for general audiences has been produced and released as well.

Significance

Sandia national security mission contribution:
Having machines that learn from their experience and respond to human directives would benefit several of Sandia's key security customers. Some examples of applications and the customers they would benefit include the following:

1. Department of Homeland Security. Airborne border surveillance robots could learn better to recognize suspicious patterns and increase their survivability by periodically interacting with a remote human coach.
2. Army: Verbally directed improvised explosive device (IED)-detecting robots would require less supervision and would free up their controllers to be perform other tasks, such as maintaining situational awareness.
3. Navy: Automated materiel transport systems on aircraft carriers would require less-explicit instructions and would be able to automatically re-route around blocked passages or inaccessible paths.
4. Marines: High-payload robots carrying supplies could trail ground forces with only occasional instruction from their human director.
5. Coast Guard: Unmanned surface vehicles could become more adept at surveillance by learning from their experience and receiving occasional verbal feedback from their remote human operators.
6. Department of Energy: Sensor networks in security systems for high-consequence assets could decrease their false-positive rates and improve the specificity of their target identification by learning from their experience and incorporating human feedback.

General S&T community contribution:
Creating directed robots requires addressing several longstanding technical challenges. We are finding answers to several hard questions:

1. How can machine learning be made as rapid as possible without sacrificing the breadth of things that can be learned?
2. How can we generate concepts directly from experience, rather than having a programmer enumerate them?
3. How can we make a machine that can handle truly unfamiliar situations gracefully, the way humans are able to?

These questions impact several fields, including robotics, machine learning, cognitive psychology, neuroscience, and neural computation.

Identifying Objects in Bright Fields Using New Ultradark, Tunable Nanorug

130709
Year 1 of 1
Principal Investigator: J. E. Massad

Project Purpose

Recent breakthroughs in the development of materials with controllable nanometer-sized structure have provided tough thin films with unprecedented properties. One such discovery was that by aligning vertical tubes that are nanometers in diameter and hundreds of microns long, one creates a surface in which incident light can barely escape. The purpose of this project was to evaluate nanorugs for an expanded range of wavelengths and incident angles and to study the dependence of performance on material properties. In this exploratory study, we discovered that nanorugs have tremendous potential.

Summary of Accomplishments

We performed exploratory research activities to evaluate the reflective capabilities of nanorugs across a range of wavelengths and incident angles. We interrogated samples of varying character with scanning electron microscopy and hemispherical directional reflectance measurements. We also investigated modeling approaches that may provide a starting point for simulating novel material behavior. Ultimately, this exploratory project has revealed that these nanomaterials can provide unprecedented optical properties.

Significance

We have analyzed a new nanomaterial and provided a basis for understanding its optical behavior, advancing the DOE goal for scientific discovery and innovation.

Malware Attribution Through Binary Analysis

130715
Year 1 of 3
Principal Investigator: S. A. Mulder

Project Purpose

One of the difficult problems in computer security is the lack of attribution of malicious activity. Even if malicious programs are discovered, tracing them back to an original source is often extremely difficult, if not impossible. Even correlating the activities of a single group using multiple tools can be challenging. Sandia is in a unique position, through our Footsteps Lab and other related efforts, to develop advanced capability to respond to national level threats to our information systems. We propose to build the foundation for a long-term program in the area of collecting evidence for attribution.

Most attribution work is currently done manually by experts. This process is slow, relies on extensive reverse engineering capability, and is naturally error-prone. Sandia has been one of the leaders in solving these problems manually through our access to interesting data and ties to various government organizations. The focus of this research effort will be to dramatically improve the speed and accuracy of our current attribution efforts through automation and to make new discovery possible through a normalization process.

Our current model of automated malware fingerprinting is to extract a variety of features from a binary and compare them to a corpus of "normal" programs that would exist in a similar environment. A composite of the unique or unusual features of the malware constitute the fingerprint. This existing capability provides the theoretical underpinnings of the proposed research effort.

Summary of Accomplishments

In FY 2009, the team has demonstrated two key accomplishments that lay the foundation for further work. The first is a demonstration of clustering malware based on build environment. This is a key piece of evidence and forms the foundation for the next stage of research which is normalization of build environment influences. The second major accomplishment is the clustering of malware with known attribution using rich feature sets. The preliminary results in this area are positive and by the end of the fiscal year we will have a strong foundation of test data for our further work. In addition, core infrastructure in the form of algorithms, database structure, and tools have been advanced and developed to provide a platform for further research.

Significance

The inability to apply attribution to malicious computer network behavior is one of the primary limiting factors in current security models. This research would directly contribute to our ability to understand the threat space, providing insight into who our adversaries are and what capabilities they possess. It also provides a basis for appropriate response to malicious activity. This directly addresses one of the primary gaps in our national cyber defense capability.

Next-Generation, High-Bandwidth Electronics Substrate Technology for Future Satellite Systems

130717
Year 1 of 1
Principal Investigator: S. E. Garrett

Project Purpose

The delivery of electronic modules for a recent program was costly and inefficient. Sandia designs pushed the state-of-the-art well beyond US printed circuit board (PCB) manufacturing capability. Typical yields for complex PCB production lots were <10%. For future systems, these PCB complexities will become the design standard, with a continued push toward reducing size, weight, and power requirements.

In addition to these aggressive design challenges there are other serious external challenges in fabricating PCBs with today's technology and materials: 1) To comply with restriction of hazardous substances (RoHS) directives, materials and components for future fabrication and assembly must be compatible with the lead-free solder processing temperatures. Sandia exemptions to RoHS directives are expected to end within two years. 2) The number of quality PCB vendors in the US has significantly decreased in recent years. Supply chain management (vendor qualification, fabrication lead-times, incoming quality control [QC]) will continue to be difficult as US vendors go out of business or move offshore.

Active and passive components will also follow the trend toward miniaturization. Currently, surface mount assembly pitch is down to 0.4 mm and is expected to decrease further. In the future, chip level flip-chip dimensions will be used directly on high density interconnect (HDI) system boards similarly to what is currently done with ball grid array (BGA) substrates. Design for manufacturability will need to be considered along with advanced board fabrication and assembly processes. Both "chip and wire" and die level flip-chip interconnects will be more prevalent. Known good die issues will be mitigated with chip scale packages. Component miniaturization will challenge existing assembly processes such as pick-and-place, solder reflow, inspection and rework.

Clearly, a new approach for next-generation electronic modules is needed. Further miniaturization will require moving well beyond current PCB technology. To support future anticipated programs an improved technology must be identified and developed within three years.

Summary of Accomplishments

The ultimate goal of this one-year project was to identify a robust, high-density interconnect technology that delivers high performance and high reliability. The main objectives of this project were to, 1) Perform an assessment of advanced technologies and select a viable technology for next-generation Sandia applications; 2) Translate an existing design into the new technology selected; 3) Fabricate a new technology demonstration board; and 4) Perform cursory acceptance tests on the demonstration board.

This project was valuable in that it identified an enabling technology for upcoming applications that enables substantial reduction in the size, weight and power of electronic assemblies. The translation to HDI technology resulted in significant miniaturization in the PCB design. The total layer count was reduced from 20 to 12 layers and the total board thickness was reduced from 0.093 inches (2.362 mm) to 0.055 inches (1.397 mm). Several HDI attributes were incorporated into the design such as, via-in-pad technology, extensive use of microvias on three separate sequential build up layers and embedded resistors. Significant improvements in quality, performance, cost and delivery times are likely to be realized within the next three years. Also important was the experience gained by designing and fabricating the first lot of high density interconnect printed circuit boards.

Significance

One of the critical enablers of advanced Sandia systems is high-bandwidth electronics. As design complexity continues to increase, we must look beyond PCB technology to find suitable packaging alternatives for the future. As a national laboratory with an interest in high-performance, high-reliability applications, Sandia is uniquely positioned in the US to working with commercial vendors to develop a robust, high-performance substrate technology that is capable of delivering small numbers of highly reliable, complex modules.

This work has taken the first step in indentifying the most viable advanced technology for future Sandia applications. An advanced design was successfully translated to HDI technology and a proof of concept board was fabricated that will provide insight for the future work.

Next-Level Technology Development for Satellite Based Processing Architectures

130720
Year 1 of 3
Principal Investigator: J. L. Kalb

Project Purpose

Sandia is currently developing new satellite payload processing and data communication architectures that are integral to providing intelligence about worldwide threats to our nation's security. These architectures focus on increasing mission flexibility, accommodating enhanced sensor performance, and optimizing payload size, weight and power consumption. The focus of this effort is to define a network-based architecture that is scalable, reliable, and reusable. By leveraging investments made by Sandia's LDRD and work for others programs, Sandia has been able to make significant progress in the specific architectural areas of network communication, model based design, sensor data processing algorithms, and reconfigurable computing. In the area of network communication, much progress has been made evaluating high speed serial protocols and potential topological configurations, developing tools to easily automate communication performance modeling, and evaluating communication performance once recovery from faults has taken place. Results from prior analysis indicate two major findings that affect the system communication design and performance, both prior to and after fault scenarios. These findings are that node placement and routing algorithms are critical to communication performance.

These architectures are based on two fundamental components: network communication and reconfigurable field programmable gate arrays (FPGAs). Several areas relating to these fundamental components pose technical challenges that need to be addressed in order to effectively implement these architectures. These challenges include mitigating single event upsets (SEU) in static random access memory (SRAM)-based FPGAs, reducing the large size of FPGA configuration bit files, placing processing nodes in a distributed, network connected architecture, and recognizing and recovering from fault conditions. The objective of this work is to investigate efficient approaches to SEU mitigation and device configuration, design methods to optimize architecture topologies for communication performance, and to effectively handle fault detection and recovery.

Summary of Accomplishments

A literature survey was performed to identify algorithms and solvers for node placement optimization. The Guide to Available Mathematical Software (GAMS) package was evaluated and two routines were acquired. A first iteration of a node optimization algorithm has been developed and implemented. These simulated topologies were compared to results from a previous LDRD project. Initial results displayed a 30-40% improvement of optimally placed networks versus "intuitively" placed networks.

Investigations into quality of service and fault detection parameters started with services provided by the Consultative Committee for Space Data Systems (CCSDS) Spacecraft Onboard Interface Services (SOIS) standards. From these services a set of metrics were determined for which a "system monitor" would be responsible. Also investigated were the types of network protocols that mitigate these failures through hardware. One promising area is the new plug-and-play (PnP) standard for the SpaceWire protocol being developed by National Aeronautics and Space Administration (NASA) Goddard.

Bit file compression research began with investigations of both hardware and software lossless compression algorithms. Two algorithms were identified and commercial intellectual property evaluation licenses have been obtained for further study. An industry standard file set was collected to benchmark the compression products against one another. After analyzing the results, an algorithm was down-selected and an IP license procured.

We reviewed past research on partial reconfiguration, completed tutorials and test designs to become familiar with partial reconfiguration flow and tools, investigated trades for using SelectMAP vs. ICAP for space applications, and finally, demonstrated reconfiguration concept by loading a soft core processor application over the SpaceWire network into a partially reconfigured region of the FPGA.

Progress to date has been focused on developing mitigation approaches so that a SiRF Technologies device can be flown in space. These approaches have been tested by leveraging the Xilinx Radiation Testing Consortium to validate these approaches. One area is to mitigate the PowerPC (PPC) in the SiRF chip. These processors cannot be mitigated using traditional triple modular redundancy.

Significance

To keep pace with new emerging threats, we must continually advance the capabilities of our intelligence systems. The availability of this architecture can address the challenges of design complexity, design reuse, bandwidth, and redundancy so that future design resources can be better spent developing capabilities to meet the needs of our DOE, DHS, and national security customers.

Nontraditional Implementation of High Processing Gain via Standard RF Transceivers and Low-Power Microcontrollers

130723
Year 1 of 1
Principal Investigator: D. A. Wiegandt

Project Purpose

This project will tackle the problem of size, power, and complexity asymmetry in today's tagging and communication devices. By researching and applying better a priori knowledge at the receiver via incorporation of novel methods for noncoherent bit-to-sequence encoding, increased processing gain without increased transmitter power or added hardware complexity is expected. Specifically, by utilizing standard technologies, like the commercial off-the-shelf (COTS) parts used in Sandia's current active tags, we intend to create a symmetric architecture that will enable high processing gain without the need for complex field programmable gate array (FPGA) or power hungry processors at the receiver. Benefits include increased range and penetration, enabling greater use of lower capability batteries, and the potential for symmetric tag/interrogator designs.

Summary of Accomplishments

The results of this project prove the capability to noncoherently add gain to a COTS-based architecture. Specifically, gains were observed in the packet based systems. More work is necessary to explore the full extent of the gains possible and determine which aspects of the bit-to-sequence mapping are more important. The results shown to date with respect to the non-packet based system are encouraging. Trends expected in spread spectrum systems can be observed in the initial results achieved. Beyond performance gain, a number of other items have been proven.

Significance

This work will provide Sandia and DOE with a unique capability to assist US government agencies with national security technologies. This strategy is applicable to current tag systems.

Phase-Based Geolocation

130725
Year 1 of 2
Principal Investigator: J. J. Mason

Project Purpose

The geolocation of radiofrequency (RF) emitters is a crucial element of many electronic systems used in national security. RF emitter geolocation is becoming ubiquitous as communications systems are more routinely expected to provide not just signal content but location of the signal source. A significant example of this is the coming location capability mandated for wireless phones (E911).

Most RF emitter geolocation systems use time of arrival (TOA) measurements. A limitation of this approach is that the accuracy of the location estimate is proportional to the signal bandwidth so that narrowband signals like voice (e.g., two-way radio) can typically be located to within only a few kilometers. Narrow bandwidth signals can also be located with moving collection platforms using frequency of arrival (FOA), but again, a typical FOA fix is a few kilometers. Another physical observable is carrier phase and it is sensitive to emitter location variations of centimeters or millimeters depending on RF wavelength. This indicates that phase measurements have the potential to provide the basis for very accurate geolocation. How to use phase of arrival (POA) measurements to accurately locate an emitter is an open problem and is the goal of this proposed research.

We believe this work has the potential to significantly advance the state of the art for geolocating a wide variety of RF emitters and will be of interest to operators of signal collection platforms. The research is high risk because there are sources of phase errors that must be removed and because phase measurements have many-fold ambiguities that must be resolved. This high risk makes this work a better candidate for LDRD than for programmatic funds.

Summary of Accomplishments

In the first year of this two-year project, we have developed and demonstrated a phase-based geolocation technique that is capable of giving better accuracy than a comparable frequency difference of arrival (FDOA)-based system. We have found that our technique is closely related to the FDOA method but improves with a parameter that we call baseline, where as the FDOA method does not have this property. Baseline is the distance that the satellite-based receivers move during the reception of the signal. For the systems we have worked with so far, the phase difference of arrival (PDOA) technique works better than the FDOA technique for signals that are longer than 0.1 seconds, but this breakpoint varies with signal center frequency. We have used our technique to locate a commercial GPS receiver that recorded phase measurements from a number of GPS L1 band and L2 band signals. We also used our technique to locate a receiver we built from test gear that recorded phase measurements from several GPS S2 band signals. We have also created simulation codes that model these processes and shown that we can predict the outcomes of these tests.

Significance

Our goal is to greatly improve the performance of existing Sandia tagging, tracking, and locating (TT&L) systems currently using time of arrival (TOA) and/or frequency of arrival (FOA). If successful, these techniques would be of interest to other government agencies involved with global awareness and national security.

Science and Implementation of Microbatteries

130726
Year 1 of 1
Principal Investigator: S. J. Hearne

Project Purpose

We propose to develop a science-based understanding, as well as the technological capability, to address key enablers needed to develop and manufacture ultrahigh energy density, 1 mm^3 batteries capable of energy storage at 100 µA-hr (~1 J). Much of the need for these batteries is driven from autonomous microsystems that require onboard power to provide enough energy for them to fulfill their field mission. This power may be harvested through solar, radio frequency (RF), or thermal energy for systems requiring a few microwatts of power. In many cases it is desirable for the microsystem to be functional when the harvester is inactive, such as at night. This requires energy storage to be included in the system. Past efforts to realize mm^3 microsystems have been unsuccessful in large part because the available batteries with sufficient capacity were orders of magnitude larger than the systems. Therefore, a concerted effort to increase the energy density and decrease the form factor of microbatteries is needed.

This project will team existing battery development and fabrication expertise with science-based understanding of nanostructured materials. The team will identify and address technical hurdles that currently hinder production of microbatteries and strive to produce cells that demonstrate key aspects of the microbattery. A second focus will be on developing an understanding of the fundamental science of charge transfer through nanostructured electrolyte and electrodes. It is anticipated that the impact of the project will extend beyond the 1 mm^3 battery systems specifically under investigation here to large-scale, high-energy systems where the potential for decreased mass and volume are beneficial. As such, there are broad applications within the nuclear weapons (NW) investment area that will benefit from secondary (rechargeable) batteries with significantly higher energy densities than are currently available.

Summary of Accomplishments

In the modeling effort we examined various atomistic modeling efforts associated with lithium ion batteries in the literature. We have identified several key areas Sandia may contribute, including solid electrolyte interphase (SEI) formation mechanisms at anode-electrolyte interfaces, Li^+ intercalation barriers at electrode-electrolyte interfaces in general, and the possibly amorphous cathode-oxide surface structure.

In the battery assembly effort, we successfully fabricated a lithium iodide (LiI) battery using a dispersion technique and then hand assembled the battery into a “jelly roll” type battery. The resultant system demonstrated the viability of the materials and techniques. Several improvements could be made to increase the capacity and performance of the battery, given the relatively rough assembly of the first set of batteries. In particular, targeting a higher LiI to poly(2-vinylpyridine) (P2VP) ratio in the coating, along with an increase in carbon loading, would improve the electrical performance of the battery and likely lead to higher capacities of the system. Also, charging and discharging at an acceptable C/10 rate, rather than the (likely) 5–10C rates that were used in this study, should also improve the capacity of the battery.

Significance

This project focuses on demonstrating the most valuable and challenging enablers of high energy density storage. Through this effort, we will demonstrate a new capability to provide high performance batteries for customer-driven national security applications and develop a path forward to future architectures.

Silicon Microphotonic Backplane for Focal Plane Array Communications

130727
Year 1 of 3
Principal Investigator: M. Watts

Project Purpose

A silicon microphotonic backplane is being developed to enable high-bandwidth (ultimately >100 Tb/s), low-power (<100 fJ/bit or 1 mW at 10 Gb/s), and scalable communication off of a large focal plane array (FPA). The proposed solution will fit into the current FPA electrical backplane solution developed by the FPA LDRD Grand Challenge (Project 95211). All data will be transferred on and off chip with a single optical fiber thereby simultaneously minimizing thermal conductance and susceptibility to electromagnetic interference in an integrated package. Further, the silicon microphotonic backplane will dissipate 10-to-100 less power than electrical or competing optical solutions and the optical source will be located off-chip and outside the cryostat. Ultralow power silicon microphotonic modulators will enable terabits/second of data to be transmitted off of the focal plane array while requiring only milliwatts of power dissipation. The silicon microphotonic modulators required for data transmission have been demonstrated under a pair of Defense Advanced Research Projects Agency (DARPA) seedling efforts achieving error-free data transmission at 10 Gb/s, representing the smallest, lowest power, and highest speed resonant silicon modulators demonstrated to date. What remains are challenges associated with real-world implementations including the following: 1. Integration with advanced complementary metal oxide semiconductor (CMOS) driver and receiver circuitry; 2. temperature stability; 3. low-temperature operation; 4. wavelength division multiplexed implementations; and 5. cross-wafer communications. All of these challenges will be addressed to ensure that a stable, reliable solution will be available for implementation into real applications within 2-to-3 years of the completion of the LDRD project effort. Further, the proposed solution, if successful, will enable complete dowloading of data (to the compute engine) of future very large FPAs (~10^8 detectors) that may have off-chip bandwidth requirements approaching 100 Tb/s, a capability not possible with present electrical or optical technologies.

Summary of Accomplishments

Accomplishment 1: CMOS driver design developed for IBM 90 nm CMOS. Simulations indicate it should reach 10 Gb/s. Design has been submitted for fabrication in a trusted foundry run.

Accomplishment 2: A CMOS-7 driver directly integrated with a silicon modulator, fabricated at Sandia, has been designed, and experimentally demonstrated yielding data rates as high as 2 Gb/s. This direct integration with CMOS-7 greatly reduces the packaging complexity and offers a path toward radiation-hardened operation.

Accomplishment 3: CMOS control circuit design for thermal control of modulator structure has been submitted for fabrication in the IBM 90 nm CMOS run.

Accomplishment 4: Demonstrated thermal tuning of microring resonators over 400 °C, bringing us a step closer to meeting our thermal control objectives. The demonstration also represents the lowest power (4.4 µW/GHz) and highest-speed (1 µs) thermo-optic control ever reported.

Accomplishment 5: Demonstrated fiber-to-waveguide v-groove attach with only 3 dB loss for highly reliable fiber attachment to the silicon microphotonic backplane.

Accomplishment 6: Gave over five invited talks on our modulator work.

Accomplishment 7: Implemented a modulator with integrated heater, sensor, and modulator structures. The structure has been tested at the wafer scale and the temperature sensor appears to track the temperature of the modulator as confirmed by driving the integrated heater. This is the first such structure ever proposed and demonstrated and brings us even closer to cryogenic operation.

Accomplishment 8: Demonstrated germanium on silicon diodes with low dark current for future implementation of germanium detectors in our CMOS compatible process.

Accomplishment 9: Won an R&D100 Award.

Significance

This project fits directly within the Defense Systems and Assessments (DS&A) program call by addressing 1. space situational awareness, 2. strategic surprise, and 3. techniques for intrasatellite wide-band data communications. Silicon microphotonics enables ultrahigh-bandwidth, low-power communications off of a focal plane array in a highly disruptive manner and is therefore an enabler for nuclear nonproliferation programs.

Refereed Communications

M.R. Watts, W.A. Zortman, D.C. Trotter, R.W. Young, and A.L. Lentine, "Low Voltage, Compact, Depletion-Mode, Silicon Mach-Zehnder Modulator," to be published in *Journal of Selected Topics in Quantum Electronics*.

Velocity-Independent Continuous Tracking Radar

130729
Year 1 of 3
Principal Investigator: D. W. Harmony

Project Purpose

Existing radars are severely limited in their ability to follow individual vehicles over typical velocity changes experienced while maneuvering in traffic. All ground moving target indication (GMTI) radars rely on vehicle motion for detection against ground clutter. When a vehicle slows or stops, tracking becomes difficult and is virtually impossible for present systems. If successful, the research proposed here would permit continuous tracking through all phases of motion, including full stops.

The thrust of this project is to develop techniques and algorithms for following a mobile high value target with radar by combining VideoSAR (video synthetic aperture radar) and azimuth monopulse GMTI processing methods. The effort combining these techniques into a new radar mode for continuous tracking is divided into six main tasks: clutter attenuation, azimuth location measurement, tracker development, antenna guidance, image formation, and mover focusing.

Summary of Accomplishments

An important accomplishment this year has been the development of tracking algorithms that work with monopulse clutter cancellation and azimuth angle measurements to create an integrated model that combines videoSAR and GMTI signal processing in a manner emulating real-time radar data streams. Existing K_a-band data has been processed into movies demonstrating current algorithm performance. Ongoing tracking efforts are developing algorithms for maneuvering and slowly moving vehicles in the presence of ground clutter. Image formation techniques to support continuous antenna pointing along an arbitrary path are also being developed.

Significance

Sandia's national security customers are relying more heavily upon monitoring mobile targets. DOE proliferation detection customers have explicitly stated the need for continuous tracking of vehicles. DOD customers have expressed a similar need for their applications. The research proposed here is the best approach for meeting these needs.

Wavelength-Division-Multiplexed (WDM) Free Space Optical Communication Using a High Repetition Rate Coherent Broadband Femtosecond Laser

130731
Year 1 of 3
Principal Investigator: J. Urayama

Project Purpose

Robust communication links among static and mobile platforms for situational awareness in areas of channel congestion or in absence of conventional links require new strategies for high-speed transmission and high-level security. Scenarios such as the "last mile" connection in emergency disaster areas (e.g. 9/11 in NYC), access in remote or denied areas, and air-to-ground and air-to-air links fall into this important category of communication. Free space optical communication (FSOC) using line-of-sight atmospheric delivery of encoded laser beams has been proposed as a means of addressing these needs. We propose a new FSOC implementation using wavelength-division-multiplexed (WDM) femtosecond lasers which will provide a significant enhancement in transmission bit rates (tens to hundreds of Gbps) over existing radio frequency (RF) technologies and offer new capabilities for secure communication. The key solutions to the bit rate demand are the generation of massively parallel channels in the broadband spectrum associated with ultrashort optical pulses and the high repetition rate (MHz to GHz) technologies of the laser source and optical encoder. Secure operation will be achieved through the selective usage of available optical encoding and decoding techniques via direct control of the amplitude and phase of the transmitter using optical pulse shaping. This femtosecond FSOC effort will leverage existing resources within our organization, most notably the femtosecond laser technology, pulse shaping techniques, and laser propagation expertise. For mitigation of challenging atmospheric effects during transmission, we anticipate the incorporation of adaptive optics which will enhance beam delivery and phase preservation.

Summary of Accomplishments

The work on FSOC began with the development and characterization of the laser source and available encoding technologies. For the source, a Ti:sapphire-based oscillator was optimized, and required diagnostics were installed. This allowed for the pumping of photonic crystal fibers which were used to generate a supercontinuum encompassing ~600 nm–900 nm at a repetition rate of 80 MHz. The pumping conditions were varied to characterize the controls on the spectral content of the supercontinuum. In order to begin the WDM effort, a zero-dispersion pulse shaper was constructed and optimized to minimize aberrations. Steps were taken to determine the channel number generated in this shaper (~1 nm per channel) taking into account the spectral resolution limitations and requirements for cross-talk limitation among the channels. Commercial off-the-shelf (COTS) hardware for encoder technology was assessed using an acousto-optic tunable filter and an acousto-optic pulse shaper. In each of these devices, amplitude and/or phase controls were characterized for encoding applications. Amplitude and phase sensitive diagnostic tools (Grenouille and SPIDER) were installed for these measurements. Assessment of these modulator technologies along with further literature research provided level of shortfall in these existing devices. Based on these lessons learned and availability of equipment, the decision was made to transition to a 1.5-µm short pulse laser and telecommunication amplifiers and modulators. Construction was started for this new optical train. Preliminary performance models based on OptSim were evaluated for a communication link based on a 1.5-µm source.

Significance

The project addresses a critical area of national security by improving secure commercial and military communications to greatly enhance data rates with minimal risk of interception. If successful, the FSOC link operating under amplitude and phase bit encoding protocols would provide a higher level of security. The capacity for data streams would enhance data transfer rates which are currently limited and present bottlenecks in high-demand connections. These capabilities could be developed and incorporated into existing tactical and strategic links relevant for surveillance and reconnaissance for national security purposes. The results of this project will benefit other programs for intelligence gathering.

High-Frequency RF Effects

131503
Year 1 of 3
Principal Investigator: L. D. Bacon

Project Purpose

Satellite communications provide an important capability to military/civilian operations. Today the loss of a small number of satellites could greatly influence the global economy as well as reduce the US military's ability to exert their influence around the globe. We propose to conduct an effort composed of theoretical, numerical, and experimental work to understand the potential of high-frequency (HF) radio frequency (RF) to disrupt satellites or other electronic systems. It is our understanding that previous electronics requirements and testing may not have uncovered all of the effects that may be enabled by modern equipment. The primary goal is to understand the fundamental mechanisms of effect and their scaling. Achievement of this goal will provide the information needed to determine if an adversary can design and build a system to disrupt our critical electronic systems. Public domain literature indicates that high-powered HF RF systems that might be able to achieve previously unstudied effects may be due for implementation in less than a year.

Summary of Accomplishments

In FY 2009 we pursued the understanding of the most fundamental aspects of RF effects on electronics: coupling/propagation and component/circuit models and measurements.

We have characterized the behavior of high frequency signals in printed circuit boards (PCBs) made from FR10 (Frontier Electronics Co., Ltd.) substrate material, the most common for conventional electronics. Circuit traces of linewidths varying from 15 mils to 120 mils have been measured. This measurement characterizes the propagation loss in FR10 up to 100 GHz, where the loss reached ~0.35 dB/mm.

Having established propagation loss behavior in FR10 PCBs, we have embarked on characterizing high-frequency interaction with circuit devices. We have started with the ubiquitous 1N914 silicon diode, with the goal of performing device and circuit simulations to compare with the measurements. To measure the response of the 1N914 to high frequency RF, we employ multiple measurements of the waveforms, depending on frequency. The RF generator is also amplitude modulated at 1 KHz, as we are interested in the behavior of the diode in generating signals at frequencies that are potentially disruptive to operating systems. To detect DC shifts and AM response of the diode to extremely high frequencies up to 95 GHz, we employ lock-in detection of amplitude modulation of the RF signal applied to the diode with extremely high sensitivity.

In order to obtain all the parameters necessary for the simulation calculations, it is necessary to carefully determine the parasitic capacitances and inductances involved in device package. We have done this by mechanically dissecting the device and measuring the dimensions of the packaging using detailed microphotography. We have begun transient simulations using Spice. The startup transient response requires many cycles (100,000 in this case) to begin to approach steady state. This is typical of systems involving nonlinear dynamics, and is one of the challenges to which we will be developing approaches.

Significance

DOE, DOD, and other federal agencies rely on satellite communication systems for day to day and special operations. Loss of these systems would compromise the ability of the US to defend itself and would leave assets at risk. Determination of vulnerability will enable efforts to protect valuable electronic assets. Determining that vulnerability does not exist prevents unnecessary costly modifications.

Security Through Unpredictability

131541
Year 1 of 3
Principal Investigator: M. J. Berg

Project Purpose

Information system defense is currently engaged in an unfavorably asymmetric struggle with sophisticated adversaries. Standardized instruction sets, protocols, and hardware interfaces make our systems too uniform and predictable, allowing our adversaries to exploit these systems en masse using minimal reconnaissance. Today's defense systems do very little to directly address this asymmetry, relying instead on reactive technologies such as signature matching and patching. Truly effective information security measures must focus on eliminating the attacker advantage intrinsically.

This research will develop diversity technologies that eliminate certain classes of security vulnerabilities from information systems. For example, we will develop randomized instruction sets that can hinder propagation of malicious code. These technologies will be based on fundamental theories of information system security (to be developed as part of this research), allowing us to scientifically determine where and how to incorporate diversity into systems for the greatest security impact.

We will first develop a theory for using unpredictability to achieve security in critical US information systems. We will build on this theory to create a science- and engineering-based framework for understanding and evaluating information system security. Year one will culminate with our team demonstrating a prototype of an unpredictability-based security technology: a processor system that uses a randomized instruction set. In years two and three, we will further develop our research to address information technology supply-chain threats by creating design-for-evaluation technologies as well as unpredictable functional testing strategies. Finally, we will begin building dynamically reconfigurable networks that will be robust to adversarial reconnaissance and planning. Our work will be guided by a threat model designed to represent a sophisticated nation-state threat.

Summary of Accomplishments

We have prepared a draft technical report describing a new way of scientifically reasoning about vulnerabilities, the root causes of those vulnerabilities, and the effectiveness of potential security solutions — including the effectiveness of various randomization approaches. We evaluated a number of existing vulnerability classes and security solutions as case studies to demonstrate how our approach can be applied and to highlight areas where additional research may be useful. Our approach maps information system design to a hierarchy of nested universal Turing machines. Design patterns are repeated at each layer of this hierarchy with the repeated indirections (abstractions or mappings) at each layer being the root causes of security vulnerabilities. By studying the indirections that cause vulnerabilities, techniques for mitigating the vulnerabilities can be evaluated and reapplied at other layers in the hierarchy of nested universal Turing machines.

We have modified both the GNU assembler (GAS) and Yasm to generate randomized instruction sets. We have modified the QEMU machine emulator to support our randomized instruction set and we are in the process of modifying the Bochs virtual machine to support our randomized instruction set. The BIOS (basic input/output system) used by both QEMU and Bochs is currently being modified to support our randomized instruction set.

We are also reviewing existing network randomization research and are considering new ways to incorporate randomization into networks to provide increased security. Network protocols, routing protocols, apparent network topologies, host identifiers, and network delays are some of the areas currently being considered for randomization.

Significance

Sandia is pursuing information assurance as a core capability as a result of recently expressed national need. If successful, this research will result in a computing environment that is incapable of executing mobile malicious code without significant inside information. The results of this research will position Sandia as a leader in the field and contribute to our existing missions of securing high-consequence systems.

High-Speed Hyperspectral Measurement of LNG Combustion

137805
Year 1 of 1
Principal Investigator: J. K. Roskovensky

Project Purpose

This work will include the collection and analysis of valuable hyperspectral data over very large (35-, 70-, 100-m diameter) liquid natural gas (LNG) fires in order to acquire LNG signatures for remote-sensing discrimination purposes. Data collected will be used to develop models and signatures applicable to overhead space measurements in accordance with national security missions. The discrimination of fires from space on the basis of their fuel sources has different objectives including those of environmental and battlespace characterization, military operations, domestic security, and disaster remediation. The United States currently imports a significant amount of LNG via tankers. The possible damaging of one of these massive tankers (with volumes of up to 260,000 m^2) by a terrorist is of significant domestic security interest. The detonation of one of these carriers could produce significant damage to a port/harbor area. The collection of predetonation and postdetonation signatures as may be seen by a satellite is of critical importance in initial detection, identification, and for coordination of remediation activities.

Summary of Accomplishments

A field campaign was organized extremely well in a short period of time, which included instrument characterization, mobile unit acquisition, interfaces, and personnel.

Data was collected simultaneously by three main instruments: a Fourier transform infrared (FTIR) spectrometer, a high-speed visible camera, and a thermal imager.

New algorithms were developed to import and temporally co-register the data.

New calibration techniques were created that let the maximum measurement error of the FTIR spectrometer be quantified.

LNG data was compared to other fire data (JP-8 and wood pile) for the first time.

Combustion modeling code was used to accurately simulate the measured spectral data. A two-temperature model most accurately depicted the true nature of the fire by characterizing both the efficient combustion regions and those dominated by slow burning, absorbing soot.

Significance

This effort will produce first-time LNG signatures that will benefit the Nation's space-based surveillance missions. Signatures will be utilized in future phenomenology studies and sensor development projects. The organization of instruments, personnel, and logistics on a short-time period for a field campaign will aid future endeavors. The collection of transient gas-plume signatures is also expected to be helpful to the DOE nonproliferation mission.

Enhanced Global Strike Target Location and Tracking

138740
Year 1 of 1
Principal Investigator: W. T. O'Rourke

Project Purpose

The recently concluded “Data Fusion and Communications for Global Strike Weapon-Deployed Sensor Systems” LDRD project successfully demonstrated that a fused system of ground and air sensors can detect and locate targets and reduce target location error for global strike. That project culminated in a field demonstration that used real-time fusion of air and ground sensor data to localize target vehicles. The system performance proved the ability to improve localization through fusion, demonstrated the necessary network communications capabilities and validated the concept of reducing target location error using combined air and ground sensors. The results also showed that increased accuracy in the ground sensor mobile target tracking capabilities could lead to greatly improved overall fused ground and air sensor system tracking performance. This improved level of accuracy in target localization for both fixed and mobile targets is needed to fully demonstrate the value of this concept and make it more attractive to the prompt global strike community. This project proposes to build on the results of the previous LDRD project by employing beamforming ground sensors for tracking targets, and demonstrating improved performance for both the ground sensor portion and the overall fused results.

Summary of Accomplishments

This project resulted in an acoustic beamforming–based localization algorithm that is realizable on a real-time embedded UGS (unattended ground sensors) system. In addition to the computational constraints required for embedded systems, these algorithms worked on sensor arrays that are small enough to fit on existing air-delivered sensor platforms. The algorithm performance results indicate the target location error is greatly reduced over previous time difference of arrival (TDOA) algorithms, using an advanced beamforming algorithm. Additionally, the use of extended Kalman filter (EKF) direction of arrival tracking algorithms to augment typical beamforming algorithms allows for better tracking of the moving target as it enters a field of sensors.

Significance

By significantly improving the system target location error and providing the performance required for precise prompt global strike, this project will support Sandia’s mission to address challenging national security needs. The enhanced localization capability also has application in other target characterization arenas such as homeland defense.

Mutual Focusing for Improved Correlation between Radar Images

138806
Year 1 of 1
Principal Investigator: A. M. Raynal

Project Purpose

Sandia is the leader in developing state-of-the-art, real-time imaging radar systems over the last 25 years. More recently we have worked on radar systems that require high-correlation between radar images taken from different channels or at different times. These include interferometric synthetic aperture radar (SAR), clutter attenuation ground moving target indicator (GMTI), and coherent change detection (CCD) radar systems. One of the key drivers for high correlation is that the relative focusing between the images be similar. The purpose of this project is to investigate techniques that use the two images simultaneously to improve the focus matching, with the goal of improving correlation between the images. These techniques are novel, high-risk concepts that apply signal processing methods not previously applied to imaging radar systems, such as techniques used in communications systems. If successful, these techniques would allow us to provide new capabilities for new and existing customers.

Summary of Accomplishments

Through this project, we gained knowledge about cross-disciplinary techniques for the relative focusing of images or signals. We adapted cross-disciplinary approaches to the radar image relative misfocusing problem, and investigated algorithm performance in solving our problem and the potential for outperforming the current focusing strategy. Ultimately, this project gave us a unique perspective for thinking about the relative focusing of radar images in the context of equalization and linear systems. We determined that this new perspective to approaching the problem is viable, although significant outperformance to the current strategy is yet to be established.

Significance

This effort could lead to new capabilities in surveillance and reconnaissance radars, which are fundamental to the war fighter's situational awareness and decision making. Such capabilities are important to Sandia and its customers, for detecting significant activities, nuclear nonproliferation, and border or facility monitoring.

Spectral Compression

139007
Year 1 of 1
Principal Investigator: J. P. Koplow

Project Purpose

The purpose of this project is to explore the possibility of spectral compression using Raman fiber cavities. Spectral beam combining (SBC) combines multiple spatially separated laser beams of different wavelengths into a single, spatially coherent, multicolor beam with the aid of a diffraction optic, typically a surface Bragg grating, embedded in an optical cavity. SBC is relatively easy to implement, does not impose constraints on phase control, largely avoids deleterious nonlinear effects, and preserves beam quality. But the number of beams that can be combined is limited by the spectral resolving power of the beam combining cavity, the gain bandwidth of the lasing medium, and the emitter array fill factor. Spectral compression could potentially address this limitation.

Summary of Accomplishments

The objective is to explore the feasibility of spectral compression. The primary tasks are:

1. 1. Fabricate and characterize a) a high-power (~10-20 W) Yb-doped single mode fiber-coupled activated stimulation of emission (ASE) source at 1 micron; or b) two high-power Yb-doped single-mode fiber lasers wavelength stabilized and selected for operation at 1 micron.
2. 2. Demonstrate and characterize spectral compression using the multiwavelength ASE source or the two discrete wavelength fiber laser sources.

We demonstrated 6% 1095-to-1137.5 nm conversion efficiency using a 1095 nm pump source with 5 nm of emission bandwidth and 2.6% 1039-to-1091 nm conversion efficiency using a two-channel, 0.35 nm linewidth amplified ASE source. Moreover, both pump sources were compressed from 5 nm and 0.35 nm full width at half maximum (FWHM) of bandwidth to less than 0.5 nm. Poor free space-to-fiber coupling severely limited the amount of power that could be coupled. However, we identified the sources of our poor coupling efficiency. It appears that thermal lensing of the free space-to-fiber coupling optics and spatial instabilities of the pump beam (beam wander) precluded us from achieving the high coupling efficiency needed for delivery of several watts of optical power to a single-mode fiber. Both issues will be addressed in a follow-on LDRD project that will begin in FY 2010. Furthermore, we designed, constructed, and tested a multichannel, amplified ASE source capable of delivering up to 10 W of power at 1040 nm. The number of channels, channel spacing, and channel line widths are discreetly tunable by interchanging bulk etalon filters embedded in the optical path of the amplifier without disrupting system alignment. This should prove to be an invaluable tool for quickly determining the impact of channel spacing and line width on conversion efficiency. Performing preliminary tests with the discreetly tunable amplified ASE source will thus reduce risk and save time by identifying potential problems before embarking on costly development.

Significance

This project will leverage our expertise in fiber laser technologies to enable technology that could circumvent limitations of conventional spectral beam combining, advancing the DOE scientific discovery and innovation goal, with anticipated benefit to national security applications.

Proving the Parallelizability of a New Hashing Algorithm

139008
Year 1 of 1
Principal Investigator: M. D. Torgerson

Project Purpose

One limiting factor in all of the mainstream cryptographic hashing designs is an inability to be parallelized or pipelined. Those algorithms have a natural limit on the data rates they can support, which means that, in practice, authentication is a bottleneck in high-end secure communications. This project proposes to explore the feasibility of implementing novel hashing techniques recently introduced into the cryptographic community by the Sandia SANDstorm algorithm. By implementing the new techniques on a wide range of architectures, we will collect data on the difficulty of implementing the new methods and provide actual throughput numbers to compare with the theoretical estimates.

From a theoretical standpoint, parallelizing hash functions securely is a very difficult problem. However, SANDstorm, a Sandia-developed algorithm, introduces two innovative methods for providing parallelizability and pipelinability, plus it has several other design features that add to its parallelizability. It is believed that if sufficient resources are in place, the novel methods should allow the algorithm to operate at approximately 10,000 times the speed of nonparallel implementations.

This project will explore this new space of parallel techniques in hashing algorithms by implementing the design on architectures that will support parallel computation. The hope is to produce results either verifying or refuting the SANDstorm speed estimates and providing data on the difficulty of attaining those speeds on a number of different computer architectures.

Summary of Accomplishments

This project was successful in verifying the parallelizability claims of the SANDstorm algorithm. Several different implementations focusing on different aspects of the algorithm were completed and implemented on a variety of hardware platforms. Our implementations have resided on machines with 2, 4, 8, and 64 processors. We have seen speed increases of a factor equal to the number of processors.

We have shown that the SANDstorm mode is parallelizable. The speed increase is a linear function of the resources applied. Similarly the division of round function and message schedule work is parallelizable, as are the several operations within each of the two halves. In all of the cases, the programming costs to achieve the parallelization are relatively small. The implementation techniques were simple and straightforward and did achieve a speed up linear with respect to the resources applied.

Significance

Cryptographic hashing serves as the workhorse for authentication services in all sensitive government digital transactions. Having fast and secure hashing algorithms available for use is imperative to our national security. Speed is a critical attribute in any hashing selection, so it is imperative that we are able to verify SANDstorm's speed claims and show with tangible evidence that the novel techniques are amenable to parallelization and pipelining.

Pulsed Laser Microfabrication: Effects of Wavelength and Temporal Length

139583
Year 1 of 1
Principal Investigator: B. H. Jared

Project Purpose

Pulsed laser irradiation presents a unique capability for the fabrication of devices due to its material selectivity, minimal heat effects, high resolution and precise ablation positioning. One challenge in laser-based processing at the microscale is the creation of features with minimal effects on surrounding volumes. Understanding how to precisely create small features while minimizing the impact on neighboring materials is critical, particularly in post-production processes that enable device operation (for example laser dicing activities). While ultrafast laser pulses are presented in the literature as creating no thermal damage near the ablation threshold, in practice, damage typically occurs since powers an order of magnitude or higher than threshold are often required to achieve acceptable material removal rates. Therefore, work is proposed to understand and quantify the impact of pulse laser processing on surrounding materials and structures.

Summary of Accomplishments

Work was performed to examine the ablation of materials using pulsed laser systems. Processing with a nanosecond pulsed laser was observed to involve a significant thermal component due to its reliance on material absorption during ablation. One advantage of this behavior was the selective ablation of opaque materials relative to silicon across a relatively wide power density range. Shortfalls of the nanosecond laser, however, were its potential introduction of thermal damage into structures and its propensity for melting and consolidating filler materials rather than ablating them. As a result, multiple pass processing was found to be ineffective, requiring mechanical cleaning after each laser scan. Since processing with the femtosecond laser relies on highly focused energy densities rather than material absorption, it was observed to provide more precise cuts with minimal levels of thermal damage compared to the nanosecond laser. Unlike the nanosecond laser, each material tested was ablated with the femtosecond laser after successive processing passes. The resulting disadvantage is that the power densities required to reasonably remove organics will either damage and/or ablate silicon, albeit at slower rates. While testing was not completed due to equipment problems, initial work did suggest that the femtosecond laser does have a process component related to its wavelength. Therefore, future work to tune the laser wavelength could further optimize material removal rates while overcoming the process weaknesses of both nanosecond and femtosecond lasers.

Significance

This project ties to DOE's scientific discovery and innovation mission by conducting the first research of nonlinear light-matter interactions involving variable-wavelength ultrashort pulsed radiation.

3D Track Fusion Algorithms

139615
Year 1 of 1
Principal Investigator: J. M. Griesmeyer

Project Purpose

Three-dimensional (3D) position and velocity target tracking information and associated uncertainties are important for queuing additional tracking and interception assets. Multiple two-dimensional (2D) sensors are required to generate a 3D track. To date, 2D sensor fusion algorithms have been implemented in-house for two different sampling regimes: nonsynchronized intermittent observations for one sensor at a time, and synchronized batch observation sequences from multiple sensors. The first algorithm uses a Kalman filter to generate 3D tracks by adding 2D sensor observations one at a time. The second algorithm uses a Kalman filter to generate the 3D track by adding 3D points determined by first triangulating the batched 2D observations from the sensors. The first algorithm is currently incorporated into an integrated simulation system for performing system trade off studies. The second algorithm builds on observation association software that has been incorporated into a soon to be delivered ground system. In this project, both fusion algorithms will be made available in the simulation environment so that both synchronous and nonsynchronous observations can be fused to estimate 3D tracks. Simulations will be used to evaluate the performance of the fusion algorithms for various application scenarios, determine the best approaches for transitioning between them and investigate possible system architecture impacts on the performance of the 3D tracker.

Summary of Accomplishments

We designed and implemented extended Kalman filter trackers to estimate the state vectors of targets seen by two or more pointing sensors. Both 9-state (3D position, velocity and acceleration) and 12-state (3D position, velocity, acceleration and jerk) filters were developed that can be updated with either single 2D observations or with least squares triangulation points for 2D observations from more than one sensor. An extensive test harness was developed to allow simulation of a broad set of tracking problems and collect performance statistics. The filters were tuned and used to estimate tracking performance for a wide variety of target types and sensor combinations. The studies were used to access tracking algorithms, characteristics of targets that present challenges for the tracking algorithms and the impacts of sensor characteristics and location. In the studies, the tracker performed as well and in many cases better than an existing tracker from another company.

Significance

The versatile track fusion capability incorporated into an integrated simulation system will allow Sandia to demonstrate how our sensor data can be utilized, show the benefits of our sensor products, and provide information regarding possible queuing latency reduction. In addition, this new capability will provide the groundwork for incorporating this sensor fusion capability into future decision-support ground systems.

Establishing Trust Relationships between Hardware and Software Components

139929
Year 1 of 1
Principal Investigator: C. Hoff

Project Purpose

We need low-overhead, trusted communication methods between any trusted components that have been added into a computer or other information system.

As we design more modular and flexible information systems, it becomes easier for adversaries to compromise these systems. Hardware busses are increasingly similar to network topologies and are similarly vulnerable to malicious devices attached to these busses and compromising the system. Software architectures built from modular components and leveraging interprocess communication (IPC) techniques are increasingly similar to client and server applications communicating across networks and are similarly vulnerable to service impersonation, man-in-the-middle attacks, and unauthorized sessions from malicious software components.

Alternative protocols must either be adapted or created for use in establishing trust between the embedded components within a system. This project will identify and explore techniques for using the current capabilities of modular hardware and software components to build the required authentication features between components. Different components have different capabilities and limitations that must be considered.

This project addressed the characteristics and capabilities of hardware and software components at different levels in a general purpose computing system. The success of this research will provide a basis for establishing secure communication between these trusted components and will be applicable to new security technologies that can be incorporated into high-consequence system designs.

The benefit of this R&D effort is to advance the state of information assurance (IA) in untrusted systems, specifically, how one could improve trust in a system primarily or exclusively made of commercial off-the-shelf components. This work, if successful or showing promise, could address many IA issues currently of concern to the nation.

Summary of Accomplishments

The first step of this project was to identify internal and external computer busses relevant to establishing some level of trust in a system. For our purposes, relevant busses had one or more of these characteristics: direct memory access, direct access to host CPU registers, ability to provide code for the host CPU to execute, ability to interrupt the host CPU, and shared among all connected devices. For each bus we investigated, we documented its adherence to these characteristics as well as other vital statistics about the bus, such as throughput, typical devices, and supporting standards.

After a detailed analysis of the characteristics and capabilities of each bus, we determined its potential ability for use in establishing trust. This usually resulted in one of three conclusions: not useful, very useful, or potentially useful, but needs further research. Communication channels falling into the latter two categories will be used as a basis for future research proposals into how trust in complex computer communications can be determined and in methods for securely communicating anomalous or malicious behavior to the user.

The result of this research was thoroughly documented and was made available to other LDRD projects.

Significance

This work addresses a key need in cyber security. Trusted hardware and software has been proposed as one of the most promising approaches to improving confidence in our cyber systems. This work makes a valuable contribution by exploring the characteristics of the interfaces that must be used between the hardware and software components of a trusted system.

Feasibility of Chip-Scale Integrated Phononic Delay

140160
Year 1 of 1
Principal Investigator: P. T. Rakich

Project Purpose

Numerous applications urgently require a compact, broadband and efficient true-time delay technology. This project will demonstrate a fundamentally new (reciprocal) means of converting radio-frequency (RF) signals into acoustic signals over ultrabroad (GHz) bandwidths, enabling a breakthrough in delay-line technology necessary to achieve ultrabroadband chip-scale, tunable delay lines and a host of potentially revolutionary signal processing technologies. Our novel transduction method exploits new physical mechanisms involving the interaction of electromagnetic waves with matter. In the context of delay lines, the ability to convert signals to and from the acoustic domain is very powerful, since one can, in principle, achieve signal bandwidths while occupying a footprint of less than 1 cm^2 (due to the reduction in signal velocities made possible in the acoustic domain).

This project will enable analysis of the feasibility of such technologies through the development of numerical models and potentially a fabrication and test demonstration of feasibility.

Summary of Accomplishments

In order to determine the feasibility of this new delay-line technology system for broadband signal transduction, we have: 1. developed new methods for computing transduction based on this new physical effect, allowing us to achieve a breakthrough in transducer designs, 2. performed parametric design studies to determine the optimal transducer designs, and 3. identified low-risk paths to the realization of such systems using readily available fabrication techniques.

Significance

If successful, this transduction method could enable a breakthrough in delay-line technology necessary to achieve ultrabroadband chip-scale, tunable delay lines and a host of potentially revolutionary signal processing technologies which would benefit tag and electronically steerable antenna radar applications due to the tremendous improvements in size, weight, and power that this technology could provide.

Analysis of Radiological Threat Identification Algorithms

140252
Year 1 of 1
Principal Investigator: J. L. Powell

Project Purpose

Several competing algorithms exist for assessing the threat posed by radioactive materials but no mathematical methods exist to compare approaches. Sandia currently uses a modified template matching technique that has been developed empirically over several decades. However, we have become aware of other approaches that may offer additional benefits in extracting the maximum information content from our radiation spectra. These emerging methods include principal component analysis, wavelet decomposition, and energy windowing. While each of these approaches seems to offer benefits in specific situations, currently, the only feasible method of comparing performance is through costly and repetitive testing with radioactive materials. We propose using existing spectral data sets to evaluate and compare these emerging algorithms using computational/mathematic methods that will reduce the amount of required experimentation with radioactive and nuclear materials. We will develop a maximum likelihood estimator that will weight the results of the various analyses to optimize the spectral decomposition, and consequently the isotopic identification and threat characterization. If successful, this ability to use a hybrid approach in analyzing spectra will enable improvements in the sensitivity and selectivity to radiation detection systems in assessing radioactive or nuclear threats.

Summary of Accomplishments

The mathematical bases for identifying radiological threats were analyzed and compared, noting statistical differences and similarities between the algorithms based on the properties of input data. Numerical metrics were developed to quantify identification algorithms to determine which approach is best for analyzing data gathered under different conditions. In addition, optimization concepts were hypothesized, in order to optimize the performance of each algorithm along with methodologies for comparing the results of each algorithm. This study produced a fundamental mathematical foundation to implement the radiological threat identification algorithms in a single software tool for testing and development of optimization algorithms and metrics. Going forward, it is our hypothesis that algorithms can be developed to assess the characteristics of gamma radiation spectra collected by detection systems, in particular, improving the quality of the spectra using signal processing techniques and determining the most appropriate algorithm or combination of algorithms to determine the radioactive source present with high confidence. The development of a software tool using the mathematical bases discovered in this study provides the foundation for developing this type of capability.

Significance

This research is tied to the DOE nuclear security strategic theme. Specifically, it is related to detecting radioactive materials and nuclear nonproliferation. This research is aimed at developing the most robust methodology for identifying radioactive materials for a variety of radiation detection systems.

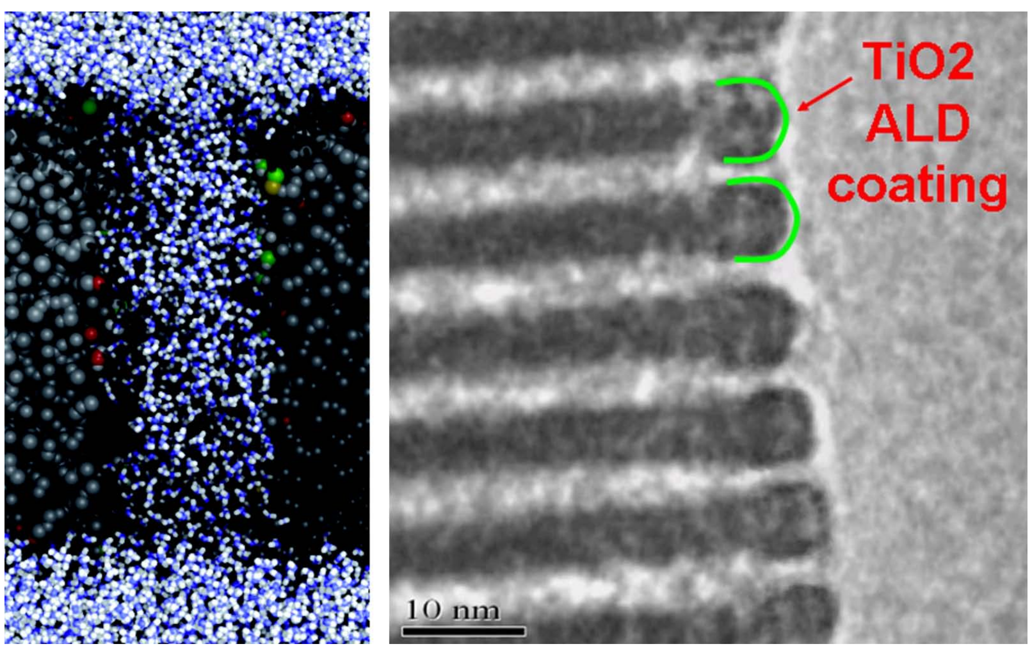
ENERGY, RESOURCES, AND NONPROLIFERATION INVESTMENT AREA

The ERN investment area funds research initiatives in energy S&T, such as solar thermal and photovoltaic, nuclear power and the nuclear fuel cycle, biofuels, liquid transportation fuels and carbon dioxide recycling, the hydrogen economy, and other areas at the cutting edge of domestic and global energy challenges.

Computational and Experimental Platform for Understanding and Optimizing Water Flux and Salt Rejection in Nanoporous Membranes

Project 117795

Clean water is widely recognized as perhaps the most critical limited resource of this century. Although they have been of great utility in purifying water of salts and contaminants, reverse osmosis membranes comprise a mature technology, one to which modifications have already shown diminishing returns. It is clear that new solutions to water purification are required, particularly in the area of efficiency. Pushing water through RO membranes requires energy, and new solutions need to address the fact that purification devices requiring lower energy consumption are crucial. Through study and modeling of biological membranes, this project is gleaning the chemical secrets that allow living cells to employ specific proteins to form both water channels through their membranes, as well as channels selective for the passage of certain salts. This project's interest lies in determining whether inorganic chemical solutions to the problem of ion and water selectivity can be discerned from their biological (organic) counterparts. Not only do researchers desire to purify water completely of its dissolved salts, but in some instances to find ways to allow certain salts to remain in the water, thus replicating naturally occurring mineral waters. Modeling has guided potential experimental solutions, for example, employing parallel silica nanotubes as water channels.



Model of a biological water channel (left). Transmission electron micrograph of parallel nanochannels of mesoporous silica (right), the entrance of the channels precisely tuned by plasma-assisted atomic layer deposition (ALD).

Innovative Control of a Flexible, Adaptive Energy Grid

Project 105865

Given the impending introduction of intermittent sources of renewable energy, such as from wind turbines, into the electricity grid, it is of critical importance to develop scalable analysis and control techniques based on thermodynamic principles. Such techniques must support the engineering of a flexible, adaptive energy infrastructure, as resilient to stresses and disruptions as possible. This is not the current situation, our existing grid operated at extremes of capacity and subject to disruptions and inefficiencies, its system properties not well-understood. To introduce intermittent energy sources into this situation demands a better theoretical understanding, as well as modeling and simulation tools that can test proposed engineering designs.

Employing a combination of theory, numerical simulation, and experimental validation, all underpinned by nonequilibrium thermodynamics, this project has designed a rapid-prototyping software environment for simulation of microgrid control systems. It incorporated experimental observations of several Hawaiian power generation systems that included diesel- and gas-powered electrical generators, to which this modeling endeavor added wind turbines. This scenario revealed several important operational findings, particularly that frequency variations occur due to wind intermittency, and may cause frequency instabilities. Ultimately, the end-result of the project will be a digital architectural framework that is self-organizing and dynamically reconfigurable to cope with diverse situations, while efficiently managing excess power capacity and surplus power-generating capability.

Model of "real world" microgrid able to simulate Lanai, Hawaii power-generation system to which intermittent energy sources were added.

ENERGY, RESOURCES, AND NONPROLIFERATION INVESTMENT AREA

Geophysical Remote Sensing of Water Reservoirs Suitable for Desalination

105824
Year 3 of 3
Principal Investigator: L. C. Bartel

Project Purpose

Creating usable new water through desalination requires identifying groundwater reservoirs appropriate for any proposed desalination process. There are many economically valuable New Mexico hydrological reservoirs (e.g., in the Tularosa Basin) where the absolute level and spatial distribution of fluid salinity are not well established. Water quality varies within a reservoir, grading from potable water, to water suitable for agricultural use, to water where desalinization is necessary. Resource characterization, production, and recharge monitoring, and identification of waste disposal formations are critical issues for managing a desalination water supply. Remote assessment of salinity and aquifer monitoring via geophysical sensing methods will dramatically reduce the cost of characterizing groundwater quality compared with drilling and sampling approaches. Monitoring is crucial in cases where there may be intrusion of more saline water, rendering the designed desalination process ineffective; e.g., total dissolved solids (TDS) in excess of 5000 ppm for some processes. The goal of this research is to differentiate groundwater salinity that ranges from EPA standard of 750 ppm, and the TDS range ~ 2000 ppm to < 5000 ppm or more and provide a methodology for water supply management. Both surface and borehole seismic and electromagnetic (EM) methods have the potential for low-cost remote assessment of salinity within large volumes of an aquifer, as well as monitoring production and recharge. Pore water salinity affects the aquifer electrical resistivity and the magnitude of the seismoelectric (SE) effect. Our research will focus on: (1) utilization of conventional EM methods to determine salinity where the geologic structure is determined through seismic methods (thereby constraining the EM interpretation); (2) enhancing our existing 3D poroelastic wave propagation algorithms to include the coupling between EM and poroelastic wavefields, allowing quantitatively investigation of seismoelectric effects to determine water quality; and (3) field demonstration of seismic and EM methods.

Summary of Accomplishments

The research in this project addressed two complementary ways to utilize seismic and EM methods. The first technique uses the seismic data to constrain the geologic structure for interpretation of the EM data, and then perform a joint interpretation of all the data for electrical conductivity, porosity, and hydraulic permeability. We showed through numerical simulations a methodology of combining seismic and EM data sets for joint interpretation. The porosity is the connecting link between the seismic and EM methods. As part of this research, we demonstrated a methodology to build an earth model that is consistent for the seismic and EM model calculations. For the second, more high-risk, component of this research, we intend to utilize the seismoelectric (SE) and/or the electroseismic (ES) effect. These techniques have not been commonly tried for water quality assessment but, have the potential to provide a better measure of the salinity and pH of the target water supply (particularly in the low ppm ranges of NaCl). When combined with the first method, the assessment of the salinity has a high probability of success for determining the economic utility of the aquifer. As part of this research, we developed a 2D poroacoustic-EM algorithm to investigate the SE and ES effects. This algorithm couples two different physical phenomena that in finite-difference modeling have different spatial and temporal scales. We developed a method to extrapolate between the different spatial scales and the different temporal scales so that the seismic and EM wave propagation are calculated on the appropriate spatial and temporal scales. A field experiment was conducted to investigate the SE effect. The electric power line noise was removed using a prediction error filter; however, the results were inconclusive as to whether an electric field was observed due to a seismic source.

Significance

This research addresses DOE’s overarching mission to advance national security, and in particular, energy security, and to promote scientific and technology innovation to support this mission. The security of the US involves water supplies to support energy and economic security. Evaluation of potential water supplies aligns with Sandia’s water initiative.

Advanced Fuel Chemistry for Advanced Engines

105825
Year 3 of 3
Principal Investigator: C. A. Taatjes

Project Purpose

The relationship of fuel chemistry to ignition is a key knowledge area for emerging low-temperature combustion engines that promise to combine increased efficiency with low pollutant emission. Knowledge of ignition chemistry is central to engineering these advanced combustion technologies for a changing fuel stream, including biofuels. This project is developing a new experimental capability to measure important radical intermediates in controlled systems of chemical reactions. This investigation poses strong technical challenges, both in the experimental time-resolved measurement of transient species at elevated pressure and temperature, and in the interpretation and analysis of complex systems of chemical reactions. The experimental capability builds on optical methods for probing intermediates in high-pressure systems and extends these methods with a novel application of molecular-beam mass sampling. This new approach overcomes the historic inability to measure the critical fuel-based radical species in ignition chemistry. The interpretation of these systems involves a multiple-scale computational approach combining state-of-the-art detailed theoretical kinetics to rigorously characterize the most important reactions with automated reaction mechanism generation and modeling to capture the global behavior. Success will hinge on close links between experiment and modeling. The anticipated outcome is a fundamentally new knowledge base of fuel-structure effects on ignition pathways in poorly characterized but technologically crucial fuels such as ethanol, butanol, naphthenes (components of oil-sands-derived fuels) and methyl esters (biodiesel). This knowledge base is a foundation for the simultaneous optimization of advanced engines and advanced fuels, an historically unique opportunity afforded by the concurrent revolutions in combustion and fuel technologies.

Summary of Accomplishments

Autoignition chemistry is central to predictive modeling of many advanced engine designs that combine high efficiency and low inherent pollutant emissions. This chemistry, and especially its pressure dependence, is poorly known for fuels derived from heavy petroleum and for biofuels, both of which are becoming increasingly prominent in the nation’s fuel stream. We have investigated the pressure dependence of key ignition reactions for a series of molecules representative of nontraditional and alternative fuels. These investigations combined experimental characterization of hydroxyl radical production in well-controlled photolytically initiated oxidation and a hybrid modeling strategy that linked detailed quantum chemistry and computational kinetics of critical reactions with rate-equation models of the global chemical system. Comprehensive mechanisms for autoignition generally ignore the pressure dependence of branching fractions in the important alkyl + O_2 reaction systems; however we have demonstrated that pressure-dependent “formally direct” pathways persist at in-cylinder pressures.

Significance

This project is closely tied to the DOE missions of energy efficiency and energy security. Knowledge of ignition chemistry is key to high-efficiency engines that may substantially reduce dependence on foreign sources of petroleum. The tools developed will support diversification of the energy supply through improved use of biofuels and nontraditional petroleum sources. The new capabilities and expertise generated by this work will benefit DOE and industrial partners.

Refereed Communications

R.X. Fernandes, J. Zádor, L.E. Jusinski, J.A. Miller, and C.A. Taatjes, “Formally Direct Pathways and Low-Temperature Chain Branching in Hydrocarbon Autoignition: The Cyclohexyl + O_2 Reaction at High Pressure,” *Physical Chemistry Chemical Physics.*, vol. 11, pp. 1320–1327, March 2009.

Supercritical CO_2 Brayton Cycle Test-Loop Development, Controls, Testing, and Model Validation

105829
Year 3 of 3
Principal Investigator: S. A. Wright

Project Purpose

Research, development, and demonstration of more-efficient and -compact electrical power conversion concepts is an essential element in maximizing the energy efficiency and cost effectiveness of next-generation nuclear power plants. The supercritical carbon-dioxide (S-CO_2) Brayton cycle is considered one of the most promising power conversion cycles because it can achieve very high efficiency (40–50%) at relatively low reactor coolant exit temperatures (< 600 °C). The cycle involves compression near the critical point of CO_2 to achieve a significant part of the efficiency increase over other Brayton cycles. The nonlinear behavior in this region and the effect on compressor control and stability have to be understood and demonstrated before development of this more-efficient cycle can occur. Although no demonstration of the supercritical CO_2 Brayton cycle and compression near the critical point has been done, recent advancements in the development of turbomachinery, gas foil bearings, high speed alternators, compact high pressure heat exchangers, and advanced inexpensive power electronics make it possible for the first time to affordably evaluate and experimentally demonstrate this essential technology on an appropriate scale. This project proposed and completed the following milestones:

1. develop the world's first supercritical carbon-dioxide (S-CO_2) Brayton cycle test-loop to study these critical point compression issues;
2. operate the loop to study the coupling of reactors with S-CO_2 power conversion systems, test and understand control methods associated with supercritical phenomena, and study the scalability to larger systems; and to
3. develop integrated dynamic simulation models for supercritical compression and Brayton cycles to support the development of effective control methods.

S-CO_2 power conversion cycles are applicable to a variety of heat sources including solar, fossil, nuclear, and geothermal. Multiple interactions and future contracts in all these areas are expected.

Summary of Accomplishments

Significant progress was achieved in designing, manufacturing, assembling and operating of the supercritical CO_2 compression test-loop. All milestones were met. The test-loop was designed the first year, fabricated and assembled the second year, and nearly 100 operations of the test loop were performed in the last year. The turbomachinery has operated at speeds up to 65,000 rpm, with flow rates of 4 kg/s and with a compression ratio of 1.65. Tests were performed to validate the compressor performance maps, to investigate thrust loads, to measure rotor windage losses, to measure seal leakage flow rates, and operations on gas-foil bearings. Over eight reports that describe the supercritical loop and test results were published in a number of journals and conferences. Sandia has also filed for a patent on the high power density supercritical turbo-alternator-compressor.

The testing has shown that compression near the critical point is stable and controllable and that there is a smooth transition from single-phase operations above the critical point to two-phase operations below the critical point but within the saturation curve. Sandia and its contractor (Barber Nichols, Inc.) have operated the loop with the compressor inlet at or very near the critical point where very nonideal CO_2 gas properties are important and even in the two phase region within the saturation curves. This loop and turbomachine is now the research and development test rig to study details of compressor operation and supporting components such as seals, bearings, and thrust balance mechanisms for supercritical power generation systems.

Significance

The completion of the small scale S- CO_2 test loop and the measured test results is providing the science and engineering base for supercritical compression phenomena to support the design and development of larger-scale demonstration systems. The work that was performed in this project has provided a basis for multiple future Sandia efforts in DOE energy security programs, for Naval Reactors, for the fossil commercial industry, and for defense applications. Over $1.4 M in additional contracts has been received to perform additional testing using this hardware.

Foundational Development of an Advanced Burner Reactor Integrated Safety Code

105833
Year 3 of 3
Principal Investigator: R. C. Schmidt

Project Purpose

Global environmental concerns, uncertainties, and unpredictability in fossil fuel resources, and the ever growing worldwide demand for energy have led to a dramatic resurgence in efforts to develop, license, and build advanced nuclear power systems to provide increased safety, reduce the amount of nuclear waste, and address proliferation concerns. In the nuclear fuel cycle envisioned for the future, an advanced burner reactor (ABR) based on fast reactor technology is expected to play a key role. However, the improved system designs being proposed have not been subject to the thorough safety analysis or risk assessment that will certainly be required. Legacy reactor safety codes have received only minimal investment since the early 1990s, and modeling approaches have not kept pace with computational technology.

The purpose of this project was to develop and demonstrate the foundational aspects of an advanced multifidelity burner reactor integrated safety code (BRISC) that could be used to perform the rigorous nuclear reactor safety analysis that will be required in the future for the design and licensing of advanced nuclear reactors. A central task was to consider how best to marry the high performance computational technologies developed over the past 15 years with the phenomenological modeling capabilities embodied in legacy reactor safety codes and improvements to them. This required addressing how both old and new codes could be combined/coupled using a multiphysics driver, and also accomplished in such a way that any strongly coupled physics being treated by the different codes would properly interact and yield fully converged solutions at each time step.

Summary of Accomplishments

We developed and demonstrated a prototype multiphysics multiscale driver code for nuclear reactor safety simulations. This tool was successfully demonstrated on 2D and 3D problems that involved six different coupled physics codes (mesoscale in-vessel flow and HT, mesoscale in-vessel solid conduction, fluid-solid interface transfer, mesoscale neutronics, subgrid core-region pin modeling, and balance of plant).

We developed a general purpose multiphysics driver and Trilinos-based coupling strategy that:

1. enables new and existing applications to be combined with strong coupling through Jacobian-free Newton-Krylov (JFNK) or fixed point solution methods,
2. is not limited to codes written in one particular language, a particular numerical discretization approach (e.g., finite element),or physical models expressed as partial differential equations (PDEs),
3. and created a wide range of associated example test problems.

We developed a novel approach for multiphysics coupling across complex nonconformal mesh interfaces that uses a “surfdiver-based” interface mesh.

We developed a prototype generalized interface to multifidelity neutronics solvers and applied it using Pt-kinetics and 2D diffusion models.

We developed the following new extensions of the RIO fluid flow and heat transfer code:

4. modeling capability for anisotropic nonequilibrium porous medium
5. capability to perform physics based preconditioning
6. capability to compute global residuals.

We applied and tested the idea of variable scaling in the multiphysics driver to improve convergence robustness.

We performed additional development of the “nonlinear elimination” strategy to enable physics codes that do not provide residuals to be incorporated into a strongly-coupled multiphysics solution environment.

We created a complex 3D solid model and the associated hex-only exodus meshes of all major reactor components and regions of an Argonne National Laboratory (ANL)-designed advanced burner reactor.

We performed demonstration calculations of

7. a 2D reactor through an entire transient
8. a 3D reactor — initial few seconds (serial calculation)

Significance

This work relates to the significant energy and global environmental problems being faced by this country. It supports DOE missions to advance nuclear power systems to provide increased safety, reduce the amount of nuclear waste, and address proliferation concerns.

Nuclear Facility Counterproliferation

105863
Year 3 of 3
Principal Investigator: D. A. Jones

Project Purpose

Emerging proliferators and uncooperative nations with nuclear ambitions present increasing threats to the US, which the government must address with increasing sophistication. The purpose of this project is to develop analytical tools that: 1) formalize the integration of data from multiple sources so that integration is easier for analysts and more transparent to the users of the results; 2) assist analysts at various stages of nuclear development by a potential adversary, where different types of questions are most important; and 3) provide guidance in developing strategies to deter, delay, or deny adversaries' nuclear weapons capabilities. In the course of this project, we have developed analytical tools based on four related, but distinct, sets of ideas. These tools are intended to assist analysts in addressing a spectrum of questions that arise at different stages of development by potential nuclear proliferators. A case study focuses on nuclear weapon development in the Republic of South Africa (RSA) during the 1960s and 1970s. By doing a retrospective case study of this type, where we now know the chronology and what was actually occurring at various times, we can test how the various modeling tools would have been helpful in sorting through various types of information that became available over time as South Africa progressed toward having a small set of deliverable nuclear weapons.

Summary of Accomplishments

We developed four tools utilizing: (1) Dempster-Shafer theory (DST), (2) Bayesian network models, (3) hidden Markov models (HMMs), and (4) project network disruption.

In DST, based on the theory of evidence, the evidence comes in many forms — varying credibility and/or reliability, and pertains to varying levels of specificity or abstraction about the event or conjecture of interest. DST models incorporate "I don't know" as part of the evaluation of the evidence. This tool is useful in early stages of analysis, when data is fragmentary and questions are broad.

We created Bayesian models providing a framework to: (1) summarize current beliefs about the probability of a specific uncertain condition or event ("prior" probability); (2) characterize the quality of new data (signals) in terms of the likelihood of false positives and negatives; and (3) integrate the new data into current beliefs to create an updated ("posterior") probability.

We developed HMMs that address questions like "How long until country X achieves capability Y?" In HMMs, some "process" occupies a sequence of "states" over time and "transitions" from one state to another occur randomly. The process is "hidden" since it is not directly observable — "signals" may emanate from the process that can be detected and used to infer what state the process is in.

We developed a project network disruption model that addresses the question "What could be done about country X's acquisition of capability Y?" We utilize a "hybrid" of risk analysis fault trees and project networks. This tool calculates the time until some critical capability is achieved, including time durations for specific activities that must be completed successfully and precedence requirements. Alternate "paths" are possible — the network may include "OR" relationships. The tool computes the probability distributions on the time required to reach the "end state."

Significance

In the course of this project, we have developed analytical tools based on four related, but distinct, sets of ideas. These tools are intended to assist analysts in addressing a spectrum of questions that arise at different stages of development by potential nuclear proliferators. At a very early stage, there is likely to be fragmented and sketchy information about possible weapon-related activities, and the core questions are in a general category: "What is country X doing?" This very general question often is directed at discerning country X's intentions with respect to nuclear development. As time progresses, more data are collected, and the character of the questions becomes more detailed. A general characterization might be: "How are they going about it?" As more data are collected and there is greater understanding of activities that are underway, a third category of questions arises: "What might the US do about it?" The four types of tools we have developed span the spectrum of these core questions versus the amount and quality of information available.

Tracking Nuclear Materials Processing: Metabonomics of Indigenous Species

105864
Year 3 of 3
Principal Investigator: M. K. Alam

Project Purpose

Tracking and proving proliferation of nuclear materials production, in particular uranium enrichment and/or plutonium production, can be a difficult task. By determining the unique metabonomic signatures of different plants and animals (birds, mammals, fish, trees, algae, etc), due to low level exposure to specific chemicals, it may be possible to provide evidence for nuclear materials processing. One can envision using metabonomics for tracking other environmental perturbations, such as those induced by industrial processes, illicit chemical production, and chemical or biological weapons manufacturing. The "indigenous species sensor" can be multiplexed (many are available), is difficult to remove or alter, and is continually collecting data, making it an ideal illicit production tracking device.

As a proof of principle we have demonstrated, with the University of Texas Medical Branch, the response on rats (a mammalian model) because these animal systems are well developed in metabonomic research. During the course of this project we have developed the chemometric tools needed for the analysis of these complex, multidimensional data sets. During the first two years of the project we have focused on developing instrument transfer functions and defining the parameters of our animal experiments. The third year saw completion of the chronic studies and successful modeling of both the acute and chronic data. Models were developed for tributyl phosphate (TBP) exposure in the presence of triphenyl phosphate (TPP) for both acute and chronic nuclear magnetic resonance (NMR) data. In addition the metabolic changes within the data were identified.

Summary of Accomplishments

The use of metabolic signatures as a method to detect nuclear production was explored. Sprague Dawley rats were used as the mammalian model in this study to determine the efficacy of biological systems as indigenous sensors. By tracking of indigenous flora and fauna and their metabolic response (metabonomics) to environmental release of chemicals associated with nuclear materials processing, one may be able to address the counter/nonproliferation puzzle of when and where nuclear production is occurring. We have shown that the metabolic response of our mammalian model is indeed altered by exposure to both acute and chronic levels of TBP, an extractant used in nuclear fuel rod reprocessing. The signature found was to be distinct, not only from the background, but from a homolog chemical, TPP, used in industrial processing. Further, in anticipation of field application of our sensor, we explored and developed methods for instrumental model transfer, needed for general application of the sensor.

Significance

Current counter/nonproliferation efforts have focused on detection of isotopic species produced from nuclear (re)processing. While an important piece of the puzzle, detection of chemicals used in nuclear processing is also a key piece of the puzzle necessary as evidence for the international community. The ultimate goal is to develop a new analytical method/sensor that will enable our nation's security by detecting covert nuclear processing. In addition to tracking nuclear materials processing this metabonomic research has the potential to impact other areas where toxic chemical exposure may be of concern, including water surety, and environmental monitoring.

Refereed Communications

T.M. Alam, M.K. Alam, D. Volk, M. Neerathilingam, and B.A. Luxon, "Investigation of Chemometric Instrumental Transfer Methods for High-Resolution NMR" *Analytical Chemistry*, vol. 81, pp. 4433-4443, June 2009.

Innovative Control of a Flexible, Adaptive Energy Grid

105865
Year 3 of 3
Principal Investigator: D. G. Wilson

Project Purpose

Although the US energy infrastructure remains very reliable, it has shown its volatility through power grid disruptions and fuel supply shortages. Some challenges within the energy infrastructure can be attributed to it being operated beyond its original intent, primarily for economic and market driven reasons. Deregulation has also complicated the system and has facilitated the transfer of power across state boundaries and over congested lines. These changes have resulted in an incomplete understanding of the system, and not an improvement. Additionally, the energy infrastructure is in a state of transition where emerging fuel options (e.g., hydrogen) and intermittent electricity generation sources (e.g., wind and solar) are being proposed as major elements of the future energy mix. Many uncertainties exist as to how these technologies will impact the energy infrastructure reliability and efficiency, because they are not designed for "easy" integration and are intermittent in nature. Additionally, the electric grid is being operated closer to the instability limits, primarily because of the need to use existing infrastructure elements to the greatest extent possible. Consequently, better approaches are needed to understand, engineer, manage, and control the energy grid. By closing the waste-mass cycle for the entire energy system and maximizing the use of exergy (useable energy), a more-efficient and reliable infrastructure could be designed.

In this project, we propose the development of a scalable closed-loop nonlinear analysis and control based on exergy and irreversible entropy production that can support engineering of a flexible, adaptive energy infrastructure which is more resilient to stresses and disruptions. Our initial focus will be on the electric power grid, and the challenges associated with incorporating diverse sources of intermittent power.

Summary of Accomplishments

- Developed exergy/entropy power flow control methodology for power engineering systems.
- Developed nonlinear/adaptive power flow control algorithms for nonlinear multi-input multi-output systems with information feedback applications.
- Two test case electrical power grid (EPG) systems have been developed with exergy/entropy control applicability.
- Validated key scenarios with analysis that will help drive and assess renewable integration for Kauai and Lanai Islands.
- Verified baseline hybrid real-time digital simulator that provided validation for exergy/entropy advanced control for the Lanai EPG system with renewables (photovoltaics).
- Performed evaluation of PSCAD® model (and identified submodels) of the Kauai microgrid system. This model was used to evaluate the stability/potential of renewable (wind) exergy assessments.
- Employed dynamic programming optimization to determine/assess best way to integrate renewables.
- Identified several potential approaches to bridge between large grid and detailed dynamic modeling:
    1. The larger model is based on a nonlinear, hybrid dynamical power grid models using finite state approximations. The finite state approximations research is expected to aid in the exergy analysis of large power systems, by serving as an intermediate between the original nonlinear dynamic

representation and application of exergy analysis. This will allow for a control and stability study that can be performed with a more computationally realizable model.

2. Distributed agent based control (implementation large scale).
3. Supernode model reduction with virtual hierarchical architecture (will require novel/new developments EPG similitude and scaling techniques).

- This project has delivered a challenging mix of science-based engineering activities (theory, modeling, experiment) that resulted in: i) participation in four national/international conferences; ii) presentation of a one-day workshop at the 47th IEEE Conference on Decision and Control; iii) formally documented results in five engineering technical archival journals; iv) generated four patent pending applications; and v) one book contract.

Significance

This project will have impact on maintenance and protection of the nation's critical infrastructures, such as, distributed supervisory control and data acquisition (SCADA) systems, networks of electrical power grids, or nuclear security systems. Many of our nation's critical infrastructures will benefit from an architectural framework that is self-organizing, self-healing, self-adapting, dynamically reconfigurable and resource optimizing, with efficient management of excess capacity and surplus capability.

Refereed Communications

R.D. Robinett III and D.G. Wilson, "What is a Limit Cycle?" *International Journal of Control*, vol. 81 No. 12, pp. 1886-1990, December 2008.

R.D. Robinett III and D.G. Wilson, "Exergy and Irreversible Entropy Production Thermodynamic Concepts for Nonlinear Control Design," *International Journal of Exergy*, vol. 6, pp. 357-387, March 2009.

R.D. Robinett III and D.G. Wilson, "Collective Plume Tracing: A Minimal Information Approach to Collective Control," *International Journal of Robust and Nonlinear Control*, vol. DOI:10.1002/rnc, p. Online Publication, March 2009.

R.D. Robinett III and D.G. Wilson, "Hamiltonian Surface Shaping with Information Theory and Exergy/Entropy Control for Collective Plume Tracing," to be published in the *International Journal of Systems, Control and Communications*.

R.D. Robinett III and D.G. Wilson, "Nonlinear Power Flow Control Design: Utilizing Exergy, Entropy, Static and Dynamic Stability, and Lyapunov Analysis," IEEE CDC, December 2008, 47th IEEE Conference on Decision and Control Workshop.

R.D. Robinett III and D.G. Wilson, "Nonlinear Power Flow Control Design: Utilizing Exergy, Entropy, Static and Dynamic Stability, and Lyapunov Analysis," Springer-Verlag, to be published in July 2010.

Decision Support for Integrated Water-Energy Planning

105867
Year 3 of 3
Principal Investigator: V. C. Tidwell

Project Purpose

Currently, electrical power generation uses about 140 billion gallons of water per day accounting for over 39% of all freshwater withdrawals, thus competing with irrigated agriculture as the leading user of water. Coupled to this water use is the required pumping, conveyance, treatment, storage and distribution of the water, which requires on average 3% of all electric power generated. While water and energy use are tightly coupled, planning and management of these fundamental resources are rarely treated in an integrated fashion. Toward this need, a decision support framework has been developed that targets the shared needs of energy and water producers, resource managers, regulators, and decision-makers at the federal, state and local levels. This modeling framework is designed to be open and interactive, providing a real-time environment for evaluating competing policy and technical options relevant to the energy-water nexus. Specifically, the model will help answer such questions as the following:

- What are possible energy and water shortfall scenarios for a particular region?
- What are tradeoffs between alternative energy futures to meet projected shortfalls?
- What are tradeoffs between alternative water allocation schemes?
- What technology options can be employed to mitigate water and energy demands?
- Where are coupled energy-water demands likely to be most acute?

The framework integrates analysis and optimization capabilities to identify tradeoffs, and "best" alternatives among a broad list of energy/water options and objectives. The decision support framework is formulated in a modular architecture, facilitating tailored analyses over different geographical regions and scales (e.g., national, state, county, watershed, North American Electric Reliability Corporation [NERC] region). An interactive interface allows direct control of the model and access to real-time results displayed as charts, graphs and maps. Ultimately, this open and interactive modeling framework provides a tool for evaluating competing policy and technical options relevant to the energy-water nexus.

Summary of Accomplishments

The primary accomplishment of this effort is the development of an integrated energy-water planning model. The tool is formulated within a system dynamics architecture, designed to operate on an annual time step. The spatial extent of the model includes the continental United States, Alaska, and Hawaii. At its highest level, the model is organized according to three primary sectors, demography, electric power, and water. The demographic sector model simulates changes in population and gross state product that drives the demand for electric power and water. Within the electric power sector the growing demand is satisfied by the construction of new power plants. The analyst has control of the type of plant (i.e., coal, oil, natural gas, nuclear, hydroelectric, geothermal, wind, and other) as well as the type of cooling system (i.e., once through, recirculating cooling tower, recirculating cooling pond, or air cooled) employed in the new construction. Water demand for the new power plants is calculated and included as a demand to the water sector. Within the water sector, the demand for water (both use and consumption) is calculated according to the other primary uses, municipal, industrial, mining, livestock, and agriculture. These demands are then compared to a variety of water supply metrics to identify locations of potential water stress. Additionally, the demand for electricity by the growing water industry is computed and included as part of the growing demand for electricity.

A key feature of this tool is the ability to perform analyses at a variety of disparate scales (national, state, county, NERC region and watershed). To aid in visualization of model results a link to Google Earth has been developed. Additionally, linkages have been developed with optimization tools for automated siting of power plants according to alternative siting criteria.

Significance

This project addresses DOE's mission to ensure a reliable, affordable, and environmentally sound energy supply for our nation. Energy extraction, processing, and transmission are dependent on the availability of water. The ability to meet growing demands for energy could be compromised by rapidly increasing demands placed on our nation's water supply by municipalities, irrigated agriculture, and the environment.

Phenomenological Basis for Safety Assessment of Nuclear Process Facilities

117791
Year 2 of 3
Principal Investigator: D. A. Powers

Project Purpose

This project's purpose is to develop mechanistic phenomenological models of key hazards that can arise in the aqueous reprocessing of reactor fuel. During the first year of the project, efforts were focused on modeling the formation and transport of combustible ammonium nitrate aerosol and the development of models of the chemistry and radiolysis of aqueous and organic solutions used in fuel reprocessing. In the second year, the aerosol model will be augmented by including the effects of particle bounce and breakup. The chemical models developed in the first year of research will be used to investigate conditions that lead to:

- explosive decomposition of hydroxylamine nitrate in highly acidic solutions (up to 15 molal)
- conditions for the formation of plutonium hydroxide precipitates and the accumulation of these precipitates that can lead to criticality hazards
- conditions for the formation of explosive metal azide compounds in the highly acidic solutions used for fuel reprocessing.

The models being developed in this effort are generic in nature so that they can be incorporated into systems-level models of particular fuel reprocessing facilities. The availability of mechanistic models will lead to better safety analyses that are not unnecessarily conservative and help to provide technical support for the administrative limits imposed on the operations of fuel reprocessing facilities. The models should find use in support of projects within DOE's efforts to close the nuclear fuel cycle and its efforts to dispose of excess weapons-grade nuclear fuel.

Development of mechanistic models of hazards in fuel reprocessing facilities is technically challenging because of the many pertinent phenomena that must be addressed in the high concentration irradiated solutions, and requires integration of state-of-the-art descriptions of individual processes into reliable predictive models to reliably predict hazards of fuel operations.

Summary of Accomplishments

Work in this effort has been divided into three broad categories: 1. aqueous modeling, 2. organic phase modeling, and 3. modeling of ammonium nitrate aerosol. The first year of work was focused on aqueous modeling. In the second year, the focus has been on organic phase modeling and aerosol modeling. Progress in these latter two areas is summarized in as follows.

Organic phase modeling

The organic phase of a solvent extraction process is an aliphatic hydrocarbon containing about 30 weight percent tributyl phosphate. Radiolysis of the organic phase will produce hydrogen. More importantly, it can produce reactive unsaturated and saturated high molecular weight species that can react to form combustible nitrates. The understanding of organic phase radiolysis is less detailed than the understanding of aqueous radiolysis. Consequently, it has been necessary to take a more empirical approach to the modeling and rely on data for the prediction of radical formation due to the ionizing radiation dose.

Ammonium nitrate aerosol modeling

Ammonium nitrate aerosols are formed from radiolytically produced ammonia vapors and vapors of nitric acid. The aerosol formation is being modeled as the Brownian agglomeration of primary particles to form particles of fractal dimensionality. A survey of methods to model coagulation of fractal particles has been completed. Modeling of particle deposition with facility ducts by turbulence has been completed. A probabilistic description of the potential for depositing particles to bounce has been devised based on particle kinetic energy. Significant has been the development of a computational technique for examining the potential of breakup when a fractal particle impacts a surface. A topical report on this development has been drafted.

Significance

The work has been undertaken in anticipation of DOE needs for safety analysis at fuel reprocessing facilities in support of its Global Nuclear Energy Partnership. The work also supports DOE's effort to develop a mixed oxide fuel fabrication facility for the disposal of weapons-grade plutonium at the Savannah River Site. The availability of mechanistic models of hazards will help avoid overly conservative designs and provide technical foundations for administrative limits on facility operations.

Development of a New Generation of Waste Form for Entrapment and Immobilization of Highly Volatile and Soluble Radionuclides

117792
Year 2 of 3
Principal Investigator: Y. Wang

Project Purpose

The US is planning to revive its nuclear power industries through the initiative of Global Nuclear Energy Partnership (GNEP). One of the key components of this initiative is the safe disposition of various waste streams to be generated in spent fuel reprocessing. Immobilizing these waste streams into durable waste forms for long-term disposal is a great technical challenge. The existing waste forms are unable to meet such needs. Disposition of iodine (I-129) and technetium (Tc-99) is particularly problematic, because of their long half-lives and mobility. During fuel reprocessing, a majority of ^{129}I will enter into the dissolver off-gas stream, and it is highly desirable to develop a material that can effectively entrap gaseous iodine during the off-gas treatment, which then can be directly converted into a durable waste form for long-term disposal. We here propose a completely new concept for developing a future generation of waste forms based on nanoscale radionuclide immobilization and encapsulation. We will first engineer a suite of nanostructured materials that are able to effectively sequestrate a specific radionuclide and form nanometer precipitates of that radionuclide inside nanopores. The radionuclide precipitates will then be encapsulated by a glass matrix or a crystalline mineral phase so that they will effectively be isolated from any contact with outside moisture or liquid water. The resulting waste form is expected to have an unprecedented flexibility to accommodate a broad spectrum of radionuclides, especially volatile or highly mobile ones, with high waste loadings and extremely low leaching rates. In this project, we plan to focus on I and Tc. Success of the project will open a new avenue to the development of new generation of waste forms that can significantly improve waste isolation, expand the waste envelope, and reduce costs related to waste disposal.

Summary of Accomplishments

Since the inception of the project, we have made very significant progress and completed milestones as planned: five invention disclosures filed, one patent application submitted, and one patent application in preparation. We have developed a general route for synthesizing nanoporous metal oxides from inexpensive inorganic precursors. The synthesis can be conducted under relatively simple ambient conditions. We have completed baseline material synthesis. More than 300 materials have been synthesized. These materials have been characterized with x-ray diffraction (XRD), BET (Brunauer, Emmett, and Teller) method, and transmission electron microscopy (TEM). The materials have been tested for their sorption capabilities for radionuclide I and rhenium (Re) (as an analog to Tc); the results have confirmed that nanoporous aluminum oxide and its derivatives have high I sorption capabilities due to the combined effects of surface chemistry and nanopore confinement. We have developed a suite of techniques for the fixation of radionuclides in metal oxide nanopores. We have identified appropriate glass-forming frits for the formation of glass-ceramic waste forms. Our leaching tests have demonstrated the existence of an optimal vitrification temperature for the enhancement of waste form durability. Our work also indicates that silver may not be needed for I immobilization and encapsulation.

Significance

Given the issues of global warming and energy security, the US is posing to revive its nuclear power industry. Development of appropriate waste forms for spent fuel reprocessing and disposal is a necessary component for an advanced nuclear fuel cycle. Success of the project will open a new avenue to the development of new generation of waste forms that can significantly improve waste isolation, expand the waste envelope, and reduce costs related to spent fuel reprocessing and waste disposal.

Refereed Communications

Y. Wang, H. Xu, E. Merino, and H. Konishi, "Self-Organizational Origin of Banded Iron Formation from Oceanic Crust Leaching," to be published in *Nature Geoscience*.

Y. Wang, H. Gao, and H. Xu, "Nanogeochemistry: Nanostructures and Their Reactivity in Nature Systems," to be published in *Contribution of Geochemistry to the Study of the Planet,* A. Parker and H. Russell, Eds., Wiley Blackwell.

Y. Wang, H. Gao, H. Xu, M. Siegel, and H. Konishi, "Surface Chemistry and Stability of Nanostructured Materials in Natural Environments," *Geochemica et Cosmochimica Acta*, vol. 72, p. A1002, 2008.

Metal Fires and Their Implications for Advanced Reactors

117793
Year 2 of 3
Principal Investigator: S. P. Nowlen

Project Purpose

The proposed work aims to establish a general metal-fires expertise, experimental capability, and analysis capability at Sandia to address a key safety issue for the next generation of nuclear reactors. The anticipated nuclear power renaissance hinges on public acceptance and the resolution of safety issues. A cornerstone of the DOE Global Nuclear Energy Partnership is the advanced burner reactor (ABR). The fast-reactor designs being considered for the ABR all use liquid sodium as the primary and secondary coolant (as do other advanced reactor concepts). Some reactor concepts are also based on the use of metallic-form fuels rather than metal-oxides. These reactor concepts introduce a unique risk; namely, metal fires. Fire is a dominant contributor to total plant risk even for current generation reactors. Given "passively safe" advanced reactor designs, some elements of plant risk will diminish substantially. Unless the metal-fire hazards are mitigated as an integral part of plant design, fires may represent the dominant risk contributor. Metal fires have unique characteristics such as very high temperatures and fire suppression challenges. An enhanced understanding of metal-fire behaviors and the availability of appropriate analysis tools will be needed to achieve and demonstrate the mitigation of metal-fire hazards. The objective of the research is to establish a "path forward" for the treatment of metal fires. This project will advance Sandia expertise in the science and safety/risk aspects of metal fires, and will establish and demonstrate a metal-fires predictive modeling capability to supplement existing Sandia fire-modeling capabilities. The work will also establish the foundations of a metal-fire experimental capability and will demonstrate that capability through a set of sodium-fire discovery experiments focused on key phenomena of interest. A working collaboration with Japanese researchers will also be pursued to complement existing agreements between Sandia and the Japanese in areas of advanced reactor design and safety analysis.

Summary of Accomplishments

During FY 2008, the sodium fires knowledge base review was completed and an electronic library of sodium fire literature established. A review of past sodium fire experiences was also completed and the identified events have been documented in summary format (SAND2007-6332). A preliminary review of proposed advanced fast reactor designs was completed and a prototypical plant design developed to support the phenomena identification and ranking table (PIRT) exercise. The PIRT itself was completed in FY 2008 (SAND2008-6855). Based on a predefined set of nuclear power plant (NPP) metal fire scenarios, those phenomena of high importance with a poor state of knowledge were identified. During FY 2009 the lead test engineer, Tara Olivier, participated in the Sodium Handling Technology Training Course at the MONJU reactor in Japan. Based on the PIRT results and insights gained from the MONJU training, a test plan was developed covering both outdoor and in-vessel sodium pool and spray burn tests. Preparation of the experimental facilities was completed, and testing has begun. All of the planned outdoor sodium fire experiments have been completed and the first two indoor tests have also been completed. Analytical efforts have focused on supporting experimental design and assessing existing modeling correlations and approaches. For example, burn/quench calculations for a burning sodium pool and comparisons to existing experimental data have been performed based on pre-existing modeling correlations. Modeling needs for spray fires are also being addressed.

Significance

Ensuring safe secure energy is a central DOE mission. Development of advanced reactors is key to our energy future. Acceptance of new reactors hinges on their assured safety, and metal fires present a unique hazard to future reactor-design concepts. This project will directly impact reactor safety assurance, benefiting DOE by establishing Sandia's expertise in metal-fire issues and physical phenomenology, a key step in the development of a safety case for advanced reactor designs.

Design and Evaluation of Border Management Systems

117794
Year 2 of 3
Principal Investigator: R. A. Duggan

Project Purpose

There are as many unique and disparate manifestations of border systems as there are borders to protect. Border security is a highly complex systems analysis problem with global, regional, national, sector, and border element dimensions for land, water, and air domains. The complexity increases with the multiple, and sometimes conflicting, missions for regulating the flow of people and goods across borders, while securing them for national security. These systems include frontier border surveillance, immigration management and customs functions that must operate in a variety of weather, terrain, operational conditions, cultural constraints, and geopolitical contexts. In FY 2008, we examined the applicability of the existing physical security design and evaluation process outline (DEPO) and found that the fixed facility model does not fit well for the border. We now understand that borders are not easily controlled nor secured at the desired level and therefore, the risks at the border must be managed. We have developed a systems analysis methodology to identify potential system enhancements. We also developed a universal border management systems reference architecture that facilitates and guides thinking about border management and is scalable and customizable for the various domains and specific elements. This generalized architecture is relevant to both domestic and international borders. Tools are needed to aid and support the analysis of these systems and for optimizing the design of enhancements. These tools must be able to analyze the impacts of recommended security enhancements to the flow of goods and people at points of entry, assess the performance of frontier border systems, and provide the analyst the capability to explore and trade off technological and procedural enhancement options. These tools will provide the basis for consistent border management systems analyses and enhancement designs, allow for comparative analyses processes, and provide consistent reporting of results.

Summary of Accomplishments

In year 2 of this project, we accomplished the following:

- Advanced our border management methodology through engagement with international colleagues
- Developed a process for providing intelligence-based background reports for border analysis enhancement to provide a foundation for site assessments
- Developed prototype tools such as:
  - Trends analysis on frontier borders based on Google Earth to show chronological and event history data
  - Ports of entry and checkpoint analysis using Sandia's Umbra simulation framework to show how flow analysis can be easily accomplished
  - Quality function distribution (QFD) tool for identifying commodity interdiction gaps
- Analyzed the role of tunnel detection, unattended aerial vehicles, remote communication systems, and the utility of synthetic aperture radar and satellite imagery for illicit path detection under dense foliage conditions
- Analyzed border interdiction data to gain knowledge about techniques used by smugglers
- Presented of analyst tools at Institute of Electrical and Electronics Engineers (IEEE) Homeland Security Conference 2009

Significance

This project supports the NNSA mission to detect nuclear and radiological materials and related equipment, United Nations Security Council in meeting the requirements of UNSCR 1540, DHS Prevention and Service Objectives, and Department of State (DOS) agendas for defeating global terrorism, defusing regional conflicts, and cooperative actions. As a national security laboratory, this work helps to uniquely position Sandia within the complex as the leader in formal border management methodologies.

Computational and Experimental Platform for Understanding and Optimizing Water Flux and Salt Rejection in Nanoporous Membranes

117795
Year 2 of 3
Principal Investigator: S. L. Rempe

Project Purpose

Lack of potable water plagues half the world's population, causing death, disease, and international tension. Furthermore, energy and water are inextricably and reciprocally linked, with production of one requiring use of the other. The best current solution to clean water lies in reverse osmosis (RO) membranes that remove salts from water with applied pressure, but this technology is mature and expensive. Incremental improvements, based on engineering solutions rather than fundamental changes to the materials, have yielded only modest gains in performance over the last 20 years. In order to progress, a breakthrough in materials research is needed. We propose to achieve a potential breakthrough with a fundamental research and development effort that exploits and extends recent advances by our team in theory, modeling, nanofabrication and platform development. A combined theoretical and experimental platform will be developed to understand the interplay between water flux and ion rejection in precisely-defined nanochannels. Inspired by protein channels in biological membranes, we seek to understand the molecular design principles of natural systems that filter water far more efficiently than conventional RO membranes, transcribe them into robust synthetic porous membranes, and optimize them for industrial working conditions. Scientific insight gained by establishing structure/transport property relationships in nanopores will inform new membrane processing strategies amenable to economic large-scale manufacturing. With guidance from worldwide experts in macroscopic membranes, our microscopic membranes will have the potential to be scaled up into practical systems that could enhance the quantity of fresh water supplies at an affordable cost for the nation and the world.

Summary of Accomplishments

We have significantly enhanced our science-based understanding of the principles for optimization of water flux and select salt rejection. In an important theoretical success, we completed a study of pressure-driven water and salt permeation through model nanopore membranes, with chemically decorated/undecorated mouths, using nonequilibrium molecular dynamics simulations. We found a general phenomenon of pressure dependence of salt rejection, even for decorated pore mouths, which highlights the importance of moderate pressures for high salt rejection. We also identified the structural origins of the dual-acidity constant behavior observed at silica-water interfaces, and submitted it to *Science*. This acid-base behavior governs the net charge inside silica pore membranes, which in turn affects desalination performance. In a major experimental success, we achieved liquid-phase atomic layer deposition of peptide-decorated biomimetic nanopores based on self-assembled mesoporous silica. This result reveals the role of the interplay between amine and carbonyl groups in a water channel, and also supports our prior predictions of the behavior of "dipolar" water channels. To understand the role of surface charge on ion transport through nanopores with pore sizes smaller than the Debye screening length, we measured the zeta potential (an indication of surface charge) of nonporous silica at different pH, and found that the isoelectric point is pH≈3-4, in contrast to pH=2.5 for flat silica. These studies help us design energy-efficient water channels. We are designing a new platform, in which we will be able to apply a gating bias to determine ion type (anion/cation) that moves through the nanopores, the potential needed to gate ion transport, and determine type/density of charge carriers, and thus understand ion transport behavior within nanopores. Also we are investigating the desalination potential of hydrophilic (titanate) molecular nanotubes as a hydrophilic surrogate of carbon nanotube and better mimic of water channels.

Significance

Affordable clean water is both a global and a national security issue as lack of it can cause death, disease, and international tension. Furthermore, efficient water filtration reduces the demand for energy, another national issue. This work supports Sandia's commitment to water, energy, national security, and public health.

Refereed Communications

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S. Moghaddam, E. Pengwang, Y.B. Jiang, C. J. Brinker, R.I. Masel, and M.A. Shannon, "Nanoengineering of a New Generation of Proton Exchange Membrane for Fuel Cells," to be published in *Nature Nanotechnology*.

Development of Efficient, Integrated Cellulosic Biorefineries

117796
Year 2 of 3
Principal Investigator: C. R. Shaddix

Project Purpose

Existing starch-based bioethanol production facilities in the US have low energy efficiencies and limited long-term expansion opportunities. In contrast, cellulosic ethanol, generated from lignocellulosic biomass sources such as grasses and trees, is a much more promising alternative in terms of potential ethanol production, CO_2 impact, and economic competitiveness. However, the lignin component of these biomass sources cannot be converted to ethanol through biochemical means and must be extracted at some point in the biochemical process. Lignin does have a relatively high heating value and is suitable for use as a feedstock for thermochemical conversion systems. Existing cellulosic ethanol plant designs call for combustion of the lignin for steam generation because of the extensive heat requirements for current pretreatment and ethanol distillation technologies. Improvements in these technologies should free a substantial portion of the lignin residue for gasification to synthesis gas for conversion to methanol or higher alcohols. This project aims to determine the optimal integrated plant design options for conversion of biomass to liquid fuels with consideration of lignin gasification. We are considering characteristic US feedstocks (such as corn stover and switchgrass) and promising pretreatment approaches such as aqueous ammonia and dilute sulfuric acid. The extracted lignin residues will be evaluated for combustibility and fed in both wet and dry forms into a gasifier, where both the ease of feeding and the gasification rate of the extracts will be evaluated. A system model of the entire integrated alcohol production facility will be developed and used to evaluate the energy efficiency and exergy flow of the integrated system as a function of the biomass feedstock and the type of pretreatment employed. We will work with the National Renewable Energy Laboratory (NREL) to evaluate suitable dilute acid process residues and to collaborate in constructing suitable system models.

Summary of Accomplishments

Significant progress has been made in the primary task areas of this project: (a) biomass pretreatment and generation of lignin residues, (b) lignin handling, combustion, and gasification, and (c) biorefinery system analysis.

A promising low-cost pretreatment technique known as “soaking in aqueous ammonia” (SAA) that yields lignin residues directly from the pretreatment process and is easy to scale-up was implemented. This technique has not been widely used as part of biochemical ethanol production processes because a sizable portion of the hemicellulose is removed with the lignin and therefore is not available for subsequent fermentation to ethanol. However, this is just the type of process that might prove to have promising synergies for biorefineries that utilize integrated biochemical and thermochemical processing. Two different corn stover samples and a eucalyptus wood sample were processed using the SAA technique and substantial lignin residue was generated from these runs.

Ball milling of the dried residue was initially used but found to produce a very fine dust that tended to agglomerate and proved difficult to feed into combustors or gasifiers. Consequently, this material was redissolved in water, dried, and then passed through a knife mill, which gave a product output with a suitable size range for effective particle feeding and analysis of combustion and gasification reactivity. A sample of the lignin-rich residue from dilute-acid pretreatment and enzymatic hydrolysis of corn stover was obtained from NREL and was also milled and sieved, as was raw corn stover.

An exergy analysis of the NREL design process model for thermochemical biomass-to-alcohol conversion was completed, showing an overall exergy efficiency of 50%. The analysis identified biomass gasification and subsequent syngas clean-up (in particular, tar reforming) as the two most inefficient steps in the conversion process, due to the low operating temperatures and pressure (1000 K, 1.7 atm).

Significance

This work aims to substantially improve the nation's ability to efficiently and cost-effectively use biomass feedstocks for production of liquid transportation fuels and other high-value commodities. The US can produce over 1 billion tons/yr of lignocellulosic biomass and through efforts such as that proposed here can significantly reduce the need to import crude oil. Success would also reduce emissions of CO_2 that contribute to global climate change and related geopolitical instabilities.

Intelligent Power Controllers for Self-Organizing Microgrids

117798
Year 2 of 3
Principal Investigator: S. V. Spires

Project Purpose

Increased energy security, decreased dependence on fossil fuels, and reduction of CO_2 emissions are primary drivers for future DOD/DOE military installation and civilian infrastructures. These goals suggest decreased dependence on a) fossil fuel-based electricity generation technology, and b) the traditional centralized architecture of electricity infrastructure. Instead, greater reliance on distributed energy resources (DERs), particularly those utilizing renewable energy, is indicated. A microgrid is a collection of one or more DERs serving one or more loads that can operate autonomously in standalone mode when required. To achieve maximum energy reliability, modularity, and security, the DERs must function as part of an "intelligent" microgrid that can self-configure to meet a diverse set of generation requirements. Most DERs are connected to the grid via power conversion systems (PCSs) to maintain both the electrical stability of the generation/storage sources as well as controlling their operation to maximize some economic or operating benefit.

When a microgrid is built from multiple small DERs, no single DER has control over the entire system; they must work cooperatively to share load and maintain system stability. The PCSs on the market today do not have this capability. The technical challenge is to create a distributed control architecture that results in a robust and reliable distribution of PCSs. To that end, this project is creating agent based controls that will be implemented in the Sandia microgrid test bed. This test bed will be created from custom research grade PCSs. This new research test bed enables hardware experimentation for this project and will serve as an enduring resource for advanced microgrid design. This project ties together Sandia's considerable research base in microgrid technology and distributed agent-based control architectures.

Summary of Accomplishments

We have now completed the construction of three research inverters (MMIs) that will enable further research. We have also purchased two different off-the-shelf control platforms (Versalogic and CompactRIO) that can be coupled via fiber-optic connectors to the MMI and provide closed-loop feedback for the power electronics. Both these control platforms are capable of networked communication with other, similar controllers. The CompactRIO is the less powerful of the two, but it has been able to show results quickly, since it is programmed in LabView and we have LabView experts available who have used this platform before. The Versalogic platform is more capable and is more likely to support our agent-based control algorithms, but as a new (to us) platform, we expect that integrating it will take a little longer. We are incorporating our initial control algorithms into the CompactRIO now. We have also completed modeling and simulation of the inverters themselves, closed-loop control of individual inverters, and open-loop control of multiple inverters. Results so far have been encouraging and no significant challenges or roadblocks have occurred. However, the real challenge will come in FY 2010 when we begin to implement true distributed, multi-inverter closed-loop control on the real hardware.

Significance

The micro-inverter project will impact Sandia's efforts to provide the DOD with secure and reliable energy to meet critical asset energy demands for tactical operations, forward operating bases, and fixed base operations. The project also ties to the DOE Solar Energy Grid Integration Systems and Renewable System Interconnection programs along with the DOE Hawaii Clean Energy Initiative and Smart Grid.

Spectroscopic Radiation Detectors for Extreme Environments

117801
Year 2 of 2
Principal Investigator: M. A. Grohman

Project Purpose

This project will evaluate the ability of spectroscopic gamma radiation detectors to survive the extreme environments (i.e., high-g/vibration/temperature) that will be experienced in mobile land-based, maritime, and air-delivered radiation detection systems. While work has previously been conducted to investigate the ability of small scintillation crystals to survive the high-g environments experienced in certain industrial applications, there is a need to conduct additional research into the survivability of larger room-temperature scintillation crystals (e.g., sodium iodide, cesium iodide, lanthanum halide) in harsh environments for the detection of radioactive materials. Identification of radioactive materials, rather than just detection, is paramount in applications where the flow of commerce should not be interrupted when naturally occurring radioactive sources are detected, or in very high consequence applications where the presence of specific materials indicates a threat. We define "survival" of a radiation detector as the ability of the sensor system to continue to identify materials via analysis of measured gamma ray spectra using the Sandia-developed radioisotope identification algorithm, FitToDB. This project will analyze, through modeling and experimentation, the ability of different materials, scintillator geometries, and photomultiplier tubes (PMTs), including the bonding of the PMTs to the scintillation crystal, to survive extreme environments. This project will further include a sensitivity analysis of the isotope identification algorithm to understand how sensor failure modes affect the analysis accuracy.

Summary of Accomplishments

This project conducted a thorough evaluation of the ability of spectroscopic gamma radiation detector components to survive the extreme environments (i.e., shock/vibration/temperature/electromagnetic) that could be experienced in mobile land-based, maritime, and air-delivered radiation detection systems. Although work has previously been conducted to investigate the ability of small scintillation crystals to survive the environments experienced in certain industrial applications, there was a need to conduct additional research into the survivability of larger room temperature scintillation crystals in the harsher environments of military and homeland defense use for the field detection of radioactive materials. Identification of radioactive materials, rather than just detection, is paramount in applications where the flow of commerce should not be interrupted when naturally occurring radioactive sources are detected or in very high consequence applications where the presence of specific materials indicates a threat. At the end of the effort, we were able to specify particular commercial components along with packaging techniques to meet most of the extreme environments specified in the various radiation detection standards issued by the American National Standards Institute (ANSI). Additionally, through modeling and experimentation, we analyzed the ability of different scintillator geometries, photomultiplier tubes (PMTs), and the bonding of these components to survive extreme environments.

Significance

The results of this work are applicable to the future development of land, air, and maritime based detection systems to support the nonproliferation and national security goals of DOE/NNSA, DOD/Defense Threat Reduction Agency, and DHS/Defense Nuclear Detection Office.

Biosafety Risk Assessment Methodology (Biosafety-RAM)

117805
Year 2 of 3
Principal Investigator: S. A. Caskey

Project Purpose

Laboratory biosafety includes the facility, the equipment, and the practices used in bioresearch to protect against the risk of accidental exposure to an individual or the community. The biological properties of agents, pathogens and toxins, define the necessary biosafety measures for safe manipulation of the agent. Biosafety experts have historically provided institutions with biosafety recommendations based upon their expert opinion and experience. These recommendations are valuable, but there is no formal methodology on which they are based. This causes an inability to explain or defend recommendations. Often multiple recommendations are also in conflict.

Sandia is an international leader in understanding biological risk, and has developed a standard methodology and software tool for conducting biological security risk assessments. This project continues the creation of a biosafety methodology than can be shared with the biosafety community and could establish a standard approach to biosafety risk assessment. The project will continue the development of a software tool that can quantify the biosafety risk for a facility based on the site environment and the agents that it works with.

Summary of Accomplishments

Biosafety is difficult to model because it is based upon several variations of practices, procedures, and physical controls. In the first year, this project developed a basic model that captures the variations and identifies both the hazards and the mitigation measures. The second year of this project was focused on weighting the criteria and formalizing the model. Working with experts in the community, we have vetted the model outline and tested the preliminary (paper based) model. Based upon these discussions, the methodology has been updated to reflect experts' thoughts and ideas, including the expansion of the models scope. The risk assessment model has been scoped to focus on infectious biological agents, now including both recombinant DNA and plant agents. Criteria have been classified into potential and consequences categories and the mathematical relationships among all the criteria have been determined. The model consists of hazard criteria that are based upon biological agent properties and laboratory hazards. The model has also identified the criteria that will be used to calculate the consequences of an accidental biological agent release. The scope of the model defines several scenarios, each of which will have a unique risk calculated. These scenarios include the risk to humans in and out of the laboratory, and the risk to the human and animal communities. Each of these scenarios consists of a unique set of hazards and hazard mitigation measures, along with a unique set of consequences. Each criterion has been ranked, and the level of detail under each criterion reflects its overall importance.

Significance

This project proposes an innovative, science-based solution to a national security problem: reducing biological threats. Facilities worldwide work with and store biological materials which pose a biological threat if improperly handled. The development of a method & tool to enhance biosafety would directly reduce the biological threat. The tool would strengthen national security, and contribute to Sandia's mission by augmenting the technical capacity of its biological threat reduction program.

Investigation of Ultralow-Power PMT-Based Radiation Detectors

117806
Year 2 of 2
Principal Investigator: B. D. Schoeneman

Project Purpose

Continuous radiation detection monitoring is essential when the size of the detector is limited. Long dwell-time measurements with small, less-expensive radiation detectors can collect the same information as larger detectors operated for a shorter interval. Cost, size, and operational advantages of smaller detectors motivate continuous radiation monitoring. In many applications, the radiation monitor must operate continuously over weeks or years using batteries of limited capacity due to their size, cost, safety, or weight restrictions. Likewise, the monitor must often have both high detection efficiency and low cost. This combination of requirements leads to the near-term choice of radiation detectors based on scintillators and photomultiplier tubes (PMTs). Recent advances in room-temperature semiconductor radiation detector materials as well as alternatives to PMTs have not yet overcome their detection efficiency and cost problems. Consequently, there is a great need for low-power PMT biasing and readout electronics. Previous PMT-based detectors have been designed with little emphasis on reducing power consumption. The limited research on low-power designs does not adequately describe the radiation detector performance tradeoffs. We propose a two year project to design, build, and characterize the relative performance of several variants of state-of-the-art PMTs, high-voltage (HV) biasing networks, and signal amplifiers utilized to develop novel designs to meet the requirements of future radiation monitors.

Summary of Accomplishments

This research consisted of three areas of investigation for conserving energy while providing the HV bias for a PMT based spectral gamma detector. These areas were the bias supply, the oscillator driving the bias supply, and a performance evaluation of the integrated bias power generation circuits. Although this research was originally intended to investigate other biasing techniques (e.g., tapered bias) only research on the low-power generation of bias voltages was possible given the resources that were available. There are many areas where it may be possible to reduce the energy required to sustain the operation of scintillators and photomultiplier tubes as gamma detectors. In pursuing this research, we decided to investigate the area that represented the greatest potential impact on this detector configuration’s power consumption, the high-voltage bias network and generation. The results of this research demonstrate that PMT based detectors are viable for use in cost-effective, low-power applications. PMT biasing power was shown to be reduced by 88% relative to conventional techniques, substantiating this viability. There are additional significant gains in this technology area that remain to be investigated. This research resulted in the successful development of two, low-power photomultiplier tube biasing systems for battery-operated monitoring devices. A grounded-cathode biasing system required a total power demand of 31 mW and a grounded-anode biasing system required a total power demand of 12 mW.

Significance

Sandia could demonstrate next-generation designs of low-cost, ultralow-power radiation detectors for our national and global security customers. With the significant investments by these customers and commercial vendors in new scintillator materials that have excellent gamma-ray energy resolution, room-temperature radiation detectors that utilize PMTs will increase in the future. Ultralow-power optimized PMT systems will be crucial for unattended and continuous spectral monitoring applications. True spectral capabilities for long-term unattended sensor applications mandate ultralow-power devices to support this need. Typically, pager type radiation detectors are designed for short duration operation (12 hrs) before requiring recharging. As a result of this project, considerably longer operation for scintillator gamma radiation detectors with spectral capabilities can be realized. It has been demonstrated through this research that the continuous power demand for supporting the HV bias of a PMT based detector can be reduced from ~250 mW down to ~12 mW. If this approach is utilized in a sensor that multiplexes the detector, such as the secure sensor platform (SSP), years of unattended operation can be realized.

Anticipating the Unintended Consequences of Security Dynamics

117807
Year 2 of 3
Principal Investigator: G. A. Backus

Project Purpose

Globalization, in the societal sense, will continue to make international security less amenable to military force and more dependent on managing human behavioral interactions. Nearly all unintended consequences occur from discounting the cultural and behavioral determinants of responses beyond the initial reaction to interventions.

Neither conventional socioeconomic models, nor their developers, attempt to simulate security related issues. New behavioral-simulation methods (qualitative choice and cointegration) recently developed at Harvard and the University of California, San Diego (UCSD), explored by Sandia for the DHS Motivation and Intent program, and utilized in the behavior-aware decision-support system LDRD project (1007337, FY 2006-2007), appear to be compatible with conventional socioeconomic modeling approaches. Further, advances in agent-based simulation can efficiently capture emergent phenomena and naturally address uncertainty. The combining of agent-based and system-dynamics methods with other recent LDRD efforts on verification and validation can ensure that simulations provide robust conclusions despite uncertainty. From radical Islamists, to the mass societal upheavals from climate change, to the resurgence of a furtive Russia, to the failed expectations in China, such a collective approach can simulate the impending dynamics, delineate the intertwined social-behavioral phenomena, and determine intrinsically secure engagements that alleviate the cascading, unintended consequences that cause enduring global destabilization.

We would develop a calibrated, agent-based, macroeconomic framework (a first) and combine it with behavioral decision making within the populations and governments, while incorporating cultural, institutional, and political distinctions. The key novel distinction is the incorporation of conflict dynamics, their evolution and the spillover across boundaries into the socioeconomic analytical tool set. We would include detailed intra- and inter-regional interactions as well as aggregate rest-of-world feedback dynamics. Russia, China, and trading-partner country interactions are the intended focus of initial efforts.

Summary of Accomplishments

The database (other than verification) is now complete for the entire globe, and the model can automatically configure itself to any inter-regional analyses among 224 nation-states. The current configuration we are using for testing is a six region configuration composed of China, Russia, US, European Union, Middle East and rest-of-world. The modeling framework now includes the primary policy options and contains 90% of the response mechanisms we anticipate in the final model.

Significance

Future security activities will embody complex, social-behavioral interactions for which Sandia does not yet have proficiency. If Sandia is “the primary national security laboratory that federal agencies call on to help solve the nation’s most difficult problems,” it has an obligation to ensure that it can address the approaching threats the nation will face. The military and intelligence community can call on Sandia for support in making security decisions that go beyond kinetic responses.

Novel Instrumentation for Selective Photoionization and Trapping of Fine Particles

117810
Year 2 of 3
Principal Investigator: R. P. Bambha

Project Purpose

The collection and in situ analysis of fine particles is a major challenge for multiple global security and energy applications. One of the few available indicators of proliferation activities is trace quantities of uranium transported from production sites on fine particles; detection becomes the proverbial "needle-in-a-haystack" problem. In the energy sector, use of petroleum diesel and alternative fuels is severely limited by the generation of toxic aerosols that are notoriously difficult to measure. Better soot diagnostics would directly benefit development of clean-burning, highly efficient engines. Progress is hampered in other areas of aerosol detection and measurement (e.g., biological aerosols, chemical agents, explosives) because of problems associated with handling fine particles. Particles of interest can be highly mobile because of their small sizes (a typical diameter of diesel soot is ~150 nm) and difficult to distinguish in a background of interfering particles (e.g., trace uranium particles among ambient aerosols). We propose efficient collection of nanoparticles and reduction of background interference using wavelength-selective ultraviolet (UV) photoionization and electrostatic trapping. This powerful and flexible method of collection will allow us to convey the particles to a wide range of diagnostics (e.g., mass spectrometry, chemiluminescence, laser-induced fluorescence, absorption, and laser-induced breakdown spectroscopies) for real-time analysis. We will exploit Sandia's expertise in compact high-energy lasers and nonlinear optics to generate narrow-band UV radiation. Selective fine particle trapping and concentration techniques coupled with miniaturized UV laser sources will allow the development of fieldable instruments that are smaller, more sensitive, and more versatile than current state-of-the-art particle detectors. This project leverages investments in fiber-laser development through a Grand Challenge LDRD and particle diagnostics through the DOE Basic Energy Sciences (BES) program and will have broad application to multiple Sandia missions. It will culminate in the development of a high-efficiency photoionization controlled aerosol trap (HEPCAT).

Summary of Accomplishments

Thus far we have met the planned milestones of configuring the laboratory laser system, building the compositional separation tube, and demonstrating temporal selection. Having reduced the technique to practice, we have submitted an invention disclosure. We have modeled the electron optics using Simion. We have configured a tunable UV laser source using a flash-lamp pumped neodymium-doped yttrium aluminum garnet (Nd:YAG) laser (1064 nm, 532 nm), dye laser (550-820 nm), and doubling (275-410 nm) and tripling crystals (198–273 nm). The system produces 1–10 mJ in the UV with an available UV wavelength range of 198–410 nm. We have implemented several methods for particle generation and have characterized them with a scanning mobility particle sizer (SMPS). We have used a burner to generate carbonaceous soot (carbon:hydrogen ratio of ~8) from ethylene and air and have installed an arc-discharge particle generator, which uses graphite electrodes to generate pure carbon aerosol with controllable size distributions (20–200 nm). We have built a drift tube with electrical and optical access to our controlled aerosol stream. We have used an atomizer to generate CeO_2 particles, which serve as a surrogate for uranium oxide and can be added to our mixed aerosol stream. Using a biased microbalance and SMPS, we have demonstrated trapping of photoionized soot and CeO_2 aerosols. Using a differential mobility analyzer, we have selected ~100-nm sized soot particles from a flame and have studied the number of charges per particle as a function of laser pulse energy, average power, and wavelength. We have begun developing a compact laser source for HEPCAT using Nd-doped phosphate glass (lasing bandwidth ~20 nm around 1054 nm) and small tunable holographic mirror (0.25 nm bandwidth) to produce ~190 µJ/pulse, which will eventually be frequency-converted to the UV.

Significance

This project addresses critical detection needs in global security and energy and will position Sandia at the forefront of particle analysis technology. Our approach leverages expertise from basic and applied organizations within Sandia, e.g., in lasers, fiber optics, combustion, and detection for nonproliferation. It will advance core capabilities in these areas. The generality of our approach will benefit applications in key areas for DOD and DHS, e.g., explosives and chem/bio agent detection.

An Ion Beam Platform for Screening and Studying Materials for Use in Fast Neutron Environments

130744
Year 1 of 3
Principal Investigator: L. N. Brewer

Project Purpose

Our country's energy needs are driving a renewed interest in power generation and waste management by reviving fast neutron reactor technology. While promising, fast neutron reactors will drive materials requirements in different directions from the more standard thermal neutron reactors. In order to support programs such as the Advanced Fuel Cycle Initiative (AFCI) and the Global Nuclear Energy Partnership (GNEP), we must find a way to measure, understand, and predict materials properties at high temperatures and under high energy irradiation. However, there are presently no operating fast neutron reactors in the United States. To address the lack of fast neutron availability for fuel cladding materials development and screening, we propose the use of high energy (MeV) ion irradiation combined with a novel, in situ, microscale test bed to characterize the mechanical behavior of advanced cladding materials as a function of stress, temperature, and irradiation damage level. The mechanical properties will be determined by expanding the extant in situ capabilities of the ion beam line to include high temperature and mechanical testing capabilities. In particular, we will develop a novel, microscale test based on the recent work in focused-ion beam produced micropillars. We will determine the ion-fast neutron damage equivalence for fuel cladding steels through ion irradiation experiments, ion cascade simulations, and molecular dynamics simulations.

This new capability will benefit AFCI and related programs. This project will provide irradiation-informed mechanical properties and microstructural stability information that will benefit nuclear fuels modeling efforts. This ion beam approach will also provide a screening capability for studying the irradiation damage and irradiation effects in new alloys, so that the relatively precious experimental time on actual neutron reactors can be reserved for samples that have passed an initial screen.

Summary of Accomplishments

We performed benchmark experiments on 316L stainless steel. We were able to compare these results with previous work in the literature to examine bubble densities and sizes as a function of temperature. Our results compared somewhat favorably, but also provided new information as we extended the damage levels from 40 dpa (displacements per atom) to 100 dpa. We are preparing a publication on this work.

We have developed a test matrix for steels of three types: ferritic, austenitic, and ferritic-martensitic that includes tests as a function of temperature and damage level that should allow us to thoroughly evaluate our ability to simulate literature data from neutron irradiation with our ion irradiation experiments.

We have found literature on molecular dynamics simulations of the Fe-Cr system in body centered cubic structures. We are currently preparing to do simulations based on this previous work to create an accurate embedded atom potential for simulating ion scattering and damage in the ferritic and martensitic steels of interest.

Development of Micromechanical Test Methods:

We have made much progress on further developing and applying the micropillar compression technique to irradiated material. The initial results are very promising. We are preparing a publication describing these results.

In addition, we are setting up experiments to use spherical indentation to measure both the yield behavior as well as the creep behavior of irradiated metals. If successful, this approach has great potential as an in situ diagnostic.

Alloy Screening Capabilities:
We have started a dual-purpose collaboration with Prof. J.C. Zhao at the Ohio State University: 1.) He will help us to apply the diffusion multiples approach to create a compositional array of steels for screening. 2.) He is applying novel, laser-based thermal properties measurements for measuring the change in thermal properties.

Significance
The success of this project will provide Sandia with a materials testing platform that will support the development and screening of structural materials for use in an advanced fast-neutron burner reactor. The DOE is keenly interested in the support and success of programs such as AFCI and GNEP. This proposal addresses technical needs for these programs.

Cognitive Stakeholder Modeling for Resource Management

130745
Year 1 of 3
Principal Investigator: Z. O. Benz

Project Purpose

A key national challenge is identifying and engaging in policies that motivate strategic changes in resource production and utilization. The difficulty lies in selecting management or policy options that achieve particular goals while minimizing potential for conflict. Furthermore, the success of a policy decision can hinge more on human factors than on the technical merits of the policy. Our approach is to create a simulation environment that integrates cognitive behavioral models of stakeholders with traditional system dynamics (SD) models of resource constraints and economics. Existing approaches tend to focus purely on economic aspects of policy decisions, ignoring other important factors that drive stakeholder actions. The proposed technical approach expands beyond economics to include factors such as stakeholder desires, needs and biases, and influence. Stakeholders include government authorities, consumers, commercial, and community interests. The resultant sociotechnical system model will aid development of candidate solution sets to streamline negotiation processes by providing perspective to all parties about decision tradeoffs. It will also provide an early assessment methodology to identify potential conflicts. These insights have the potential to be applied in the form of assisted decision-making applications for customers in government and industry across all aspects of natural resource allocation problems, particularly as an aid to water planning efforts related to supply, quality, demand management, water market design, and habitat restoration. We will use water planning and management in the Upper Rio Grande basin as a specific motivating application for combining technical resource models with individualized cognitive models. Prospective customers for the developed technology include agencies, organizations, and commercial entities with a need to conduct strategic long-term decision making for complex, uncertain, and potentially conflictive situations, including in the resource scarcity management, energy production, and nuclear waste storage domains.

Summary of Accomplishments

We refined our approach to modeling during the initial design phase. Our current approach uses a layered, or ensemble, model consisting of three pieces: an initial roughed-in model of stakeholders and their interactions with an SD model created by the team, an automated refinement of stakeholder-SD interactions using statistical text analysis, and a final model automated refinement based on online learning in which computationally based automated knowledge capture is used to monitor and learn from the activities of actual stakeholders role-playing in relevant scenarios. Inspiration for this approach was taken from current literature, with a focus on automating as much of the modeling process as feasible as well as automating the generation of useful feedback to stakeholders in real-time. It is intended that this layered approach will be generic enough in design and implementation that it can be applied to novel problem domains in a straightforward manner that achieves efficiency and fidelity beyond the current state of the art. As a result of our pursuing the refined approach, we have focused first on the integration of the Cognitive Foundry with Omega-AB in order to support the initial roughed in modeling. Two-way communication between these two codes has been achieved. Simultaneously we pursued the implementation of statistical text analysis codes into the Cognitive Foundry in support of the second layer of modeling. The decision to perform text analysis within the Cognitive Foundry rather than through the use of the STANLEY code was made based on many factors. Most importantly, the Cognitive Foundry provides rich code for performing efficient sparse matrix algebra and machine learning that does not exist in STANLEY, allowing the exploration of techniques such as latent semantic analysis.

Significance

Ensuring future resource (e.g., energy, water) stability is a critical national security mission of Sandia. Through modeling and analysis, we will provide mechanisms to guide dialogue in a way that minimizes the potential for conflict while identifying options for effective policy development. There exists the potential to modify the proposed test-bed application for other domains with complex stakeholder based decision problems, such as for nuclear waste storage or energy production.

International Physical Protection Self-Assessment Tool for Chemical Facilities (IPPSAT-CF)

130746
Year 1 of 3
Principal Investigator: C. R. Tewell

Project Purpose

International efforts to prevent malicious use of chemicals focus on verifying destruction of chemical weapons and export control of dual-use chemical technologies. No international standards exist for determining the appropriate level of physical protection for hazardous chemicals or to prevent sabotage at chemical facilities. Sandia's existing risk assessment methodology for chemical facilities, RAM-CF™, tools have been adopted by multinational companies, but are export-controlled and best-suited to large, complex facilities with complete safety and operational analyses. Target identification in RAM-CF is driven by lists of controlled chemicals in US regulations rather than by a comprehensive facility consequence analysis. Because comprehensive consequence analysis of chemical facilities that do not belong to multinationals is seldom, if ever, required, chemical facilities remain at risk for malicious attack. The risk is greater in areas of the world with the greatest likelihood of attack and the lowest standards for safety and security. We propose to develop a methodology that will assist chemical facilities in such global regions to improve their physical protection posture cost-effectively. This requires assessing where the greatest consequences of an attack or theft might be (target identification) on a facility. There are two existing classes of target identification methodologies, neither of which is useful in reducing risk in our targeted global regions. The first is a comprehensive facility safety analysis. This approach requires time and resources that are untenable in regions with little or no regulatory oversight. The second involves list-based approaches that could never identify every potential target of malicious attack. We are developing a new target identification methodology that takes a facility inventory of chemicals and chemical processes in order to identify a list of potential targets prioritized by potential consequence. Such prioritization is challenging because of the limited information that is available in economically developing regions of the world.

Summary of Accomplishments

We have developed a methodology for a chemical facility to identify potential chemical targets to protect, based on the consequences the facility wants to avoid. The methodology requires the facility inventory of chemicals and processes and identifies the possible target category: theft of chemical weapon agent, precursor or chemical identified as attractive to terrorists, energetic chemical, flammable chemical or sabotage by ignition of highly flammable material, creation of a toxic cloud, detonation of explosive material, use of stored process energy (pressure), or use of chemical energy (heat of reaction). Part of the potential burden is finding physical data to determine the target class or to rank a chemical within a target class. In developed countries, this data may be available in reference guides or required safety documentation, our experience shows that this information is not easily accessible in our targeted regions. In addition, toxicological data is usually only available on the most common industrial chemicals. There is a lack of reliable and extensive toxicological data on the majority of chemicals. To compensate, we have utilized simple algorithms for computing physical data such as flash point and lower flammability limit using only the boiling point of a chemical. We identify potential explosives using only the molecular formula of a chemical. The identification of indirect sabotage targets will require information that is not readily calculated from molecular formula or boiling point. To identify potential runaway exothermic reactions, we have devised a parameter — the potential adiabatic temperature rise rate. This parameter can be used to rank the runaway potential of different chemical reaction processes within the facility. Calculation of this parameter will require knowledge of the chemical kinetics, heat of reaction, and overall process heat capacity.

Significance

Weapons of mass destruction (WMD) nonproliferation is part of Sandia's mission, and encompasses biological and chemical threats. The objective of this proposal, reducing the risk from the malicious use of chemicals and chemical facilities, fits well with our national security mission.

Intrinsic Security for Insider Threats

130747
Year 1 of 2
Principal Investigator: F. A. Duran

Project Purpose

The objective of this project is to create a systems-based process with principles, methods, and practices for designing, evaluating and operating security systems that are resistant to insider threats. Computational modeling and subject matter expertise provide the basis for interdisciplinary research and development to create a process that can be applied to: (1) integrate security practices; (2) analyze effectiveness and costs of different sets of protection measures against a broad range of insider types and capabilities for multiple target types; and (3) define intrinsic security practices and system architectures to deter, detect, and neutralize insider attacks. Discovering basic principles and developing methodologies, technologies, and analysis tools that make possible and enable intrinsically secure systems requires addressing the insider threat. Insiders are among the most ubiquitous and capable security threats. Current protections against insiders are expensive, intrusive, and implemented piecemeal (e.g., material/access controls, personnel security, Human Reliability Program, two-person rule, contraband detection, cyber security). Insiders continue to be revealed, indicating that many current protection strategies can be defeated. High-asset facilities (DOD, DOE, DHS) need to demonstrate effective insider security while simultaneously improving operational efficiency. Individual protection approaches demonstrate varying levels of effectiveness, but no understanding of integrated protections or overall effective insider security for a given facility. Achieving intrinsic insider security requires comprehensive reassessment of operational activities and security disciplines and their interdependencies. This project, therefore, is not suitable for funding of piecemeal areas by individual customers, but is appropriate for LDRD funding. Insider threats are a major security concern across the DOE complex and across high-security facilities in general. Intrinsic insider security will provide a more integrated application of insider protections to achieve reduced costs, improved operational efficiency and greater security performance. This project is relevant to energy security, homeland security, and defense mission areas.

Summary of Accomplishments

To determine current insider threats and protections, the project team had group and individual meetings with subject matter experts (SMEs) in different security domains and programs, including physical security, cyber security, counterintelligence, security incident management, information security, operations security, personnel security, the human reliability program. This information provides the basis to describe a baseline insider security "system" (Task 1) and to update the system dynamics model of the employee life cycle (Task 3). Generally, results from this effort indicate that different programs and strategies are used to address the insider threat, most often in a stove-piped manner. Tremendous opportunity exists to develop an integrated systems-based approach to insider security. We developed a glossary of insider security terms and counterintelligence case studies and investigated requirements and security metrics to support our systems-based approach and modeling efforts. We also developed an initial set of objectives and principles (Task 2). The preliminary employee life cycle model was peer reviewed, and we have used these comments to incorporate revisions into the model (Task 3). The model development has been extended to include a complementary system dynamics model on information protection and control (Task 3). We established contacts with agencies in the intelligence community that have interest in addressing the insider threat, discussed our approach with these contacts, and gathered critical comments. Generally, the focus on the employee life cycle and a systems-based approach has been well received. We submitted papers for the Institute of Electrical and Electronics Engineers (IEEE) Security and Privacy Special Issue on The Insider Threat, International System Dynamics Society Conference and Institute of Nuclear Materials Management Annual Meeting.

Significance

Establishing a systems-based process for intrinsic insider security will provide Sandia unique capabilities to support DOE's nuclear security strategic goals and help the nation defend against the insider threat. Also, this work supports DHS strategic goals related to prevention and protection, which are to detect, deter, and mitigate threats to our homeland and to safeguard critical infrastructure and property of our nation.

Refereed Communications

F.A. Duran, S.H. Conrad, G.N. Conrad, D.P. Duggan, and E.B. Held, "Building a System for Insider Security," IEEE Computer Society, *IEEE Security & Privacy Technical Magazine — Special Issue on the Insider Threat,* November 2009.

Linking Ceragenins to Water-Treatment Membranes to Minimize Biofouling

130748
Year 1 of 3
Principal Investigator: S. J. Altman

Project Purpose

Biofouling impacts membrane separation processes for many industrial applications such as desalination, wastewater treatment, oil and gas extraction, and power generation. We propose to use ceragenins to create biofouling resistant water-treatment membranes. Ceragenins are synthetically produced antimicrobial peptide mimics that display broad-spectrum bactericidal activity. They are simple to prepare and purify on a large scale and are amenable to broad usage because it is anticipated that they will not engender resistance. Our goals are to determine the best attachment method of ceragenins to water-treatment membranes, the optimal density and configuration of the ceragenins without compromising the permeate flux, the impact of sustained releasing versus permanently attached ceragenins, and whether the ceragenins will affect the permeate water quality. We will evaluate three methods for attaching the ceragenins to the membranes. Testing the efficacy of ceragenins will include measurement of minimum inhibition concentrations and minimum bactericidal concentrations, measurement of bacteria attachment and an assessment of percentage of bacteria killed on the membrane surface, and measurement of biofouling (flux reduction and bacteria concentration on the membrane surface) in a high-pressure cross-flow system. We will collect relevant source waters (e.g., waters used for steam extraction of heavy oil, surface seawater used for desalination) and culture critical bacteria from these waters. Our testing will expand to controlled single- or multi-species cultures of these critical bacteria and finally, less controlled tests on the actual source waters. Finally, we will test the permeate waters to determine whether the ceragenins will pass through the membranes. To date the research on the antimicrobial effects of ceragenins have focused on testing drug-resistant bacteria and studies with medical devices. The application of ceragenins to water-treatment membranes is novel. Development of biofouling resistant membranes will assist in creation of clean water and energy with lower energy usage.

Summary of Accomplishments

Four different ceragenins have been synthesized and immobilized on reverse osmosis membranes. The best method of immobilization to maximize the ceragenin density on the surface of the membrane with minimal impact to membrane performance is still being evaluated. Hyperspectral imaging with multivariate curve resolution and infrared spectroscopy have been used to measure ceragenin density on the membrane surface. A protocol to use hyperspectral imaging to differentiate fluorescence from membrane autofluorescence, a fluorophore-tagged ceragenin, and live and dead bacteria has been developed. After carefully characterizing all of the possible sources of fluorescence present, we have decided to switch our fluorophore from a nitrobenzoxadiazole to DY-520XL. The emission spectra from DY-520XL will have less overlap with the membrane autofluorescence as well as the live-dead stain. Infrared spectroscopy has confirmed the attachment of the epoxyalkenes although the expected polyacrylate peaks were very weak. As larger batches of ceragenins are prepared, concentrations will be increased and the density of attached oligomers should also increase. Batch test and drip-flow test protocols have been developed to test the biocidal activity of the ceragenins. Batch testing and drip-flow testing have shown that immobilized ceragenin decreased biofilm formation by *Pseudomonas fluorescens* by over 90% and over 80%, respectively. Several membranes have been tested on the cross-flow system to measure the impact of the treatment on permeate flux. These tests indicated that the ceragenin attachment methods will not have a significant impact of membrane performance. Water samples have been collected from the Colorado River, agricultural drainage, seawater, and groundwater. These samples were assayed for culturable organisms. Colony colors and morphologies are consistent with *Pseudomonas spp.* for many of the colonies. To accurately identify the species cultured, we have grown up the organisms, extracted DNA, amplified it via polymerase chain reaction (PCR), and prepared primers coding for the 16S region of the ribosome.

Significance

The continued security and economic health of the United States depends on a sustainable supply of both energy and water. These two critical resources are inextricably and reciprocally linked; the production of energy requires large volumes of water while the treatment and distribution of water is equally dependent upon readily available, low-cost energy. Through creation of biofouling resistant membranes, this research allows for creation of more clean water with less energy use.

Membranes and Surfaces Nanoengineered for Pathogen Capture and Destruction

130749
Year 1 of 3
Principal Investigator: M. D. Nyman

Project Purpose

With increasing population and wealth, we are approaching a critical state with respect to producing enough potable water to sustain the human race. Consequently, radical alternatives such as wastewater treatment, by necessity, become more common. Pathogens in wastewater are among the biggest threats to the health of communities that rely on these challenged resources. We propose to design coatings for water filtration media (including membranes and sand) that can help address these issues via controlled capture, destruction and release of pathogens. The proposed coatings are complex ion nanocomposites that are effective for microorganism capture via chemical affinity; and controlled pathogen destruction/release via complex state-changing mechanisms. Pathogen capture is accomplished by electrostatics, hydrophobicity, and surface disorder/roughness. Photoactive species in the coating control pathogen destruction, initiated by UV irradiation. Simultaneous change in electrostatics, order and hydrophobicity result in release of the inactivated microorganisms. Characterization of nanocomposite coatings will identify the active components of the coating, and their collective characteristics such as supermolecular ordering and enhanced photoactivity. Collective coating features control efficacy of pathogen capture, destruction and release; and therefore will be identified and optimized. Efficacy of coatings will be tested by filtering contaminated water through the coated media. Pathogen populations on the filtration media and in the filtered water will be quantified. Pathogen destruction/release will be similarly quantified, following irradiation of contaminated filtration media. Attractive/repulsive forces between coatings and microorganisms will be investigated via advanced atomic force microscopy techniques.

The coatings developed in this work are foundational to a number of other applications in which detection, mitigation, capture or destruction of microorganisms is required. The broad applicability of these coatings, potential impact at both the fundamental and applied level, and the challenge of developing novel state-switching complex materials provide an ideal profile for an LDRD project rather than programmatic project.

Summary of Accomplishments

In the first half-year of this project, we have focused on the pathogen-capture components of the hybrid coatings for pathogen-capture/release. We developed a protocol for testing coatings for pathogen affinity. We chose MS2 bacteriophage as the test pathogen, in that it is an excellent model for infectious viruses, featuring many of the same physical characteristics. Furthermore, the small diameter of the virus (27 nm) ensures that its retention on the column is truly due to chemical affinity for the surface coating rather than gravitational settling or clumping, which often contributes to retention of larger pathogens such as bacteria. This provides a greater challenge to optimize the coatings for pathogen affinity, and reduces the possibility of false results.

We identified several coatings that could remove ~99% (one log reduction) of the MS2. Namely, diethylene-triamino-propylsilane (DE-TA-PS), and polyaluminum cations tethered to disilane coupling agents. We also noted that hydrophobicity is another factor that increases virus affinity, but not the dominant feature. The key to pathogen capture appears to be high cationic charge density, and covalent bonding of the cationic species (rather than electrostatic self-assembly) to the filtration media. We are in the process of optimizing our coating techniques based on the solvent composition for coatings, and the sequence of heating/drying between coating steps.

In the second half of the first year, we identified a photocatalytic component for the composite coatings that is both highly effective and can be fixed to a stationary surface for a filtration process. The effective photocatalyst is a delaminated layered titanate that is functionalized with peroxo ligands. Scoping studies utilizing the catalyst in a powder form and methyl orange dye as a model contaminant showed that very small amounts of the photocatalyst could quickly decompose the dye.

Significance

The proposed discovery-based research has potential for impact in a variety of disciplines including materials, environmental, interfacial, and inorganic sciences; thus contributing to DOE's scientific discovery and innovation goals. Alignment with DOE's mission areas includes the environment and national security; based on potential applications involving mitigation, detection or destruction of pathogens. The research may be applied in DOD field-based operations for producing reliable water.

Modeling of Advanced Nuclear Fuel Pins

130750
Year 1 of 3
Principal Investigator: T. J. Bartel

Project Purpose

With renewed interest in nuclear power as a domestic source of clean, economical and sustainable energy, DOE, the Nuclear Regulatory Commission (NRC), and commercial entities are initiating programs, strategic planning activities, and license applications for nuclear power facilities. All of these entities will require the ability to simulate both the operational performance and transient response of nuclear fuels to complement the traditional time-consuming and expensive in-pile experiments. Sandia has been developing the capability to simulate the behavior of materials under large, simultaneous thermal and mechanical stress gradients for defense applications. We propose to extend this capability into a computational tool to simulate nuclear fuel pin performance at the mesoscale that can simulate material segregation, grain restructuring, fission gas bubble transport, and the mechanical interaction between fuel and clad due to swelling. This tool will be based on MPALE, a 3D code which couples discrete particle modeling using kinetic Monte Carlo with a particle-in-cell method for unsteady continuum level elastic/plastic material mechanics.

This project will develop algorithms and capabilities to incorporate the necessary multiple, coupled physical phenomena into MPALE. Microstructural evolution such as grain growth and restructuring will be handled by kinetic Monte Carlo (kMC) models while plasticity will be handled by mesoscale informed continuum crystal plasticity theory. These major methods will be further developed to include new physics such as fission gas bubble at the mesoscale, solid mass transport and fracture. The core challenge and deliverable of this project will be to combine the kMC and plasticity methods within a material point method (MPM)-based code to provide a detailed physics-based simulation capability of the thermomechanical behavior of a fuel pin, that is, both fuel and clad, to a transient thermal environment in a computationally reasonable timeframe. The primary comparison will be the Sandia shock thermodynamic applied research (STAR) experiments on fuel and clad relocation.

Summary of Accomplishments

- Coupled Physics
  - Physics coupling using three strategies has been formulated and implemented: diffusion, kinetic, and continuum.
- Lower Length Scales (LLS)
  - Identified the different LLS physics mechanisms for the fission gas swelling problem and investigated various density functional theory (DFT) codes to obtain the transport probabilities. These mechanisms are: energy (i.e., conduction) transport, atomic structure, atomic species transport, gas cluster transport, and vacancy transport. Collaborations with other DFT groups at Sandia and Los Alamos National Laboratory have been established so that transport coefficients in actinide materials can be obtained. The Einstein formulation to obtain Fickian diffusion coefficients from random walk processes will be used.
- Mechanics
  - Verification and validation (V&V) of both Monte Carlo and gradient based crystal plasticity models in MPALE was performed. A time implicit strategy was developed and partially implemented into the Lagrangian grid based strategy in MPALE. A preliminary diffusion operator was also implemented into MPALE.

  - Material properties (e.g., grain boundary energies, elastic coefficient, bulk energies) for UO_2 at high temperatures were obtained using power fit extensions to available literature values.
  - Alternative strategies for the mechanics operator are being evaluated and compared with the current MPM formulation.
- Calibrated Monte Carlo
  - The time calibration strategies for both 2D and 3D configurations have been developed and the direct coupling between the calibrated Monte Carlo kinetics operator and the continuum mechanics model in MPALE has been demonstrated for texture evolution with plasticity. Kinetic transport of gas bubbles has been demonstrated in MPALE; direct coupling requires implicit time integration.
- Documentation
  - Thesis of the coupling between MPM and texture evolution finished.
  - A journal paper on the 2D calibrated Monte-Carlo was submitted and three more papers are in progress: 3D, Monte Carlo plasticity, direct coupling.
  - An MPM V&V paper is also in progress.
  - A preliminary manual for the MPALE has been written.

Significance

Sandia has had a long-standing and well-established mission in safety technologies for nuclear reactors. The development of these computational capabilities will allow us to support transient fuel experiments and maintain our unique capabilities in this area to support both DOE and NRC missions. In addition, many NNSA technologies will benefit from this project, such as ceramics for microelectronic packaging, solder joints, PZT ceramics, cermets, microsystem technologies and solid oxide fuel cells.

Novel Radiation Detection Technology for Active Interrogation

130751
Year 1 of 2
Principal Investigator: M. A. Grohman

Project Purpose

Various government organizations are funding active interrogation (AI) techniques for substantially increasing the detection signal in numerous national security applications. While there is some small amount of funded effort in the detector systems for AI projects, the majority of current funded efforts is focused on the generation of the actual AI beam. It has been assumed in several government organizations that the existing passive radiation detectors could be used for this other application. However, AI systems involve the operation of detectors in very harsh environments for which they have not been designed.

Sandia has been developing a novel microcapillary detector array based on tiny tubes filled with either high pressure helium-3 for neutron detection or with xenon for gamma detection. Because of the miniature size of the individual elements, they are far less susceptible to upset and saturation caused by operation in the harsh environment of a generated radiation beam during AI. Furthermore, the inclusion of many detector elements in a precisely controlled array allows for both spectroscopy and imaging from scattering events, both of which are extremely important to separate the signal from the target with the signal from the beam. An additional benefit is that the inherently massively parallel nature of the devices can lead to very high dynamic range in terms of data rate.

A related issue with AI techniques being pursued today is the lack of understanding of the signal to be detected. Sandia is one of the world leaders in developing algorithms for radiation detection and can apply this vast expertise to the new AI focus area.

Such technology could have widespread national security applications, such as DOE nuclear nonproliferation, DHS nuclear detection, and DOD standoff detection to locate and track nuclear materials.

Summary of Accomplishments

Shortly before this project began, the extreme difficulty of containing highly pressurized gas in the individual microcapillaries was discovered under separate basic technology safety tests. Because of those manufacturing difficulties, the work in this project was changed in the very first month to include a metal pressure vessel as containment for the gas. This pressure vessel has since been designed, built, and delivered to Sandia. Sensor elements have been constructed and tested external to the laboratory prototype system. In the near future, these sensor elements will be housed inside the pressure vessel. Next, the vessel will be sealed and pressurized to 20,000 psi with helium gas. After this is completed, the device will be tested in a Sandia accelerator laboratory.

The initial neutron modeling work was completed, and the radiation transport model results are currently being combined with the wall interaction model and the electronic drift estimates to simulate the expected signals for algorithmic discrimination of fast neutrons from gamma background. This model will then be used to predict the results of the accelerator testing over the summer, with subsequent model updates after the testing. We expect to meet the milestone to demonstrate the sensor effectiveness of the new technology as compared to existing bulk macrotechnology such as the Sandia neutron scatter camera.

Significance

Radiation detection, location, and identification are keys to, and share common requirements with, a number of DOE/NNSA, DHS/Defense Nuclear Detection Office, and DOD/Defense Threat Reduction Agency national security missions. Because the range of detection using passive techniques is limited, all these agencies are funding active interrogation technologies. All such techniques will require detector schemes that are likely to be substantially different from detectors deployed today due to a significantly increased background from the AI source.

Scalable Microgrid for a Safe, Secure, Efficient, and Cost-Effective Electric Power Infrastructure

130752
Year 1 of 3
Principal Investigator: A. L. Lentine

Project Purpose

Distributed renewable energy generation is a key element in transforming society from its reliance on fossil-fuel based energy to a carbon-neutral, sustainable, and secure energy infrastructure. A new power grid architecture is needed that uses information to enable real-time cooperative generation, intelligent metering, load management functions, and to provide decentralized coordination of potentially millions of generation sources and loads.

We propose a fundamental shift in the management and distribution of electricity at the home, local, regional, and ultimately national scale. This consists of developing a "micro-grid" that is scalable at multiple levels.

In this project, we will:

- Develop a revolutionary control architecture and requirements for the evolution from the current grid to the scalable microgrid approach, using the theoretical foundation from our team's work in physical and information exergy and multiagent based control systems at the community, regional, and national scale.
- Apply innovative microsystems technologies to build a low cost, compact power management, sensing, and secure communications module to provide information for managing the microgrid.
- Demonstrate the use of this module for power management of a representative portion of the scalable microgrid at the distributed energy technology laboratory (DETL).

The project will benefit the proposed National Energy and Water Grid Infrastructure Development Center (NEWGRID), which aims to establish a new power grid technology center of excellence that brings wide-ranging experts together with the required data, sources, sinks, and hardware to assess new technology concepts in a systems context.

Summary of Accomplishments

- Completed a reference architecture for modeling, simulation and test at DETL; the architecture includes intelligent control of generation, storage, and loads, both within individual entities and in communities.
- Developed models of the macromodular inverter and an advanced model-based control scheme for simulation of multiple inverters on a grid.
- Began development of the general software control architecture.
- Generated a set of preliminary requirements for intelligent sensor/actuators, both inside and outside the home.
- Developed a preliminary approach to information aggregation that will also be refined by the results of the modeling and simulation.
- Investigated optical sensing as a means of providing noninvasive high-voltage sensing; we are now investigating new science and technology in microsystems sensing that can complement commercial products.

Significance

Transitioning the electric grid from its current centralized structure to a distributed intelligent scalable grid is required to enable the transition of the US energy infrastructure from fossil-fuel based energy to a carbon-neutral, sustainable, reliable, and secure energy infrastructure with reduced dependence on foreign oil. We propose key innovations in grid architectures, intelligent distributed controls, and microsystems information technology that will play a key role in this transition.

Space Reactor Impact-Criticality Modeling for Launch Safety

130753
Year 1 of 2
Principal Investigator: R. J. Lipinski

Project Purpose

The purpose of this project is to develop the tools needed to analyze the risk from launch of a nuclear reactor into space. The National Aeronautics and Space Administration (NASA) is anticipating using fission reactors for lunar, Mars and deep-space missions. Launch approval for the reactor must be obtained from the Executive Branch. The codes used to obtain launch approval for radioisotope power systems (RPS) are well-established and are used at Sandia for RPS launch approval, but none exist for fission power systems.

Preliminary studies show that the safety requirements for a reactor launch would be easily met unless the reactor goes critical during a launch accident. Reactor criticality might occur at any stage of the deformation resulting from impact on the ground, or impact by large structures onto it. The main technical hurdles that must be overcome are the following: 1) modeling an impacting reactor with sufficient detail for criticality assessment without excessive computer run times, 2) coupling the impact code results with a neutronics code to track the event with millisecond resolution, and 3) accommodating negative thermal feedback effects which could curtail a criticality event in a manner similar to a pulse in the Sandia Annular Core Research Reactor. At the end of the project, Sandia would possess a key tool that could support DOE and NASA in future reactor launch safety analysis.

Summary of Accomplishments

We developed computer aided design (CAD) models (SolidWorks) for an 85-pin reference space reactor, a 19-pin simpler reactor, and very simple single fuel pin test cases. We modeled the impact of a simple test geometry (one fuel pin) onto concrete at 40 m/s and a 19-pin core at 40 m/s with both Pronto3D and Presto. The bottom half of all the fuel pins deformed until they touched each other in the 19-pin simulation. We established a contract with the University of Wisconsin for assistance with the direct accelerated geometry Monte Carlo (DAGMC) code. (DAGMC is the base code that we are modifying to handle the criticality calculation using the deformed geometry output from Pronto3D or Presto runs as input.) We ported DAGMC to Sandia successfully and calculated the change in reactivity in one large fuel pellet. We discovered that the fuel density changed, so correction factors were introduced to ensure conservation of mass. An impact simulation of an 85-pin reactor was performed. We discovered that shell elements, which are needed for timely impact simulations, need special handling in DAGMC. We performed scoping studies for an 85-pin reactor assuming the bottom half of all fuel pins deform until they touch using MCNP (Monte Carlo n-particle code) and found a 5% to 8% increase in k_{eff} (neutron multiplication). We wrote a paper for the American Nuclear Society Topical Meeting on Nuclear Emerging Technologies for Space summarizing our results.

Significance

Sandia was assigned the lead role for nuclear launch safety analyses in 2004. Besides being cutting-edge research, this project is strengthening our core capability in safety analysis so that we can be prepared for any future mission that might use a reactor. The US has only launched one reactor and that was in the 1960s. Currently there are no missions planned that would use a reactor power source although periodically the topic is discussed. Consequently this work is anticipatory of a future need. This project helps Sandia prepare for future DOE needs so that when a mission is funded the techniques can be implemented in a production code in a timely fashion to meet the launch schedule. While DOE would be expected to fund the development of any production code should the need arise, the work being done in this project is examining modeling options and is exploratory in nature.

Additionally, there are other applications of this technology. The techniques being explored in this project can be used to assess the criticality margin for the impact of shipping containers with nuclear fuel or impacts in the transport of small reactors. At present, such analyses are not performed because they are not feasible. Hence, this work offers the hope of developing techniques that can be used for multiple DOE applications.

Engineering Framework for Complex Adaptive Systems of Systems (CASoS) and Applications to the Global Energy System (GES)

134529
Year 1 of 3
Principal Investigator: R. J. Glass Jr.

Project Purpose

Complex adaptive systems of systems (CASoS) are ubiquitous, they include cities, infrastructure, government, armed forces, nations — in short, systems that are socioeconomic-technical in nature. As a national laboratory with an engineering mandate, nearly every important problem which we confront is within a CASoS; problems include nuclear stockpile management, nonproliferation, energy surety, and critical infrastructure protection. We must recognize this CASoS context to properly pose and solve problems while not producing unintended consequences: that they are feasible solutions, robust to uncertainties, and enhance system resilience. Of essential importance to this engineering process is the actualization of the solution within the CASoS, a step that is often neglected. We will develop a general CASoS engineering framework for the definition, design, testing and actualization of solutions within CASoS. This development must be done through focus on high priority, specific applications while keeping an eye on the general. We choose the global energy system (GES) as our CASoS of application. The GES contains both complex earth and complex adaptive human systems including economic, socio-political, and technical systems. The GES is currently the nation's and humankind's highest priority, largest, most important CASoS. In context of the framework, we will first define and evaluate several critical issues of high potential impact within the GES. Based on this evaluation, one to three of these initial applications will be chosen for extension into the design and testing phase. The development of a CASoS engineering framework for application to the GES and beyond to the myriad of socioeconomic-technical problems within DOE/NNSA/DHS/national security missions is vital and cannot be accomplished within current programmatic context.

Summary of Accomplishments

In FY 2009, this project pushed CASoS engineering at Sandia forward on many fronts. We:

1. Began development of a CASoS engineering framework that addresses the unique aspects of CASoS activities, various strategies for engineering solutions for CASoS, engineering processes, and possibilities to leverage efforts if multiple aspirations are undertaken for a given CASoS.
2. Began development of a CASoS engineering cyber space that can accommodate emergent theory, algorithms, and tools, the rapid integration of new CASoS engineers and CASoS projects, and effective use of high performance computing,
3. Set the context for our work in the GES with links to interdependent issues of climate and international negotiation, including an initial survey of global climate and integrated climate and economic models,
4. Defined the two GES CASoS applications that would work synergistically with each other: global energy surety and strategic energy intelligence. For each of these applications we defined objectives, conceptualized required CASoS models and analyses, charted a path towards implementation and began to implement.

Significance

DOE's overarching mission is to advance the national, economic, and energy security of the United States. Energy and infrastructure assurance is a mission area for Sandia. The GES is the arena in which both DOE and Sandia carry out their missions. The GES is a CASoS, but it is rarely treated as such. Bringing CASoS approaches and techniques to analysis of the GES will improve Sandia's and DOE's ability to optimally perform their respective missions.

Responding to Biological Threats Raised by the WMD Commission Study, World at Risk

139458
Year 1 of 1
Principal Investigator: J. M. Gaudioso

Project Purpose

In December 2008, the Commission on the Prevention of WMD Proliferation and Terrorism report, *World at Risk*, highlighted the threat of bioterrorism and specifically called for bioscience laboratories that handle dangerous pathogens to implement a unified laboratory biorisk management framework to enhance their safety and security. This report asserted that laboratory biorisk management was perhaps the most effective defense against terrorists acquiring dangerous pathogens and developing biological weapons. Although safety and security pose separate risks and must be assessed independently, the system to manage these risks must be cohesive and unified to be effective from the laboratory perspective. A risk management framework has seven main phases: preassessment, risk assessment, concern assessment, risk characterization, risk evaluation, decision-making, and implementation. The bioscience community has tools for implementation, and is developing standardized processes for risk assessment and risk characterization. But they lack the ability to determine which of these tools are the most sustainable and effective. Thus, this project focused on research into the best approaches for preassessment and decision-making for biorisks. This project developed a series of technical recommendations for laboratories to implement a unified laboratory biorisk framework, helping them meet the WMD Commission's recommendations for addressing biological threats in laboratories.

Summary of Accomplishments

This project developed an integrated approach to implementing a unified laboratory biorisk management framework by adapting the International Risk Governance Council's new integrated analytic framework for the development of comprehensive assessment and management strategies. This report analyzes the value in implementing integrated formal biorisk management systems. The report also identifies key technical approaches and gaps in the current state of the art that are crucial for laboratories adopting a formal biorisk management system. Recent laboratory biosafety and biosecurity incidents were analyzed to understand common causes of failure and we identified a set of drivers that could be used to encourage institutions to implement an integrated biorisk governance approach. We substantively revised and updated specific risk assessment methodologies for assessing relevant biosafety and biosecurity risks and wrote a set of technical requirements for assessing the relevant risks separately but managing them in a unified framework. We explored existing laboratory risk management approaches and identified important technical gaps that often lead to biorisk incidents. We enumerated sets of technical recommendations to close those gaps. Finally, we drafted a set of requirements for using new communication tools to effectively implement an integrated framework.

Significance

This project should facilitate bioscience institutions' efforts around the world to better implement effective risk management systems, helping to ensure that work with dangerous pathogens is conducted in a safe, secure, and sustainable manner. The results should also be useful to the international community's work to develop a guidance document for implementing the international laboratory biorisk management standards.

Model Framework Development for Penetration Options in the US Energy Supply

139460
Year 1 of 1
Principal Investigator: P. S. Pickard

Project Purpose

The purpose of the project was to develop a systems dynamics (SD) framework for the analysis of a broad range of energy technology and policy questions and demonstrate an initial version of this SD framework on an illustrative energy question on low carbon energy source penetration into the US energy supply mix. Sandia has developed numerous SD models over the past 10 years to address energy questions, resulting in the development of a number of SD codes that could be used to some degree to address future energy policy issues. The first objective of this project was to develop a framework to apply this previous investment in SD models to current energy policy or technology questions. The second objective was to develop an initial set of models utilizing some of the previous Sandia models combined to address a low-carbon energy source questions and demonstrate this framework on the more specific question of what would be the carbon and import implications of expanding nuclear electric capacity to provide power for plug-in hybrid vehicles. The types of energy policy issues and questions being asked in current discussions generally involve how best to achieve some overall societal objective where energy may be one of the key elements and can include functional or performance goals, economic objectives, environmental constraints, and energy security issues. These goals or objectives are often interrelated, and require consideration of a complex combination of factors that interact. An integrated system dynamics framework based on Sandia SD models is an efficient and effective simulation tool to examine the interaction and implications of various energy policy and technology options.

Summary of Accomplishments

1. Fifteen Sandia SD energy models were reviewed for relevance and future adaptability. Ten of these were evaluated to be relevant to aspects of current energy issues, and five of these were evaluated to be very good to excellent. More recent models were generally developed in a more structured and documented approach, making them more likely to be useful in a broader framework.
2. The US energy and greenhouse gas model (USEGM) was identified as most relevant Sandia energy model to track carbon emissions, costs and petroleum requirements for a range of energy supply options and new types of transportation vehicles (e.g., plug-in hybrid electric vehicle [PEHVs]). The global energy futures model (GEFM) was identified as suitable to model electric generating capacity of the nuclear power fleet and future expansion.
3. A simple US transportation model was created to model how the US fleet changes as PEHVs gain penetration with respect to gasoline usage, electricity usage, and greenhouse gas emissions.
4. The results of the initial model runs indicate that a relatively modest increase in nuclear electrical generating capacity creates sufficient off- peak power to charge a significant number of commuter style PEHVs. Current projections of PEHV efficiency range from ~1600 kWhrs/yr (12,000 miles) to more than 4000 kWhrs/yr. At the lower efficiency end of the range, one 1000 MWe plant is needed to power 2 million PEHVs. Ten new plants could then support 20 million vehicles (about a 10% penetration) with an associated nominal 10% reduction in carbon and oil imports from transportation. Based on these results, the adoption rate of PEHVs would be the limiting factor in achieving these levels of reduction in carbon and imports.

Significance

A systems dynamics framework was demonstrated utilizing Sandia SD models resulting in a capability to more efficiently address a wide range of energy policy and technology questions. The approach demonstrated in this project could be applied to future Sandia energy analyses. The initial analysis results indicated that a very achievable level of nuclear electric expansion can support of significant penetration of PEHVs to reduce carbon emissions and imports. The results of this project can be used to provide informed input to US energy stakeholders.

Microsystems Technology Opportunities for Next-Generation Renewable Energy Systems and the Intelligent Electric Power Grid

139861
Year 1 of 1
Principal Investigator: R. C. Pate

Project Purpose

This project will develop several advanced integrated device and module designs and process engineering concepts, utilizing innovative Sandia microsystems and nanomaterials technologies and capabilities, needed to implement advanced renewable energy systems (i.e., solar, wind, geothermal), energy storage, and new smart grid architectures. Widespread adoption of renewable energy technologies that are so vital to building a sustainable energy future, is being hampered by the inability of the current transmission and distribution grid infrastructure to handle load management, bidirectional power flows, and the time-variability of power generated from renewable resources. Also an impediment is the relative immaturity (in terms of cost, reliability, dynamic sensing, monitoring and control capability) of wind, solar, and geothermal renewable energy generation systems, energy storage systems, and load systems. Revolutionizing the power grid demands implementation of new architectural concepts that integrate advanced renewable energy generation, storage, power conditioning, energy management, sensing, and control. This requires development of advanced power flow control and energy storage technologies. Numerous barriers remain to be overcome to realize this vision. Advances are needed in power electronics device and module design, materials and processing, packaging, and integrated sensing and control systems to enable increased electrical power grid reliability, stability, security, and efficiency while at the same time decreasing installation and operating costs. Key gaps in the enabling technologies required include cost-effective solid-state power switching devices and modules with improved, high-temperature performance and reliability, dynamic energy system sensing, monitoring and control, and advanced energy storage. This project will address several of these gaps. LDRD investment is needed to enable the leveraging of Sandia's unique multidisciplinary capabilities to effectively address the gaps in this application area.

Summary of Accomplishments

The purpose, goals, and approach for this LDRD project were to develop selected conceptual designs for devices, systems, and/or processes that leverage Sandia's microsystems and materials capabilities to enable improved technologies for renewable energy generation, energy storage, and the future smart grid. The project succeeded in developing several design concepts by a multidisciplinary team of Sandia content-experts spanning energy, applied storage, materials, microsystems, physical protection systems (PPS), and basic sciences. The results of the project are summarized below.

We established a multidisciplinary team that formed into four task subgroups that developed selected microsystem-enabled concepts for: smart grid (sensing, secure communications and control), wind turbine blade sensing and control, solid-state high-power switching, and other energy storage and renewable energy related concepts. The S&T and applications criteria and goals were as follows: leverage Sandia microsystems capabilities; leverage Sandia nanomaterials capabilities; address problems with S&T content; and address challenges to increased renewable energy use and penetration into the emerging smart power grid. Project next steps and recommendations include the following: publish and distribute final project report; submit and present selected work at conferences; submit selected work for journal publications; use project results to inform new LDRD proposals to pursue in-depth R&D; and use the project results to inform proposals for external funding opportunities with DOE, DOD, and industry.

Significance

This project leverages unique Sandia capabilities in microsystems, nanomaterials, renewable energy, energy storage, and power switching to enable improved performance and reliability of next generation renewable energy generation, storage, and smart electric power grid architectures. It likewise contributes to improved energy security, increased deployment of renewable energy and power generation, reduced carbon footprint, and economic benefits associated with more efficient energy and power management and use.

Reduction of Uncertainties in Remote Measurement of Emissions and Uptake of Greenhouse Gases

139863
Year 1 of 1
Principal Investigator: B. D. Zak

Project Purpose

Recent discussions with climate research colleagues from National Aeronautics and Space Administration (NASA)/Jet Propulsion Laboratory (JPL), Los Alamos National Laboratory (LANL), Lawrence Livermore National Laboratory (LLNL) and the National Oceanic and Atmospheric Administration (NOAA) reveal that all recognize the need for a greenhouse gas information system (GHGIS) to provide global and regionally resolved greenhouse gas (GHG) emissions and uptake data based on remote and in situ sensor output combined with atmospheric modeling. Such a GHGIS would facilitate both US management of its own GHG emissions and monitoring of future global GHG treaties. The objective of this project is to use sensitivity analysis to investigate atmospheric and GHG sensor data fusion with transport models to reduce uncertainties in point and regional GHG emissions and uptake measurements. This project will allow Sandia to lead in developing the technology for a future GHGIS analogous to national technical means for nuclear test ban treaty monitoring.

On February 24th, the JPL Orbiting Carbon Observatory (OCO) was launched, but failed to achieve orbit. OCO (to be replaced in 2–3 years) and similar other nation GHG orbital sensors (like the Greenhouse Gases Observing SATellite [GOSAT] launched by Japan in January) will be critical sensor elements for the future GHGIS. Both OCO and GOSAT were designed to measure column concentrations of selected GHGs using surface-reflected light. OCO and GOSAT do not measure GHG emissions and uptake directly. These measurements can only come from sensor and atmospheric model data fusion. There is an emerging consensus that the DOE-ARM (atmospheric radiation measurement) sites are highly appropriate for both column concentration measurement validation and technology development for measuring GHG emissions and uptake. This project will address satellite and other sensor data integration with atmospheric models together with ARM site utilization in GHGIS development.

Summary of Accomplishments

We analyzed the principal available models used in current GHG local and regional emissions and uptake measurement techniques, and chose to focus on Carbon Tracker (CT), and the Weather Research and Forecasting (WRF) models. In collaboration with the NOAA Earth System Research Laboratory, we ported Carbon Tracker to Sandia's Thunderbird machine along with supporting meteorological data, and got CT running using meteorological and GHG data identical to CT runs that had earlier been carried out on a NOAA machine. We discovered that there were small but significant discrepancies between the output from the present Sandia and the earlier NOAA runs that require further analysis. We also ported WRF to a Sandia machine, got it running and began working with it. We met with NASA regarding the prospects and potential characteristics for a replacement for the Orbiting Carbon Observatory which failed at launch, and investigated the availability of data from the Japanese GOSAT. Preliminary GOSAT data is only now being made available internal to their team. We took part in the conceptual design of a mobile laboratory now being built at Sandia for in situ and column GHG measurements under OCO (replacement) or GOSAT overpasses and elsewhere in connection with GHG emissions and uptake measurements. The mobile lab contains extensive GHG, meteorological, and sampling capabilities. It is designed to be compatible with DOE/ARM data archiving and distribution systems. This mobile laboratory may become a prototype for GHG measurement platforms for use in this and other countries in support of GHG treaty verification. We also investigated other potential GHG measurement techniques, and focused particularly on an innovative airborne sampler called Air Core being developed at NOAA which could fruitfully be coupled to the analytical capabilities of the mobile laboratory.

Significance

This project supports the DOE Strategic Plan: Strategic Theme 1, Energy Security, Goal 1.2, Environmental Impacts of Energy: Improve the quality of the environment by reducing greenhouse gas emissions and environmental impacts to land, water, and air from energy production and use. Managing GHG emissions both in the US and globally will be greatly facilitated by techniques for accurate measurement utilizing satellite remote sensor data coupled with other data and models.

HOMELAND SECURITY AND DEFENSE INVESTMENT AREA

Projects in this investment area (IA) focus on the physical and computational tools, and the underlying science, necessary to protect our nation — its citizens, military personnel and diverse types of infrastructure — from a multiplicity of threats. From detecting the entry of biological, chemical, and nuclear threats, to lighter, more-effective armor for warfighters, to computational tools for intelligence analysts such as filters for the traffic messages along the internet and other networks, the reach of this IA extends broadly into a diversity of science and engineering areas.

Deployable Pathogen Diagnostic System

Project 130756

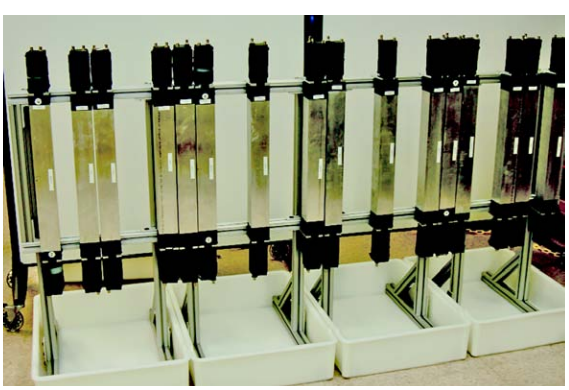
The probability of bioterrorism is increasing. Therefore, improved ability to quickly detect pathogens and treat exposed individuals is a national-security priority. Portable, field-deployable, accurate detection devices are a key countermeasure, which will allow first responders to quickly identify exposure to specific pathogens and rapidly initiate appropriate therapeutic measures. This project is designing and fielding just such a portable diagnostic device. Drawing from Sandia advances in microfluidics technology, a gel-electrophoresis lab-on-a-chip technology has been designed, which can integrate several functions. Preconcentrating a (blood or saliva) sample and mixing with a labeled antibody probe, the device then separates samples and detects and quantitates positive assays. The chip's design allows the parallel processing of samples with multiple analytes, such that multiple screens for can be performed simultaneously and with a short incubation time.

Prototype of the field-deployable diagnostic system

Active Coded-Aperture Neutron Imaging

Project 117818

The ability to detect special nuclear material (SNM) over large distances is an important component of homeland security, conferring the ability for early detection of potential nuclear terrorism, a well as serving as an aid to verification initiatives. An attractive way to perform such long-distance detection is through the imaging of the fast neutrons emitted by SNM, which are energetic enough to penetrate shielding and to travel over long distances without scattering—and whose environmental background is very low. This project combines both double-scatter and coded-aperture methods, that is, active coded-aperture imaging. The mask is made active to increase the opacity to energetic neutrons. This technique results in a better signal-to-noise ratio and efficiency of detection. A set of Monte Carlo simulation tools have been developed and calibrated by experimental results so that future detector designs can be tested. This represents the first system that demonstrates fast-neutron imaging using an active mask.



Prototype active coded aperture imager

HOMELAND SECURITY AND DEFENSE INVESTMENT AREA

Enabling All-Threat Analysis Through Intelligent Filtering of Network Traffic

105870
Year 3 of 3
Principal Investigator: J. Van Randwyk

Project Purpose

The Department of Homeland Security (DHS) categorizes the nation's critical infrastructure into many categories including energy, transportation, banking and finance, public health and healthcare, information technology/cyber security and others. Many of these sectors are interrelated, but cyber cuts across them all. In a sense, this categorization artificially restricts the approaches used to determine and address the threats in each of these sectors. Cyber data, in particular, can be useful in understanding many types of potential threats including those outside of the cyber realm.

The key goal of this R&D is to study and develop "intelligent" network filters through the use of data mining techniques such that the "signal" is extracted from the "noise." We believe that data mining cyber data for non-cyber threats will illuminate data already on US government networks that provides insight into existing and evolving terrorist plans, as well as insight into the intentions of nation-state adversaries. We intend to publish information that assists other government agencies in building databases of cyber data and analyzing those databases. Additionally, we hope to develop tools that can mine large quantities of cyber data, producing results that clearly point an analyst to threats to the US.

Summary of Accomplishments

We continued to refine our database, making it more efficient and adding a new data source. Additionally, the data-ingestion process is now sufficiently automated so that we can import new data on a monthly basis with a minimum amount of human intervention.

We continued to develop the REVELAR (Revelar environment for visual exploration of latent associative relationships) tool. REVELAR queries our database for pertinent data, mines the data using a variety of user-selectable, built-in "interesting-ness" formulas, and presents the results in an interactive, visual format. We added a tool to visualize trends over time and implemented two tools to visualize relationships between our data as expressed by the LSA (latent semantic analysis) algorithm. This tool suite provides an analyst with multiple ways to look at changes in data over time, mathematical algorithms to perform analysis of the data, and opportunities to interleave data in a single visualization that might otherwise not be looked at simultaneously.

Significance

This work has significant potential to contribute toward strengthening national security. Specifically, this work addresses the DHS goals of awareness and prevention, indirectly contributing to the third goal of homeland protection. We contribute to achieving each of these goals through tool and technique development that can be used by counterintelligence and law enforcement organizations in an analysis role. DHS contains law enforcement and counterintelligence (CI) elements charged with this mission.

Enhanced Simulation for Homeland Security Training

105872
Year 3 of 3
Principal Investigator: D. D. Djordjevich

Project Purpose

Emerging, changing modes of attack using weapons of mass destruction (WMD) — threat scenarios under investigation by DHS and DOD — require new approaches to examining detection, mitigation, and response options. This has left many of our installations at increased risk due to inexperience with the new threats. As an immediate solution, many have defaulted to "best educated guess" response plans that potentially increase losses due to incorrect threat assessment. To educate and train decision-makers in the modes of attack and response options specific to their unique requirements, we propose the use of human-in-the-loop training simulations using game technology. This would place multiple participants in the center of the simulation and allow their decisions to influence scenario evolution in a responsive environment. Simulations provide a means for decision-makers with different perspectives to explore the full complexity of a terrorist WMD defense through interactive, dynamic, "what-if" computerized "war-gaming." Exploratory live, "fire-drill," training is too expensive to use for awareness gathering and passive, paper-based, training does not present the trainee with adequate fidelity. Gaming enables users to interact within the context of a virtual scenario embedded with specific learning objectives and, in addition, to quickly and objectively analyze their responses and provide valuable post-training feedback. Ultimately, trainees gain greater situational awareness and understanding that would aid them in the development of new response plans to secure the military's infrastructure and force projection capabilities.

Investment in this research project will further Sandia's leadership role in interactive simulations with advanced gaming technology for WMD decision analysis scenarios and result in a unique capability that could benefit other government agencies.

Summary of Accomplishments

This project followed three themes of R&D to accomplish its objective to develop a game-based training platform for homeland security (HS) training: 1) provide a game-based training approach, 2) use cognitive models to replace other players, and 3) leverage automated decision support research to replace facilitators.

This project was a three-year effort with major R&D milestones in each year. For year one, the development of our open-source based R&D infrastructure was critical for positioning the project to meet the later-years' R&D goals. The second year's milestone was the successful integration of emotionally enabled cognitive models that replace other players. Year three's goal was the inclusion of adaptive scenarios to train judgment-based, decision-making skills. We tackled the technological challenge of integrating highly complex cognitive models into our infrastructure and supporting real-time operation for our scenarios of interest. In addition, we successfully included the adaptive scenario capability in a way that is complementary to the real-time demands of our infrastructure while still retaining efficacy. Each year further refined and integrated each capability, which has now culminated in the "Ground Truth" platform.

Significance

This research address key issues in using the project's proposed delivery path for HS training and analysis systems. By integrating cognitive models and decision aid research with our internal, open-source based, game infrastructure, we were able to develop rapid HS-focused prototypes.

Specifically, we developed our training platform to meet R&D needs based on open-source technology. We also successfully integrated cognitive models to replace other players within this infrastructure and leveraged automated decision support research to replace facilitators. This combination has repeatedly been demonstrated to showcase the utility of this approach for addressing HS training gaps. This project served to further establish Sandia expertise in serious gaming applied to national security problems.

This work supports a major goal of the Homeland Security strategic management unit (SMU), namely to develop and apply technologies that anticipate, prevent, respond, and recover from terrorist and catastrophic natural events. It represents a unique capability in applying advanced gaming technology to WMD decision analysis training. Further, this work complements existing programs underway or planned for DOD/DTRA, DHS Chemical and Biological National Security Program (CBNP), and NNSA/NA-22 and is broadly applicable to homeland security and emergency response.

Microbial Agent Detection using Near-Infrared (IR) Electrophoretic and Spectral Signatures for Rapid Identification in Detect-to-Warn Applications

117811
Year 2 of 2
Principal Investigator: J. A. Fruetel

Project Purpose

Rapid identifiers of aerosolized biological agents are desired by both DHS and DOD to rapidly (in 1–5 minutes) provide additional information following an alarm by aerosol particle triggering systems. Because current triggering systems false alarm frequently on non-biological particles and cannot discriminate between pathogenic and nonpathogenic biological particles, rapid identification of the source of the trigger alarm is critical to enabling rapid response actions which could save lives and protect assets. The ultimate aim of rapid identifiers is to achieve species-level specificity, as this is required in order to distinguish disease-causing organisms (e.g., *Bacillus anthracis*, the causative agent of anthrax) from benign neighbors (e.g., *Bacillus subtilis*). Current methods require sample manipulations, are time-consuming (30–60 minutes), and thus preclude their use as rapid identifiers. The purpose of this project is to demonstrate a novel identification methodology that does not require time-consuming sample preparation, but rather detects intact organisms using native near-infrared (NIR) absorbance. In this approach, organisms are sorted from each other and other particulates using capillary electrophoresis (CE), and detected by NIR absorbance spectra. Both techniques show promise of species-level identification when used alone; by coupling the two techniques, we anticipate species-level discrimination in a microfluidic format compatible with use in the field. A key challenge to implementing absorbance-based approaches in microfluidics is achieving sufficient sensitivity, as absorbance pathlengths are short (<100 µm). To enhance the sensitivity, we will implement cavity-ringdown absorbance spectroscopy (CRDS). The overall approach described here can be rapid enough (<5 minutes) and sensitive enough (~10^5 colony forming units per milliliter [cfu/mL]) for use as a rapid identifier, and can be implemented in a capillary-based format to provide a robust and low-cost platform for wide-spread use in biodetection architectures.

Summary of Accomplishments

To prove this new methodology, we have successfully demonstrated CE resolution of *Bacillus* spores—including *B. anthracis*—and vegetative bacteria at the species level for the first time. Fiber coupled incoherent broad-band cavity enhanced absorption spectroscopy (IBB-CEAS) has been shown to be a sensitive technique for absorption measurements of NIR absorbing compounds. To our knowledge, this work represents the highest sensitivity reported with respect to detection of absorbers in nanoliter samples. This detection method has broad applications for sensitive detection of aqueous solutions; however, for particulate samples, a less invasive capillary-fiber interface needs to be developed. For scattering particles, a single pass configuration was developed for simultaneous scattering/transmission loss measurements which has potential for discrimination based on scattering/transmission ratios as well as peak widths. Potential areas for follow-on development include integrating multiple wavelengths into a single fiber.

For the identification of aerosolized biological agents, this detection approach meets several desired performance parameters for rapid identifier systems: detection in less than 5 minutes, species-level discrimination for *Bacillus* spores including *B. anthracis*, low reagent use and operating costs, compact size (< 1 ft^3), and detection of 104–107 organisms/mL sensitivity. A key issue still to be resolved to realize this methodology as a viable fieldable detector is improving the capillary-fiber junction to enable cavity-enhanced detection of CE separated biothreat particles. Single-spore detection with the single-pass system is just at the noise level of the system. Because the CEAS technique increases signal (ten-fold) but not system noise, it is expected that single spore detection would be easily obtainable. Additional issues include better understanding and reproducibility of spores in the presence of vegetative cells, and implementing physical controls to eliminate particles outside the sample.

Significance

This proposal addresses critical detection needs in homeland security. Features of this approach — low capital and consumable costs, portable, extensible to new agents, potential to measure viability — match operational constraints articulated by DOD and DHS program managers, which are currently unmet with developed systems. This project will integrate Sandia capability in areas relevant to DOE missions — lasers, fiber optics, microanalytical devices, bioscience — and will advance core S&T capabilities.

Antibacterial Polymer Coatings

117812
Year 2 of 2
Principal Investigator: M. Hibbs

Project Purpose

In this project, a series of novel polysulfones with pendant quaternary ammonium (QA) groups will be synthesized and evaluated for antibacterial activity. The activity of similar agents is strongly dependent on the length of the alkyl chains attached to the QA group, so varying chain lengths will be studied for potency together with the density of QA groups in the polymers. The solubility of these polymers can be tuned by exchanging the anions present, and this will be utilized in preparing ethanol/water solutions that can be sprayed onto various surfaces to create protective coatings.

QA compounds are effective against viruses and vegetative bacteria, but are decidedly less effective against highly persistent agents such as bacterial spores (e.g., anthrax). In order for the proposed polymer coatings to address the broad spectrum biological threat, glutaraldehyde, a commonly used sporicidal agent, will be tethered to the proposed polysulfones via an alkyl chain. The tether length will be studied to allow the glutaraldehyde enough mobility to bind to and penetrate the outer layers of spores while keeping it from leaching out of the coating and into the surrounding environment. Other aldehydes will also be investigated.

If successful, the proposed coatings could be easily applied to a variety of surfaces (fabric, plastics, building materials, etc.) to provide a first line of defense for personnel, property, and critical infrastructure against biological attacks.

Summary of Accomplishments

The work accomplished demonstrated the following:

- Poly(sulfone)s with quaternary ammonium groups can be synthesized and sprayed to form coatings that kill 99.9% of both gram positive and gram negative bacteria on contact.
- These coatings still kill 99.9% of bacteria after 14 days of exposure to a simulated diurnal temperature cycle, and they still kill 87% of bacteria after 14 days of immersion in water.
- These same polymers can be modified using a “click” chemistry approach to add aldehyde functional groups.
- The poly(sulfone)s with pendant aldehydes can be sprayed to form coatings that kill up to 81% of *B. atrophaeus* spores on contact within 6 hours.
- The combination of quaternary ammonium groups and aldehydes is required for the coatings to kill any significant amount of spores.

The aldehyde coatings represent the first report of a sporicidal coating that does not rely on the release of biocides into the environment. The percentage of spores killed is perhaps not high enough to be of practical use and the long-term stability of the coatings has not been thoroughly investigated. Future work on these coatings should include efforts to develop ammonium groups that have two or more aldehydes attached to them in order to increase the ability of the coating to kill spores. Also, trialkoxysilane groups can be attached to the polymers in order to allow the coatings to covalently bond to surfaces with hydroxyl or amine groups (such as cotton and glass). Additionally, the possible use of coatings with aldehydes protected as acetals could be explored. The rate at which the acetals hydrolyze to aldehydes could be tuned to extend the usable lifetime of the coatings.

Significance

This project contributes to the development of a passive first line of defense against biological attacks. This would support the DHS strategic goal of protection by safeguarding people, critical infrastructure, property, and the economy of our nation from acts of terrorism and other emergencies.

Knowledge about antibacterial coatings and how to apply them learned from this project is being leveraged in two currently funded projects. One of these is another LDRD project in which reverse osmosis membranes are being modified to increase their resistance to biofouling to increase the lifetime of the membranes. The other is a DOE-funded project to develop hydrokinetic devices for producing renewable energy. Within that project, there is a materials task, part of which involves coatings that will prevent biofouling on the devices.

High-Volume Preconcentrator Coatings for High Vapor Pressure Compounds

117813
Year 2 of 2
Principal Investigator: L. A. Theisen

Project Purpose

There is an urgent need to increase our nation's capability to detect high vapor pressure (HVP) compounds. Sandia has already developed and commercialized a preconcentrator designed to collect low vapor pressure (LVP) compounds. HVP compounds are more reactive, do not adhere to existing preconcentrators, and are difficult to detect. Effective detection of HVP compounds using ion mobility spectrometry (IMS) requires efficient collection and preconcentration of the volatile materials for detection. This project investigates unique polymer coating materials for application onto Sandia's high-volume preconcentrator to enhance the detection of HVP compounds.

Very little is known about IMS detection of HVP compounds. This work will aid in the understanding of how HVP materials bind to coating materials, and will increase the understanding of the degradation/decomposition of the HVP compounds in relation to the IMS detection of these compounds.

Summary of Accomplishments

The team performed experiments to determine if any of the nine preconcentrator screens (eight coated and one uncoated) improved the ion mobility spectrometry (IMS) detection of HVP and LVP materials. There was a total of six different explosive analytes tested. The explosive materials all contained nitro groups and were either nitro aromatics or aliphatic nitrated compounds. One of the tested coating materials improved the IMS detection for all six analytes over the uncoated screen. The coating's binding ability was related to several noncovalent interactions with the analyte.

Significance

This project will benefit DOE and DHS missions by developing a tool to detect HVP compounds that are typically found in improvised explosive devices (IEDs) and homemade explosives (HME). Sandia researchers have a proven way to collect and preconcentrate LVP explosive materials, and we would like to explore the use of new coatings with Sandia's patented explosives collection technology to solve the problem of detecting HVP compounds.

Two-Pulse Rapid Remote Surface Contamination Measurement

117814
Year 2 of 3
Principal Investigator: T. J. Kulp

Project Purpose

We propose to develop an optical detection method to allow stand-off sensing of chemicals on surfaces. As a particular example, we will target the detection of surface deposits of low-volatility chemical warfare agents (referred to as LVAs). The remote characterization of chemical residues on a substrate is a problem for which only limited tools currently exist. It is, nevertheless, an area of fundamental importance to homeland and military defense because many threat and indicator materials exhibit low volatility and are likely to be found as a molecular or particulate surface deposition. Examples include LVAs, biological organisms and toxins, nuclear particulates, and explosives. Traditional optical remote sensing methods based on light absorption often fail in sensing trace surface deposits because their spectral signatures are masked by that of the underlying material. Methods based on fluorescence may not succeed for that reason or because the analyte does not fluoresce efficiently. As an alternative, we propose to explore pulse-probe measurements that would apply two pulses of light to the surface — one to remove the analyte (or a fragment of it) from the surface and the second to sense the removed material. For the selected case of LVA detection, the first pulse would photofragment the non-fluorescent agent to release the highly-fluorescent phosphorous oxide (PO) radical as a vapor, and the second pulse would detect the PO using laser-induced fluorescence (LIF). Thus, the first pulse would serve the dual purpose of removing an analyte fragment from the surface and converting an undetectable analyte into a detectable (fluorescent) byproduct. The work would demonstrate this measurement both in a cell in the laboratory and as a short-range (few meter) standoff detection measurement.

Summary of Accomplishments

During FY 2009, we demonstrated the feasibility of extending the pulse-probe measurement of organophosphate simulants from the vapor to the condensed phase. This was accomplished by measuring four simulants deposited on one or more of several common surfaces. The simulants were: (A) dimethyl methyl phosphonate (DMMP); (B) diethyl methyl phosphonate (DEMP); (C) diisopropyl methyl phosphonate (DIMP), and (D) diisopropyl (ethoxycarbonylmethyl) phosphonate (DIPP). The latter was determined to be the most representative LVA simulant of the four. The successful measurement of all indicates that the method is transferable among multiple organophosphate forms. The surfaces on which measurements were achieved were asphalt, cement, paint, oxidized steel, aluminum, paper, wood, lucite, and cardboard.

The above results show that the method is versatile. However, because the samples were made without quantification of the analyte, they do not test the sensitivity of the approach. This was addressed by assembling an apparatus in which a controlled density of simulant is deposited on a surface by an airbrush. The process was calibrated by weighing the substrate before and after spraying. During the pump-probe measurement, the sample was rotated to ensure probing of an undepleted layer of analyte.

The controlled deposition measurement was conducted for DIPP on aluminum, where it was found that an analyte density of 78 $\mu g/cm^2$ can be detected by a single pair of laser pulses with a signal-to-noise ratio of about 5. This is currently being extended to measurement of DIPP on concrete, which may be more difficult because of its porosity.

It is expected that the sensitivity will be improved by optimization of the measurement conditions. These include the adjustment of laser fluences and signal integration to minimize interference from laser plasma emission and by matching the probe volume to the size of the fragment plume.

Significance

The results contribute to the field of optical spectroscopic analysis and to Sandia's ability to address key national security mission areas. The pulse-probe method has been demonstrated in the vapor phase for chemical warfare agent simulants, but never in the condensed phase. Our demonstration that this is feasible will be of interest to the outside community. Pulse probe measurements have been shown on surfaces for explosives detection — however, they have only been performed in a demonstration mode and have never extended to controlled trace contaminant levels as we have demonstrated. The ability to do so and the identification and mitigation of certain problems (such as plasma emission) when this is done will be of strong value to the outside technical community.

Automatic Recognition of Malicious Intent (ARMI)

117816
Year 2 of 3
Principal Investigator: H. D. Nguyen

Project Purpose

The purpose of this project is to create a robust capability for the automatic recognition of malicious intent (ARMI) exhibited by intruders (e.g., humans, vehicles) encroaching on an extended security perimeter. A ground-based radar is employed to detect and track intruders, and optical imagers are used to establish intent. A long-range acoustic annunciator is utilized to challenge intruders in order to elicit an observable behavioral response that can be categorized as malicious or benign. The capability to automatically recognize, at distance, intruders with malicious indicators of intent has tremendous potential for reducing nuisance alarms in extended perimeter surveillance systems, and reducing the workload of security response forces.

Summary of Accomplishments

We contracted with Science Applications International Corporation (SAIC) to perform a study for the development of a “periodic table” of elemental behaviors. These behaviors form the basis for understanding malicious behaviors in the context of perimeter intrusions. A protocol for field data collection of intruder behavior scenarios monitored by ground-based radar and camera video was approved by the Human Studies Board at Sandia and a successful data collection was conducted. The intruder volunteers carried a hand-held GPS unit while their movements were observed by radar and video in order to provide position ground truth. An algorithm was devised and tested with the ability to reduce radar track position uncertainty thereby improving the interpretability of small movements at long range.

Significance

This work will significantly extend our physical-protection system capabilities with tremendous benefits to several DOD, DOE, DHS, and national security initiatives, such as physical and border security, extended-defense systems, and insider identification and detection. ARMI is a critical need for extended-defense systems and is anticipated to be a major component of next-generation, 21st-century physical-protection system installations.

Risk-Based Decision Making for Staggered Terrorist Attacks — Situational Awareness, Resource Markets and Systemic Risk Reduction Under "Reload" Scenarios

117817
Year 2 of 2
Principal Investigator: J. Ray

Project Purpose

We propose to develop quantitative, risk-based methodologies for allocation of scarce resources during the trans-attack phase of a bioattack. Using the reload scenario (where a small set of cities are subjected to staggered bioattacks over a week or two) as an example, we will investigate approaches that simultaneously minimize casualties and variation of resource utilities across all attacked sites, thus enabling a system-level "hardening." Sandia is uniquely positioned to address this problem given our resident infrastructural modeling and simulation expertise (National Infrastructure Simulation and Analysis Center [NISAC]) and recent LDRD work on the characterization of bioattacks from scarce data.

In a reload scenario, resource allocation will be performed soon after the detection of the first attack and in ignorance of the subsequent ones. Resource demand is the key uncertain quantity; however, it will become more deterministic with time. Resource allocation may be performed via "rationing" or a "market mechanism." The research element in the former approach involves modeling it as a problem of optimization under uncertainty, under the constraint that the variations in resource allocations (engendered by better demand characterization) be commensurate with transportation infrastructure capacities.

The "market" approach views cities and military bases as repositories of medical resources, with demand at attacked sites being met by surplus at the unattacked ones. The modeling challenge involves designing the market mechanism that facilitates the exchange and gauging their performance via agent-based simulations. Elements of mathematical research include characterization of the stochastic bid-and-ask streams (to determine whether the mechanism is inventory or information limited), their valuation, the calculation of equilibrium values of various measures of "market" (allocation) efficiency and the deviation of the dynamic behavior from them. Comparison of the two approaches will expose various facets/bottlenecks of the allocation problem, indicate sustainable resource allocation architectures and enable flexible and rapid response strategies.

Summary of Accomplishments

The project identified that certain combinations of the time between attacks, the epidemic and response time-scales could lead to situations where the allocation of resources under an uncertain characterization of the demand posed a challenging problem. Under such situations, the targets that conventional resource allocation techniques are designed to meet may not lead to desirable outcomes.

We devised a multistage, stochastic optimization scheme (with recourse) to perform the allocation. We first extended an existing, data-driven technique that reconstructs bioterrorist attacks to estimate resource demands as probability distribution functions (PDFs). The PDFs were used to generate posterior predictive runs to create an ensemble of possible evolutions of the epidemic ensuing from the attack. The optimization scheme was designed to provide a resource allocation that would lead to a peaked PDF of casualties, i.e., the resource allocation would, with high probability, yield an acceptable level of casualties while almost certainly eliminating the possibility of an extremely bad outcome. Traditional resource allocation schemes were seen to lead to fat-tailed casualty PDFs, wherein extremely bad outcomes had a small, but finite chance of happening.

Further, since the resource allocation technique was data-driven, allocations could be continuously refined as the resource demand crystallized over time.

The project also revealed that a “market-based” mechanism would not respond quickly enough (i.e., less than a week) to be of relevance in mounting a response.

The project initially intended to investigate bioattacks using noncommunicable diseases. However, toward the end of the project we extended it to address some of the resource requirements relevant to an epidemic of a communicable disease. The primary thrust was on obtaining demand estimates from patient data. Plague and influenza were investigated. Results with plague were surprisingly good; even with influenza, the demand estimates were within 20% of the correct result.

Significance

The proposal has direct ties to Sandia’s national security mission in homeland security threats. It seeks to develop an efficient and resilient resource allocation mechanism that is robust under demand uncertainty. The reload scenario of bioattacks is employed to stress both aspects of the mechanism. This project has the potential to identify sustainable response strategies for bioattacks by coupling new developments in inference techniques with NISAC’s infrastructural simulation expertise.

Active Coded-Aperture Neutron Imaging

117818
Year 2 of 3
Principal Investigator: P. Marleau

Project Purpose

There is an urgent national security need for systems that can detect special nuclear material (SNM) at great stand-off distances and/or when obscured by shielding. Because of their penetrating power, energetic neutrons and gamma rays offer the possibility of detecting shielded or distant SNM. Of these, fast neutrons offer the biggest advantage due to their very low occurrence in natural background. We are investigating a wholly new approach to fast-neutron imaging — an active coded-aperture system that uses a coding mask made of neutron detectors. Low-energy neutron sources have been imaged at short range with passive coded-aperture neutron detectors. However, only fast neutrons are likely to travel long distances without scattering, and the penetrating nature of fast neutrons limits the ability of passive coded apertures to modulate them effectively. Thus, the only previously demonstrated method for long-range neutron imaging is double-scatter imaging, but that method has limited detection efficiency. Active coded-aperture neutron imaging should be more efficient for improved detection speed, range, and sensitivity. This efficiency advantage is achieved by simultaneously imaging using both double-scatter and coded-aperture methods. In coded-aperture imaging, neutrons originating from different locations are very efficiently detected at the image plane as the superposition of aperture patterns. In double-scatter imaging, the incident angle and energy of any neutron that is detected in two or more different detectors can be determined. By simultaneously imaging using both coincident and anticoincident detection events, this new, dual design allows for high-efficiency imaging of sources of energetic neutrons and should lead to an instrument capable of locating SNM at a much greater distance than any existing instrument or technique. The project directly addresses a major national need in homeland security and assures Sandia leadership in a fast-neutron imaging.

Summary of Accomplishments

The first year of this project was focused on demonstrating the fundamental physics of the coded-aperture technique and determining the functionality and performance requirements of individual detectors. Based on the results of these efforts, Monte Carlo simulations were developed and calibrated against measurements in the laboratory. At the start of the project's second year, models of possible final detector designs were developed and some basic imaging algorithms were applied. The results are promising and indicate that reasonable imaging capabilities may be achieved.

Parallel efforts have been made toward exploring optimal detector cell designs and readout electronics. Our team has been working closely with developers at Mesytec, a manufacturer of electronics modules for applications with analog pulse shape discrimination (PSD) in liquid scintillators. Measurements made by our team with prototype detector cells have been crucial toward the development of a new eight-channel analog PSD module that will be used in the final project design. Several cell prototypes have been built and evaluated, and a final cell design was chosen that will allow maximal flexibility in the placement and orientation of the final detector. This will allow for several detector configurations to be explored easily in the third year of this project. The design concept is a reconfigurable array of identical bar type detectors read out by photomultiplier tubes on either end.

All mask cells have been fabricated, assembled, and evaluated. Pulse shape discrimination, decent lower energy thresholds (10-100 keV), and position resolution along the length of the bar (~1 cm) have been achieved. Construction and evaluation of initial active mask array configurations has been completed. These preliminary tests have confirmed that active masks can greatly enhance opacity and have produced the first ever images using coded aperture imaging.

Significance

Detecting hidden SNM is a central technical goal in the mission of DHS. In fact, detecting shielded and/or distant SNM is probably the highest priority of the DHS Domestic Nuclear Detection Office (DNDO). This project squarely addresses the SNM mission requirement.

High-Throughput Discovery and Validation of Biomarkers for Biodefense

117992
Year 2 of 3
Principal Investigator: G. S. Chirica

Project Purpose

Effective clinical diagnostics of early-stage exposure and infection to biowarfare agents are urgently needed to minimize exposure and to direct and monitor treatment. To date, no biomarkers have been identified to diagnose presymptomatic infection/exposure to pathogens or to monitor the efficacy of antimicrobial therapeutics. The lack of clinically actionable biomarkers is principally due to performance limitations of current methods for biomarker discovery and validation. Technical hurdles to surmount for effective biomarker discovery are primarily “needle-in-a-haystack” or biodiversity problems: 1) expected biomarkers are too dilute for accurate detection; 2) they must be picked out/isolated from complex sample matrices with thousands of similar compounds 11 orders of magnitude more abundant; 3) biomarkers’ differentiating features are often minute posttranslational modifications; and 4) host genetic and physiological variability creates large statistical backgrounds (extensive person-to-person variability). The candidate biomarkers, once identified, need to be rapidly validated in hundreds of preclinical samples for which standard immunoassays are cost prohibitive.

The focus of our biomarker research strategy is to develop and implement a set of high-performance analytical tools which are common to biomarker identification, verification/validation and constitute the basis for seamless translation to clinical assays. Revolutionary technological advances are realized by integrating modular automated processing system (MAPS) with mass spectrometry and newly discovered nanopore analysis methods to analyze multiple time-points serum samples from *Bacillus anthracis* (anthrax)-infected mice. High-throughput data will be processed using support vector machine classification and network modeling to identify candidates for biomarkers panel indicative of the stage of infection. Concurrently, we are developing higher-throughput, on-chip immunoassays to enable verification of several biomarkers simultaneously; these devices substantially improve the sensitivity, cost and speed of analysis making screening of large populations a reality.

Summary of Accomplishments

We developed and tested new modules for on-line processing of microliter-volumes of mouse serum. One module employs size-based protein fractionation for removal of high abundance proteins (HAP) that are larger than 50 kDa. This new approach to HAP removal has performance similar to immunodepletion (95% HAP removal), eliminates the 150-fold sample dilution, reduces the analysis time five-fold for a 200 µL sample, and costly immunodepletion materials are replaced with 100-fold less expensive size-fractionation packing. New modules tested this fiscal year focused on further separation/selection based on posttranslational modifications (PTM). Phosphorylation is the PTM most often encountered in signaling. We have set up a phosphorous enrichment module based on immobilized metal affinity chromatography (IMAC) using gallium as a chelating metal for selective and high-recovery enrichment of phosphorylated proteins. The 80 µL module enriches proteins and peptides and is readily integrated to the buffer exchange module to deliver purified, interferent-free microliter-samples. Glycosylation occurs in 50% of the proteins. We are currently testing a concanavalin A glyco enrichment module; nevertheless, our modular system can easily be extended to include up to 10 distinct lectin modules. This improves our chances to differentiate between anthrax exposure and other conditions with similar symptoms. As the molecular fractionation module maintains the total sample volume to microliters (rather than milliliters) we connected, downstream, the modules developed last year to test mouse serum samples.

We have established a rotary laser induced fluorescence scanning capability for high-throughput, low-cost immunoassay verification. The mechanical assembly and optical path was optimized for highly focused beam and accurate registration. The goals of spatial resolution, scanning frequency and optimization for high sensitivity were all achieved. Novel on-chip fractionation methods have been established for discrimination by isoelectric point as well as size.

Significance

Identification of early-stage biomarkers and high-throughput diagnostics will enable rapid/large scale screening of exposed/infected populations during bioterror/biowarfare attacks or outbreaks of naturally occurring infectious disease. Data generated using our high-throughput platform can provide biological insight into the immune response mechanism and enable therapeutics development. We published 3 papers, submitted 5 patent applications and 5 technical advances, presented 6 posters and 5 oral presentations at national and international conferences.

Refereed Communications

G.J. Sommer, A.K. Singh, and A.V. Hatch, “Enrichment and Fractionation of Proteins via Microscale Pore Limit Electrophoresis,” to be published in *Lab on a Chip*.

G.J. Sommer and A.V. Hatch, “Isoelectric Focusing in Microfluidic Devices,” *Electrophoresis*, vol. 30, pp. 741-757, March 2009.

A *C. elegans*-Based Foam for Rapid On-Site Detection of Residual Live Virus

130755
Year 1 of 3
Principal Investigator: C. Branda

Project Purpose

In the response to and recovery from a critical homeland security event involving deliberate or accidental release of biological agents, initial decontamination efforts are necessarily followed by tests for the presence of residual live virus or bacteria. Such “clearance sampling” should be rapid and accurate, to inform decision-makers as they take appropriate action to ensure the safety of the public and of operational personnel. However, the current protocol for clearance sampling is extremely time-intensive and costly, and requires significant amounts of laboratory space and capacity. Large numbers of samples may be required to achieve a high degree of statistical certainty, depending upon the physical dimensions of the contaminated area. The samples must then be transported to the lab for measurement of biological activity. Detection of residual live virus is particularly problematic and time-consuming, as it requires evaluation of replication potential within a eukaryotic host such as chicken embryos. We intend to revolutionize clearance sampling, by leveraging Sandia’s expertise in the biological and material sciences in order to create a *Caenorhabditis elegans*-based foam that can be applied directly to the entire contaminated area for quick and accurate detection of any and all residual live virus by means of a fluorescent signal. This novel technology for rapid, on-site detection of live virus would greatly interest the DHS, DOD, and Environmental Protection Agency (EPA), and hold broad commercial potential.

Summary of Accomplishments

We have established the laboratory infrastructure for working with RG2 viruses, as well as with the RG1 organism *C. elegans*. In progressing towards generation of *C. elegans* strains with increased susceptibility to viral infection, we found that *C. elegans* that are dying, or that have been infected with virus or bacteria, or that have been grown in liquid culture (one method for viral infection), display high levels of autofluorescence. To overcome this technical hurdle, we generated both Vesicular Stomatitis Virus (VSV), a model RNA virus with low human pathogenicity, and Rift Valley Fever Virus (RVFV) that express the red fluor mCherry. The mCherry-labeled VSV virus can infect *C. elegans* cells in culture, and we are currently developing a protocol for adult *C. elegans* infections. In addition to working with intact *C. elegans*, we have established a method for generating primary *C. elegans* embryonic stem cells in culture. We were able to use these cultured cells to identify media conditions that promote viral infection using our original green fluorescent protein (GFP)-labeled VSV; preliminary results suggest that a low pH shock (of pH 5.1) results in a higher rate of viral infection of the cultured cells. In addition, we have constructed first-generation cellular reporters of VSV and RVFV infection.

Significance

The critical need for improved methods of clearance sampling of biological agents has been emphasized by both the DHS and EPA. Our revolutionary technology for clearance sampling will be substantially faster and cheaper than state-of-the-art culture-based techniques, and will address multiple mission elements by facilitating response and recovery efforts following biological attacks on US interests here and abroad.

Deployable Pathogen Diagnostic System

130756
Year 1 of 2
Principal Investigator: A. Hatch

Project Purpose

No field-deployable devices for monitoring pathogen infection exist, even though the need is recognized. "There is a need for rapid, highly sensitive, specific, easy to use, adaptable, and cost-effective medical diagnostics for . . . laboratories, and point-of-care use to diagnose individuals exposed to and/or infected with priority pathogens or their toxins . . . so appropriate therapeutic intervention or containment can be executed" (source National Institutes of Health [NIH] website).

While Sandia has considerable experience developing deployable field-monitoring systems, the requirements are much different for medical diagnostic systems needed to monitor pathogen infection/exposure while conforming to Food and Drug Administration (FDA) requirements. We have demonstrated that Sandia's unique microfluidic diagnostic platform meets key performance criteria (rapid, specific, sensitive) but the platform has not progressed beyond a bench-immobilized system that only highly trained technical staff can utilize. We have also been constrained from demonstrating diagnostics for priority pathogens since the current format cannot be deployed in a biosafety cabinet to satisfy biosafety level (BSL)-2 containment on-site, nor can it be deployed at collaborating institutions that also include BSL-3/4 containment needs.

This effort focuses on a systems engineering approach to manufacture and refine a robust and deployable prototype system that facilitates collaborative research and development for diagnostics of priority pathogen infection. A modular first-generation prototype system was designed and built this year. The prototype will be tested in BSL-2 labs at Sandia and BSL-3 facilities at the University of Texas Medical Branch (UTMB) for evaluation and refinement during year 2, to realize a field-deployable device ready for field assessment by the end of year 2. Realizing a functional prototype is key to further develop the platform for priority pathogen diagnostics, and eventually, widespread deployment.

Summary of Accomplishments

A powerful and yet flexible generation 1 system architecture was designed, built and integrated. The modular elements can be updated as technology progresses or requirements change without requiring a redesign of the full system. A number of the modular system control elements are novel and valuable to microfluidic platform technologies in general. The high-voltage (HV) and fluidic distribution board in particular pushed the envelope for a highly multiplexed interface between the portable system and an easy-to-replace microfluidic cartridge. This module will be leveraged in the 2010 "RapTOR" Grand Challenge LDRD project. The cartridge technology itself is attractive for ultimate ease of use and disposability via manufacture suited for low-cost mass fabrication techniques. The analysis cartridge is designed to simply be dropped in place with magnetic latching (with design guides and registry) on top of spring loaded electrical contact pins and compressed gasket fluidic ports.

Other technical hurdles for realizing the first-generation system have been met including a CPU board capable of overall system control, rotary scanning and laser-induced fluorescence (LIF) detection module design, updates to HV and fluidic pumping and valving boards for compatibility, and a touch-screen graphical user interface framework with basic command and device operation infrastructure.

In addition to the more-focused technical achievements, the overall system features meet the desired goals of utility in BSL2-4 settings and field deployability. By meeting these milestones, the level of risk is substantially lower moving forward and the lab testing and refinement process will begin in these desired lab settings early in FY 2010.

Significance

This work is crucial for continued development of solutions to biological weapons and infectious disease concerns in Sandia's Homeland Security and Defense (HSD) strategic management unit (SMU). Bringing prior investments in platform development to fruition requires deployability to ultimately contain and mitigate outbreaks/attacks. The system will also bolster capabilities at Sandia to demonstrate meaningful test results and studies of infectious disease with priority pathogens by satisfying BSL-2 or greater containment criteria. The high-throughput analysis capabilities of this system are attractive to a number of external customers in the areas of infectious disease and biothreats. Notably, the National Biodefense Analysis and Countermeasures Center (NBACC) is interested in evaluating a deployable system to meet their homeland security mandate in the area of forensic analysis of potential biotoxin samples. Lovelace Respiratory Research Institute is interested in the platform technology to bolster their research efforts in basic research on biological mechanisms of actions of toxins including inhalation animal models. This system will also be leveraged for the Homeland Security and Defense SMU investment in the area of radiation biodosimetry.

Development of an Explosive Materials Threat Assessment Tool

130759
Year 1 of 2
Principal Investigator: F. A. Bouchier

Project Purpose

A bewildering array of explosive materials can be used to carry out a wide variety of illicit acts. One recent study conducted at Sandia identified approximately 300 explosive materials that might be considered realistic threats. Since the best approach to explosive detection often depends upon the type of explosive, decision-makers tasked with protecting facilities or airplanes against explosive threats require information on the types of explosive materials that are most likely to be utilized. There is at present no good source for such information. The purpose of this project is to develop a computer-based assessment tool that would allow decision makers to obtain such information by answering a series of questions about the nature of the threat being considered and the specific facility or object they are tasked with safeguarding. Different threats that could be assessed would include large vehicle bombs, mail/package bombs, airplane bombs, and small bombs planted by a perpetrator. The output of the tool would be a prioritized list of explosive materials — each given a numerical score — that would be most likely to be used to carry out the threat based upon considerations such as the mass of the explosive needed, the availability of the explosive or the materials required to make it, the explosive power of the material, the availability of knowledge to construct a functional explosive device, security equipment and procedures already in place at the facility in question, cost of the explosive or starting materials, etc. If not known, the explosive mass required to carry out a threat will be calculated using blast modeling capabilities incorporated into the tool.

Summary of Accomplishments

1. Developed extended database (approximately 120 materials) of explosive materials with explosives scored for several attributes, including: ease of obtaining explosive or starting materials, ease of synthesis, safety of synthesis and handling, availability of knowledge to make a functional device, cost per pound, prior use by terrorists/adversaries, difficulty of detection, and explosive power.
2. Developed scoring criteria for the relative importance of these attributes to large vehicle bomb (LVB) and aviation bomb scenarios using the well-known analytic hierarchy process.
3. Ranked 120 materials for use in aviation scenarios.
4. Ranked 20 materials for use in the LVB scenario.
5. Developed software to manipulate the above databases so that scoring of attributes for all materials can be changed easily and systematically. This provides users with insight into the effects of alterations to the scoring criteria.
6. Presented the ranked listing of materials for the aviation scenario to the Department of Homeland Security, the Transportation Security Administration, and the Technical Support Working Group international working group for home-made explosives.
7. Developed probability of detection database for various explosives, covering a diverse set of detection techniques. We also performed uncertainty analysis of how model outputs vary with variations in p(d) inputs and wrote a report on this topic.
8. Developed database of estimated TNT blast equivalence for approximately 87 explosive materials, including novel and homemade explosives and ideal and non-ideal explosives.

9. Developed tables of damage estimates for various construction types as a function of impulse quantity, using glass panel threshold of injury for unhardened structures and single-degree-of-freedom dynamic response for hardened structures.
10. Established a group of prospective end-users (DOE security personnel) with whom we will work early in FY 2010 to test our first-order tool.
11. Developed software that integrates all of the above into a first-order tool.

Significance

Protecting facilities or airplanes from illicit attacks employing explosives is important to a number of key federal agencies such as the Department of Homeland Security, Federal Bureau of Investigation, Department of Energy, and Department of Defense. This computer-based assessment tool will help these agencies do that by providing critical information on what explosive materials pose the greatest threats. It can also help identify explosive materials that require further study.

Intrinsic Security Principles

130760
Year 1 of 1
Principal Investigator: A. Walter

Project Purpose

Current security system design and analysis methods are based on a collection of best practices that center upon the cornerstone principle of "timely detection." However, the timely detection principle is becoming increasingly fragile in the face of highly advanced modern threats. Recently, the term "intrinsic security" has gained recognition as an important principle of future security systems solutions in a variety of domains. Yet, while many agree with the general concept of intrinsic security, a lack of a common understanding of both its fundamental principles and a working-level definition of the term itself leads to suboptimal domain-specific solutions. These obstacles create an approach to security design/analysis that is inconsistent across domains such as nuclear weapon design, physical security, infrastructure security, cyber security, food security, etc. These problems may be remedied by a thorough examination of methods and core principles in the various security domains, exploration of underlying principles and methods in the more mature safety field, identification and articulation of intrinsic security definitions and principles that cross-cut all domains, and trial application of the resulting principles and definitions to several real-world problems. This project will seek to create working-level definitions and principles that form the foundation of "intrinsic security," develop a rudimentary security design and analysis methodology based on them, and apply the methodology to real-world problems of interest.

Summary of Accomplishments

We analyzed methodologies and principles across five security/safety domains to discover first principles of security. Based on this work, a definition for "intrinsic security" and its core principles was developed. With the principles defined, a methodology was drafted that can be used to guide security designers assuring a robust, secure system. The methodology was applied to two classified nuclear weapons problems. The analysis of the problems demonstrated the potential of the methodology to uncover issues rapidly and comprehensively.

We demonstrated that taking this approach can, at minimum, identify inconsistencies across domains and identify suboptimal designs within specific domains. This approach may provide remedy for these situations since the process may demonstrate potential activities to leverage one domain to support another.

Significance

Developing intrinsic security principles advances Goal 1 from the DOE Strategic Plan, "Nuclear Weapons Stewardship," and the DHS Strategic Goal related to protection, which seeks to "Safeguard our people and their freedoms, critical infrastructure, property and the economy of our Nation from acts of terrorism, natural disasters, or other emergencies." The use of intrinsic security principles should lead to security designs that take into account the entire system in order to improve security performance, robustness, and efficiency.

This project will be able to leverage "intrinsic security" as a differentiating Sandia specialty, and apply a consistent intrinsic security methodology across all programs and customers. With a more rigorous foundation and consistent application, it could become the vehicle that allows us to more easily integrate and communicate among the disparate domains.

Nontoxic, Noncorrosive Approach for Decontamination of Anthrax Spores in Critical Infrastructure

130761
Year 1 of 2
Principal Investigator: M. D. Tucker

Project Purpose

Bacterial spores (e.g., *Bacillus anthracis* [anthrax]) are some of the most resistant forms of life and are several orders of magnitude more difficult to kill than their associated vegetative cells. Consequently, remediation of facilities contaminated with anthrax spores (e.g., the Hart Building) requires the use of highly toxic and corrosive chemicals such as chlorine dioxide gas and vaporous hydrogen peroxide (i.e., a 35% concentration of liquid hydrogen peroxide deployed in vapor form). Even the much less corrosive, Sandia-developed DF-200 formulation utilizes an oxidative chemistry that will not be suitable for certain applications such as the interior of aircraft and extremely sensitive equipment. We will demonstrate a new approach for killing anthrax spores using very mild chemicals. Sandia has recently developed a mixture of chemicals that triggers the germination process in bacterial spores and causes those spores to rapidly and completely change to the much less-resistant vegetative cells. We will use this mixture of chemicals to rapidly germinate highly-resistant bacterial spores to vegetative cells which will then be exposed to mild chemicals (low concentrations of hydrogen peroxide, quaternary ammonium compounds, alcohols, aldehydes, etc.) or natural elements (heat, humidity, ultraviolet light, etc.) for complete kill. This method could be used to kill spores on a contaminated surface, as a "fumigation" method where the germination formulation and kill formulation will be introduced sequentially as a fog/mist for facility decontamination, and as a method to decontaminate sensitive equipment. This approach will potentially result in a faster, cheaper, and much less destructive decontamination method. The method will be noncorrosive and require no safety controls beyond what is required to minimize exposure to the biothreat agent itself. It will also not require the use of specialized, expensive equipment and will allow our nation to quickly and efficiently recover from the release of a biothreat agent.

Summary of Accomplishments

In FY 2009, we developed an optimal formulation for germination of bacterial spores to vegetative cells. We identified anthrax surrogates to use and obtained stocks (*B. subtilis, B. thuringiensis, B. cereus,* and *B. atrophaeus*). We first investigated a rapid germination formulation as a starting point for experiments by conducting a thorough literature review and consulting an established microbiologist in this area. We then developed an experimental plan and conducted laboratory analysis using a variety of potential germination formulations. Effectiveness of the formulations was tested by staining methods, flow cytometry, and culturing. Through the experimental approach, we were able to identify a germination formulation that is highly effective at germinating bacterial spores. A mild kill formulation was also identified which consisted of a very low concentration of hydrogen peroxide. The kill formulation is capable of killing the vegetative cells after they have been converted from spores by the germination formulation. In-vitro and surface decontamination tests were conducted using a sequential application of the germination formulation followed by the mild kill formulation with good results.

Significance

A key need for the Department of Homeland Security is to develop capabilities to rapidly recover from releases of biothreat agents to minimize economic damage to the US. Decontamination of critical infrastructure (airports, subways, ports, urban areas, etc.) is a key element of that capability and, at present, only toxic and/or corrosive chemicals are available for this need. This method will provide a safe, rapid, inexpensive, noncorrosive, and nontoxic approach to meet this need.

Risk-Based Security Cost-Benefit Analysis Tool

130762
Year 1 of 2
Principal Investigator: G. D. Wyss

Project Purpose

Traditional approaches to risk-based cost-benefit analysis are difficult to apply to security assessment problems. Problems include reliance on linear utility theory, aggregation of disparate consequences, difficulties predicting attack likelihood, and lack of scalability to large "systems of systems." Thus, security budgets are often allocated by gut feel, as noted by Admiral Mies (2002) and the Hamre Commission (2004). This project builds on prior NNSA and Sandia LDRD work to develop a scalable risk-based security cost-benefit analysis tool. We will recast Kaplan's risk triple to replace "scenario likelihood" with "adversary resources needed for success" in order to reflect established adversary planning behaviors. The cost-benefit tool will be developed using two techniques: (1) aggregating quantitative consequence and adversary resource estimates along an optimal attack frontier whose movement serves as the cost-benefit metric, and (2) extending the revised risk triple using linguistic and approximate reasoning techniques, combined with belief/plausibility theory, to model adversary decision-making methods. These will result in implementation requirements for Sandia's production-level security risk assessment software tools (e.g., ATLAS, DANTE). Many existing obstacles to risk-based security cost-benefit analysis derive from the requirement to understand scenario likelihoods in order to develop unconditional risk estimates. Reformulating Kaplan's risk triple may overcome these obstacles. Since this would modify the basic underpinnings of risk theory, it is more appropriate for funding by LDRD than by individual customers. The resulting tool will enable risk-based security resource allocation both locally and across facilities, leading to cost-effective security across disparate targets and infrastructure systems and can enable security cost-benefit tradeoffs during for weapon life extension programs.

Summary of Accomplishments

In keeping with project plans, the project team developed an extensive list of reference adversary and cost-benefit methods, with brief descriptions and references. A 29-page document completed this deliverable. A parallel activity examined how proposed enhancements to the definition of security risk would affect security risk calculation methods. The team developed a 46-page paper describing the mathematics of such a risk formulation using quantitative and linguistic representations of adversary resources for both point-estimate and uncertainty analyses. Both probabilistic and belief-plausibility uncertainty analysis methods were addressed in the paper. The paper also builds a foundation from which the "attractive scenario frontier" method can be developed.

The project team also demonstrated coupling between genetic optimization methods and the Dante combat simulation tool. This provides confidence that it is feasible to use Dante to estimate the adversary resources required for success in a specific attack scenario, providing important insights for our FY 2010 activities.

The project team has begun work to develop a method to rank and compare the adversary resources required to successfully produce objective consequences from postulated attack scenarios. A workshop is planned to gather insights from diverse experts on adversary attack planning methods and scenario resource utilization/scenario attractiveness. This guidance will enable the project team to develop its prototype method to compare scenarios based on adversary attack resource requirements. This method will ultimately be refined through application to example problems and continued dialogue with subject matter experts.

Concurrent with this LDRD project, Congressional language tasked NNSA to justify recent and planned security investments. As a result of Sandia's participation in this tasking, our LDRD team members had the opportunity to study DOE's security investment process. We provided the Congressional tasking team with results and insights toward a new objective security investment prioritization process. The insights and process were enthusiastically received by NNSA.

Significance

A risk-based security cost-benefit tool advances DOE Strategic Theme 2, Nuclear Security (Goal 2.1), and the DHS Strategic Goal related to protection, which seeks to "Safeguard our people . . . from acts of terrorism." The resulting tool will satisfy stated needs from DOD, DOE and DHS by enabling decision-makers to perform risk-based security resource allocation both locally and across facilities, leading to cost-effective security across disparate targets and infrastructure systems.

Target Detection and Tracking in Cluttered Environments using Rapidly Deployable VPED Sensor Networks

130763
Year 1 of 2
Principal Investigator: H. D. Nguyen

Project Purpose

The ability to robustly detect, localize, and track multiple human targets in uncontrolled, cluttered environments (e.g., forested areas) is a difficult and unsolved problem in virtual presence extended defense systems (VPEDS). The two main difficulties to overcome are the wide range of operational environment conditions which cause excessive nuisance alarms and the inability to rapidly deploy these systems without time consuming calibration and testing. These difficulties contain subsets of obstacles which require the development of new algorithms. These new algorithms must be realizable in a deployed unit in varying environmental conditions that range from deserts to rain forests with an operational constraint on power. In order to address the challenge of rapid deployment, the algorithm approach must address issues such as rapid real-time installation and configuration of the system with a constraint on limited infrastructure. While these two categories appear independent, they share key enabling elements such as self-calibration and real-time vulnerability assessment. Each functional element will require the development of data aggregation algorithms that can infer detection volumes based on signal propagation and an associative algorithm that can, in near real time, assess and provide a vulnerability map. Specialized operations that require the same fidelity of situational awareness but with added mobility (i.e., ability to rapidly move the situational awareness perimeter) would benefit to an even greater degree. The payoff would be increasing system adaptability in varying terrains and providing an order of magnitude reduction in time to assess vulnerabilities by combining the installation and performance testing phases into one single action. In this concept, the actions and signatures from the blue force deploying the system would be used to generate a near-real-time detection image of the area of deployment.

Summary of Accomplishments

- Defined data architecture
- Defined/developed/implemented using real sensor data by post processing with our algorithms
- Defined visualization needs
- Completed initial data collection and have planned out 2nd year data collection efforts
- Invention disclosure / patent application (in progress)
- Presented results at Institute of Electrical and Electronics Engineers (IEEE) conference in June

Significance

This research will create capabilities that will protect our national security by providing world-class scientific research capacity, advancing scientific knowledge and engineering excellence in the field of sensor technology for surveillance and reconnaissance applications.

Uncooperative Biometric Identification at a Distance

130764
Year 1 of 3
Principal Investigator: K. R. Dixon

Project Purpose

One of the greatest challenges facing the security of public facilities and infrastructure is the rapid identification and verification of persons of interest. The problem becomes especially acute when considering that some subjects have a motivation to be deceptive or otherwise uncooperative toward identification. Some domains require a high degree of accuracy, such as granting access to a secured building or sensitive area for force protection or virtual presence and extended defense applications. Other domains require high throughput and recognition at a distance, such as the Department of Homeland Security's Transportation Safety Administration airport screening and Immigration and Customs Enforcement. This project aims to create a high-accuracy, high-throughput biometric identification system that works with both cooperative and uncooperative subjects and at multimeter distances.

The human iris is one of the most promising avenues for biometric identification for several reasons. First, the iris is believed to be one of the most stable, unique biometric measurements throughout the course of an adult's life; the iris does not change as a subject ages and is extremely difficult to alter. The project will explore new research and development with Sandia's expertise in adaptive optics and Microelectromechanical systems (MEMS) mirror arrays with research at Carnegie Mellon University, leveraging their state-of-the-art iris identification and facial-pose correction algorithms. The integrated system will provide a high-accuracy, high-throughput, multimeter distance iris recognition of both cooperative and uncooperative subjects. We will work closely with Sandia's force protection groups to validate the performance of the proposed system with human-subjects data and verify its capabilities in mission-relevant scenarios.

Summary of Accomplishments

In the first few months of the first year of the project, we have already demonstrated a multimeter iris-recognition system (up to four meters) for cooperative subjects in our laboratory using Sandia-created hardware and commercial off-the-shelf (COTS) iris-matching software. Using unique adaptive polymer lens technology and Sandia-developed autofocus, we have demonstrated an unprecedented depth-of-focus (1.5 meters) for the recognition system. We have shown very promising results using standard near-infrared enrollment of subjects and then recognition at multimeter distances with a standard charge-coupled device (CCD), which is crucial to the success of long-range iris recognition. We have already published one paper deriving from first-principles the need for adaptive optics for iris recognition for very long ranges.

Significance

The project ties to the DOE mission of "the development and deployment of technologies to replace costly and manpower-intensive physical protection strategies," and can be used to secure sensitive facilities with a standoff biometric identification of potential threats. This research addresses an acute need of the Department of Homeland Security to create a high-volume biometric identification system to protect public infrastructure and ensure continued public confidence.

Refereed Communications

J. Choi, G.H. Soehnel, B.E. Bagwell, K.R. Dixon, and D.V. Wick, "Optical Requirements with Turbulence Correction for Long-Range Biometrics," SPIE, April 2009, *Biometric Technology for Human Identification*.

Vulnerability of Multinetwork Infrastructure to Cascading Failure: Design of Robustness to Orchestrated Attack

130766
Year 1 of 3
Principal Investigator: R. J. Glass Jr.

Project Purpose

The US critical infrastructure is a network of dynamically interacting systems designed for the flow of information, energy, and materials. Experience has shown that under certain circumstances, particularly targeted attack, disturbances can cause cascading failures within and between infrastructures that result in significant service losses and long recovery times. Existing infrastructure models focus on physical components, but human behavior is essential in both controlling infrastructures during normal and unexpected conditions, and in creating the demands that infrastructures serve. This project will extend Sandia's existing infrastructure modeling capabilities by: 1) addressing interdependencies among networks, 2) incorporating human behavior models into the network models, and 3) providing mechanisms for understanding vulnerability to targeted attack. These aspects are not currently addressed in network models individually or in combination. We will apply this capability to evaluate the robustness of existing infrastructure systems against attack, and to identify changes in design and operation that will decrease the chance of large-scale disruption. The models provide a toolkit for analyzing for cascading failures in interacting networks so that the risk can be adequately mitigated. This capability has relevance within the National Infrastructure Simulation and Analysis Center (NISAC) and to DHS, as well as potentially any other system-of-systems that can be modeled as networks such as DOD logistics and net-centric operations. With modifications, the results of this project may also apply to analysis of physical and cyber security systems and lay the foundation for developing advanced security solutions that include autonomous triage and augmented cognition for infrastructure control systems.

Summary of Accomplishments

During the past year we have, (1) elaborated use cases, (2) developed multinetwork interdependence modeling capabilities, and (3) implemented behavioral representation of entity interaction.

Critical infrastructure at the national scale is the primary use-case with which we will develop and exercise our complex adaptive system of systems (CASoS) approaches. This enables us to implement and refine interdependence and behavior on a reusable, reality-based example. Briefly, this use case consists of connected components which interact among the interdependent infrastructure systems. Households are hierarchically grouped based on demographic data. Each infrastructure network (e.g., fuel, electric, communication, food, emergency services) interacts differently with households. We have also identified and articulated follow-on "stretch" use cases including warring Mexican drug cartels and migration of new virulent infectious diseases.

Concurrently we have implemented interdependency modeling capability. Interdependency is modeled as entities and networks exchanging resources. Key entity characteristics include inventories of resources, the number of connections to sources of inputs and users of outputs, and policies for searching for alternative sources and users.

We have implemented three models of entity interaction and adaptation. These models are based on decision theory, classifier systems, and a novel causal network. We are also investigating cognitive behavior models to apply to human entities.

Significance

This project will demonstrate a capability to model, including human dependencies, interdependent complex adaptive systems of systems such as US infrastructures, security systems, and net-centric warfare concepts. The project will also develop methods evaluating the human in task functions so as to optimize responses. Systems utilizing this technology will be resilient to both random and targeted disturbances, and recovery to full operational capacity will be easier, cheaper, and faster.

QCL for Standoff Explosives Detection

138733
Year 1 of 1
Principal Investigator: L. A. Theisen

Project Purpose

The purpose of this project was to investigate quantum cascade lasers (QCLs), a rapidly maturing technology, for application to standoff explosives detection. QCLs are the only semiconductor laser that can operate at room temperature at wavelengths in the mid-infrared range between 3 and 15 µm. This wavelength spectrum is important because vibrational adsorption lines within this range can specifically identify all molecules. QCLs are currently used as an excitation source for optical and photo-acoustic spectrometers. When applied to standoff detection, QCLs have been shown to detect chemical warfare agents where the signature is very large. For standoff detection of explosives where the signature is small (i.e., fingerprints), limited work has been reported. QCLs offer significant advantages over conventional IR lasers when considered for standoff detection. This feasibility project investigated emerging detection technologies utilizing QCLs to understand their potential application to standoff explosives detection.

Summary of Accomplishments

The following was accomplished during the research of QCL for optical standoff detection:

- Conducted an internet search of leading scientific and research institutes to survey the existing knowledge base of QCLs.
- Assembled and analyzed the scientific and technical papers on the subject of QCLs.
- Determined the systems equation that describes the application of optics to standoff detection that governs the application of QCL to standoff detection:
  $$n_x = P_i/h\nu \cdot \sigma_x \cdot c_x \cdot \Delta L \cdot Q \cdot S_o/r^2 \cdot \tau \cdot \eta.$$
  The equation describes the interrelationship between the initial photon energy from a laser, $P_i/h\nu$; the atmospheric adsorption, σ_x; the concentration of explosives, c_x; the spatial resolution of the laser, ΔL; the re-emission of the photons resulting from interaction with the explosive, Q; the area of the collected return signature, S_o/r^2; the characteristics of the receiving optics, τ; and the efficiency of the photon detector, η. All of these factors contribute to the final photon count that can be obtained, n_x.

Using the systems equation it is possible to identify the factors that can be influenced through further technology development. These include:

1. initial photon energy, $P_i/h\nu$
2. spatial resolution, ΔL
3. return signature, S_o/r^2
4. receiver optics, τ
5. photon detection, η

Areas of specific improvement to the application of QCLs include developing smaller source packages, wavelength tunability, robustness, and the elimination of cooling requirements. For optical standoff, in general, the following research and development is needed:

- Refined photon sources that address $P_i/h\nu$ and ΔL.
- Room temperature detectors, such as metamaterials, specifically designed for the wavelengths of interest to increase signal-to-noise that address η.

- Systems engineering in the design of a complete detection system that reduces volume and weight for portable applications.

Significance

This project will benefit DOE and DHS missions by investigating new technologies for application to standoff explosives detection. Explosives are the weapon of choice for many terrorists because explosives are easily transported, readily available, and cause significant property damage or loss of life. Sandia can contribute in the development of QCLs with broader wavelength tunability, and could perform systems engineering in the design of a complete detection system.

Sensor Integration for a Shallow Tunnel Detection System

138949
Year 1 of 1
Principal Investigator: M. L. Yee

Project Purpose

During the past several years, there has been a growing recognition of the threats posed by the use of shallow tunnels against both international border security and the integrity of critical facilities. This has led to the development and testing of a variety of geophysical and surveillance techniques for the detection of these clandestine tunnels. The challenges of detection of these tunnels arising from the complexity of the near surface environment, the subtlety of the tunnel signatures themselves, and the frequent siting of these tunnels in urban environments with a high level of cultural noise, have time and again shown that any single technique is not robust enough to solve the tunnel detection problem in all cases. The question then arises as to how to best combine the multiple techniques currently available to create an integrated system that results in the best chance of detecting these tunnels in a variety of clutter environments and geologies. The proposed work will survey the strengths and weaknesses of the existing techniques and develop a sensor system architecture that best optimizes the ability to detect both the construction and use of these clandestine tunnels.

Summary of Accomplishments

An analysis approach using the system engineering method of Taguchi analysis was developed to determine the optimal combination of sensors for tunnel detection, based on the physics of the sensor phenomenology along with environmental and tunnel characteristics. This approach was tested using the specific sensor modes of passive and active seismic, passive electromagnetic, and gravimetry. The results indicate that the optimal combination of sensors can be determined with this approach once the environmental clutter level is accurately characterized. This has implications for future work, indicating that it is critical to measure environmental clutter at potential sites prior to determining the suite of sensors that should be deployed. Once the clutter is characterized, this approach can be used to determine the suite of sensors. This approach can easily be extended to other sensors in addition to those used in this study.

Significance

This work will support our mission for homeland security and defense, and may also be potentially useful for security of special nuclear or other secure sites against illicit tunneling activity.

Defensive IO: Understanding and Modeling of Hybrid Threats

139186
Year 1 of 1
Principal Investigator: K. B. Vanderveen

Project Purpose

Sophisticated adversaries seeking to maximize damage to facilities and infrastructure will likely use a hybrid attack, in which multiple attack modes (physical, cyber/information, electromagnetic/electronic warfare (EM/EW), and insider) combine to more effectively disable defenses. Critical facility and infrastructure protection increasingly relies on information technology (IT)-based defensive sensor networks, data fusion systems, and communication networks to detect physical intrusions. An adversary may disable these IT systems through cyber or EM/EW attacks to enable a physical attack that destroys the target's functionality. Attacks may occur from one mode, or from multiple modes simultaneously or in a sequential manner. Security concepts for individual attack modes have been examined, but there has been less rigorous study of hybrid attacks (combinations of different paths, different ordering and timing, etc.), with the exception of work at Sandia, which considers combined cyber/physical attacks. Sandia has a well-established analysis capability in physical security (including insider threat) and is developing strong capabilities in cyber and infrastructure protections. Sandia also understands EM/EW attack methods. What we lack is the capability to analyze multiple combined threats where timing and order have a much stronger influence on potential damage and loss of mission. Previous work illustrates that there is greater uncertainty regarding cyber (and possibly EW) threats than physical threats. Therefore, coping with uncertainty in the threat space is necessary for a successful analysis methodology. Rather than viewing a hybrid threat as a summation of multiple individual threats, we will build on existing cyber and physical security methodologies to develop a mathematical and conceptual framework for understanding and protecting against hybrid threats holistically. This framework will enable comparison of risk and degradations to mission success across multiple attack modes simultaneously and in the presence of uncertainty, and facilitate follow-on studies to improve understanding of interactions among different attack modes.

Summary of Accomplishments

We have identified promising areas for future research, especially application of design of experiments methodology from statistics to the problem of determining where, in a security system addressing both physical and cyber threats, we can invest in additional components (or enhancements to functionality of existing components) to have the greatest reduction in our uncertainty of the response of the system to attack. Another promising area we have identified for future research is the need to capture the graph of interdependencies between different aspects of the security system, both physical and cyber, and interdependencies of components of the security system with the mission of the asset that the system is defending.

In addition, we have identified a promising candidate mathematical structure with which to express the problem of hybrid physical/cyber threats, and from which we can optimize design of security systems to maximize the expected protection given to the mission of the asset being protected. This structure is a graph in which different functions of the security system and functions of the asset being protected that relate to the asset's mission are represented as nodes of the graph. Edges in this graph represent interdependencies between the various nodes, i.e., one component of the security system may rely on correct functioning of other components, and may in turn be relied on by components of the protected asset. Each node has associated with it an assessed probability of correct functioning against a class of adversarial threats, and using methods from Bayesian statistics, we can compute overall probabilities of damage to asset mission given certain attacks. We can also compute uncertainties for these damage probability estimates. Future work (for other LDRDs or funded projects) would consist in generalizing these methods to full-fledged graphs (right now they only work for trees) and applying them.

Significance

The protection, security and surety of critical DOE assets, facilities and personnel have long been a part of the DOE and Sandia's national security missions. The expertise developed to accomplish this has also been applied to numerous other US governmental agencies and expanded to threats far beyond physical attack and theft. This work is aligned with these long-standing DOE and Sandia missions by supplying new concepts and tools for enhanced overall protection planning and methodologies.

Large-Scale Structural Armor Development using High-Performance, Cost-Effective Materials

139351
Year 1 of 1
Principal Investigator: K. J. Fleming

Project Purpose

There is a growing need for structural armor protection technologies to protect assets from acts of terror that employ explosives. Homeland Security Presidential Directive (HSPD) 19 addresses counterterrorism efforts that use explosives as a means of attack on the Homeland and related assets. HSPD-7 involves the "Infrastructure Identification, Prioritization, and Protection" from explosives-related threats and attacks. One large component of Homeland Security is the protection of federal buildings, refineries, power plants, and other critical infrastructure assets, by using building standards and materials capable of resisting blast effects (pressure, fragmentation, and progressive collapse). Additionally, all new federal building guidelines require the assessment and commensurate upgrades to resist blast effects from IEDs (improvised explosive devices).

Currently, large-scale structural armor is typically cost prohibitive, too heavy for taller structures, or lacks adequate blast analysis. Using traditional blast analysis codes are not optimal when applied to non-homogeneous materials such as concrete, masonry, or other mixes that are found in the building industry.

This effort focuses on a study to create a predictive software tool that integrates the use of novel materials that can be used on a large-scale manufacturing platform to provide good blast protection without prohibitive cost. These materials are low cost, commercially available, and usable by larger manufacturing facilities in their current plants. Additionally, blast model development to validate the new armor material is desirable for cost versus performance criteria.

Summary of Accomplishments

This project evaluated the predictive capabilities of nontraditional blast response material. This included the design, analysis, and blast response model for structural armor, and related science. The ability to rapidly design, then create test panels (at a composites fabrication company) was also assessed for effectiveness. Lastly, proof-tests of best-performer panels were performed, then analyzed to determine Sandia's blast model accuracy. The blast model correctly predicted test panel performance, using very low cost materials and fabrication techniques that can be scaled up for large scale manufacturing processes.

Overall, the concept to finished test samples was less than 4 weeks, once the materials, target dimensions, and realistic possibility of fabrication were determined. Autodyne code accurately predicted the "no spall" response for the optimal blast resistant composite design, which taught us the value of rapid modeling/test validation. The materials also met the goals of this project in that they were low cost, easy to use in a large-scale fabrication environment, and provided a minimal environmental impact for fabrication/transportation. Perlite-entrained concrete also exhibits significant R-value (approximately 1.5/inch), and has excellent fire protection for underlying structural members and walls, as used in building construction. Additional criteria for a visible overlay are that the protective structure should be both aesthetically pleasing, and should not look like an up-armored application.

The test series, although brief, confirmed blast code predictions, in that spall size and velocity in the control samples were significant, and potentially lethal from a small detonation (5 lb) source. Additionally the best performer (steel sheet/perlite) protected the underlying concrete from shock overpressure by absorbing and compressing under shock loading of approximately 23,000 psi.

Significance
This effort relates to Homeland Security Presidential Directives HSPD-14, and HSPD-19, which are concerned with mitigating the effectiveness of terrorist acts on our homeland. Potential attacks include the use of explosives in, or on structures that have little or no blast/fragmentation protection. This project evaluates/develops methods and predictive models for cost effective structural armor. This technology could be used by large manufacturers of building materials, which in turn protects buildings at threat.

Development of a System Design for Remediation of Chemical Weapon Bunkers in Iraq

141375
Year 1 of 1
Principal Investigator: B. L. Haroldsen

Project Purpose

Buried chemical weapons present an ongoing safety and health hazard; they are a major threat to the environment; and they provide a potential source of material for terrorists. The problem exists in the US, which has six large burial sites, as well as in other nations. Iraqi chemical weapon bunkers at Al Muthanna, which were bombed and severely damaged in the first Gulf War, were sealed because the munitions were deemed too damaged to destroy with the technologies then available. In China, about 700,000 abandoned Japanese chemical munitions were buried in the Haerbaling District of Jilin Province following World War II. There are few records about what was buried at any of these sites, and the condition of the munitions and chemicals is unknown. Remediation will require a system-of-systems approach to deal with all aspects of the problem including locating, recovering, characterizing, and destroying the munitions; monitoring and containing the chemical and explosive hazards; and decontaminating the site. Technologies exist to deal with various aspects of the problem, but major pieces are lacking. Technologies are needed to rapidly recover and remove large numbers of munitions, destruction methods must be faster, and multi-agent chemical detectors are needed. Our proposed solution is to use human-in-the-loop robotic systems to remove the munitions followed by destruction in an advanced version of the Sandia-developed explosive destruction system (EDS). We propose, under this project, to flesh out the details of the system and to identify specific additional research and development needs. Sandia's experience with the Non-Stockpile Chemical Materiel Program, combined with our expertise in robotics, sensors, chemistry, and systems engineering, makes us uniquely qualified to address this sort of large, but poorly defined problem.

Summary of Accomplishments

In this study we evaluated the approaches and technologies that can be used for remediation of large burial sites and sealed bunkers. We considered the different steps that might be required and identified technologies that could be used to help accomplish that step. We analyzed the benefits and limitations of the various technologies and how they could be integrated together in a system-of-systems approach to smoothly, efficiently, and safely process the large number of munitions while meeting all of the political, environmental, and social constraints. We indentified technology gaps where additional development work is needed. The biggest technical problem will be in excavating, removing, and transporting munitions and other items. We recommend using robotic to mitigate the inherent hazards, but it is important to choose carefully when and how robots will be used. Each process must have the right balance of human interaction and machine autonomy. It is important to begin developing robotic systems specifically for this application. Continued development is also needed for technologies to isolate hazards and mitigate accidental releases or detonations and to simultaneous detect and monitor many different agents and chemicals since one cannot know a priori what chemicals will be encountered once the remediation begins. Although technologies exist to safely destroy the recovered munitions, steps should be taken to increase the throughput of systems simply because of the numbers of munitions expected at these sites. In the case of sealed bunkers, technologies to rapidly and safely access the hardened structures are also important.

Significance

This work is related to the DOD objective of eliminating chemical weapons, to the DOE mission of environmental responsibility, and to the DHS objective of preventing chemical attack because the burial sites and bunkers are a threat to the environment and provide a source of material for terrorists. Chemical agent detection and decontamination technologies are also applicable to the DHS objective to strengthen our nation's preparedness and emergency response capabilities.

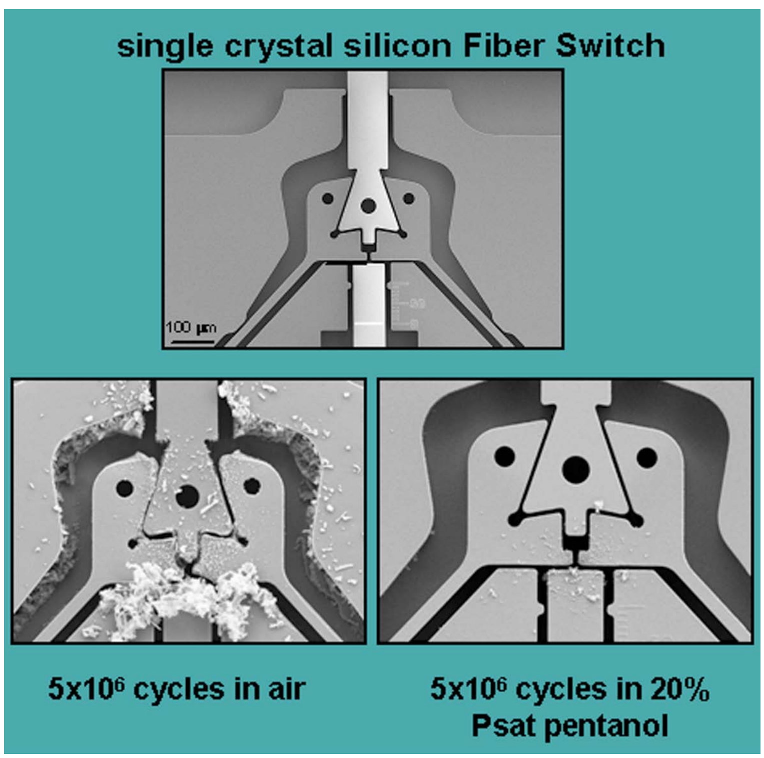
NUCLEAR WEAPONS INVESTMENT AREA

From fundamental studies into novel material combinations underlying better sensors and actuators, to more immediately employable sensors for monitoring the environment of weapon components, to improved nuclear weapons communications architectures, the projects in this investment area all aim to provide better, more-reliable methods of stockpile stewardship, with potential impacts to related mission areas (such as advanced battery construction and the role of the hydrogen economy in non-fossil-fuel energy generation).

Vapor Phase Lubrication for Advanced Surety Components

Project 130801

As weapons are continuously miniaturized, materials selected for their miniaturized-component manufacturability qualities will frequently require lubrication to reduce friction and diminish wear, thereby extending their life. Conventional solid lubricants are inadequate to this purpose, both because they oxidize, and because it is difficult to ensure uniform deposition on miniature parts. This project has developed vapor-phase lubricants, based around pentanol, that have been demonstrated to uniformly coat microstructures and increase their operating life 10,000-fold, dramatically reducing wear and debris accumulation. Implications for weapon designers include reduced variability in lubrication thereby improving ability to quantify margin and uncertainty.

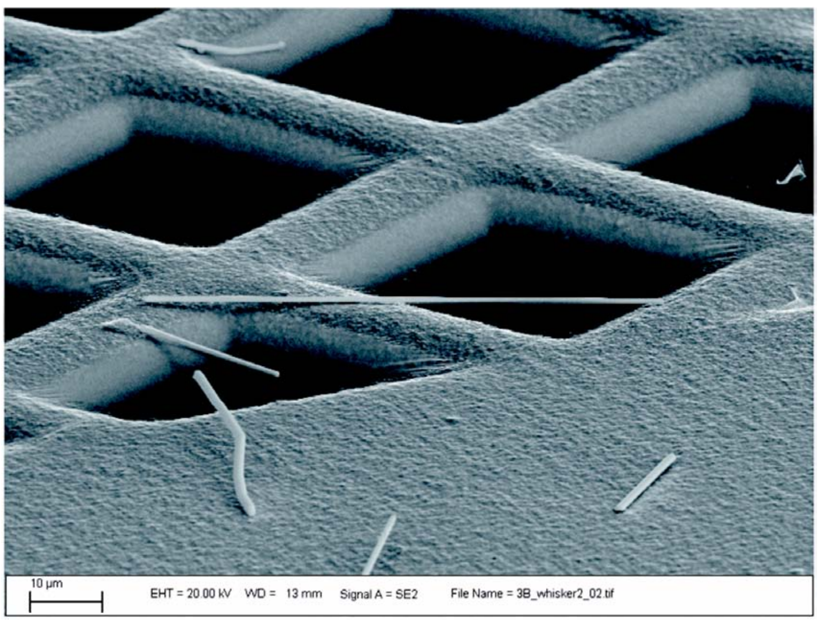


Micrographs of moving, interlocking microscale parts, showing greatly reduced debris formation and therefore wear with pentanol vapor lubrication (lower right) as compared to without such lubrication (lower left).

Understanding and Predicting Metallic Whisker Growth and its Effect on Reliability

130800

As the electronics industry continues to move toward lead-free components, engineers are encountering new issues on the microscale. This project is studying one of those circumstances, the occurrence of tin "whiskers" on the lead-free surfaces of tin-coated electronics, a phenomenon that was more rare when the surfaces were composed of a tin-lead alloy. This is problematic in that such whiskers — thin extensions of tin metal— can carry electrical current, thus raising the possibility of shorting failures between conductors, a potentially fatal flaw in a weapons system. A combination of experimentation and computational modeling is allowing project personnel to predict whisker nucleation density and growth rate, thereby assisting in establishing the important parameters that determine whisker formation, so that it can be understood — ultimately well enough so that it can be controlled or eliminated.



Scanning electron micrograph of tin whiskers on the surface of a support grid

NUCLEAR WEAPONS INVESTMENT AREA

Nanolaminate Thin Film Heat Sources for Advanced Weapon Components

105948
Year 3 of 3
Principal Investigator: D. P. Adams

Project Purpose

We address the problem that many future components will require a reliable, small, nonexplosive source of energy, which can be rapidly fabricated, allowing design-to-product in less than 36 months.

Toward this end, we propose to research how multiple exothermic nanolaminates respond to certain external stimuli, and enable function through rapid high-temperature reaction. Exothermic nanolaminates show great potential for their ability to rapidly evolve heat and irreversibly change properties through tailored reaction rates. To gain the advantages of exothermic multilayers for important applications, several critical unknowns must be addressed. The critical unknowns researched in this project include the following: 1. routes to reliable foil ignition, 2. response to electrostatic discharge and mechanical shock, 3. multilayer resiliency to deformation, 4. development of foil morphology/microstructure after reaction, 5. changes to exothermic foil properties after transformation, 6. thermal transport into neighboring materials, and 7. long-term stability.

Summary of Accomplishments

Relevant to the scientific community, we have demonstrated new reaction modes for exothermic nanolaminates. The direct observation and characterization of spin modes in nanolaminates was an unanticipated (new) discovery and adds great value to a particular community of scientists. In addition, we have discovered and reported on seven new exothermic materials pairs. This includes Sc/Au, Sc/Ag, Sc/Cu, Y/Cu, Y/Au, Y/Ag, and Y/Ir multilayers. We have determined their rates of reaction (involves self-propagating, high-temperature synthesis) and how the rates depend on multilayer design (periodicity) and reaction environment. We have additionally discovered methods for reacting these materials that lead to a desired ductile phase (B2, CsCl-type structure). These highly-ductile materials composed of one rare earth and one transition metal species could have great impact in the commercial sector. With many examples, we have explored the ignition sensitivity of reactive nanolaminates. We have determined ignition thresholds by pulsed laser irradiation. Furthermore, we have investigated how ignition depends on pulse duration (from the source), material design (periodicity and volume) and stored chemical energy density.

Our study has demonstrated thermal batteries that consist of reactive nanolaminates and examined their performance. In particular, we have shown that foils can lead to rapid activation, minimum thermal impulse and sufficient output.

Significance

In the next few years, we expect to provide a versatile technology that enables multiple, reliable "skip-generation" components and facilitates new system architectures. This should establish a more responsive laboratory infrastructure that is challenged with adapting to future, changing threats. Our technology has great potential for modular designs and reduced fabrication cycle times compared with current methods.

In particular, our results with nanolaminate thermal batteries are of immediate interest for an existing life extension program (LEP). The thermal battery prototypes demonstrated through this project are also of great interest to the DOD due to their enhanced performance.

In the scientific community, we have demonstrated new reaction pathways for exothermic nanolaminates. The direct observation and characterization of spin modes in nanolaminates was an unanticipated discovery and adds great value to a particular community of scientists. In addition, we have discovered seven new exothermic materials pairs. Highly ductile foils composed of rare earth and transition metal species could have great impact in the commercial sector. Reactive Ni/Al nanolaminates have been commercialized for various joining activities but are limited due to insufficient toughness that leads to cracking.

Refereed Communications

J.P. McDonald, M.A. Rodriguez, E.D. Jones Jr., and D.P. Adams, "Rare-Earth Transition-Metal Intermetallic Compounds Produced via Self-Propagating, High-Temperature Synthesis," to be published in the *Journal of Materials Research*.

D.P. Adams, M.A. Rodriguez, J.P. McDonald, M.M. Bai, E. Jones Jr., L. Brewer, and J.J. Moore, "Reactive Ni/Ti Nanolaminates," to be published in the *Journal of Applied Physics*.

J.P. McDonald, V.C. Hodges, E. Jones Jr., and D.P. Adams, "Direct Observation of Spin-Like Reaction Fronts in Planar Energetic Multilayer Foils," *Applied Physics Letters*, vol. 94, p. 034102, January 2009.

J.P. McDonald, Y.N. Picard, S.M. Yalisove, and D.P. Adams, "Nanosecond and Femtosecond Pulsed Laser Ignition Thresholds of Reactive Multilayer Foils," *Proceedings of the Materials Research Society*, vol. 1146E, 2008.

Multifunctional and Hybrid Energetic Components

105950
Year 3 of 3
Principal Investigator: M. K. Alam

Project Purpose

Current stockpile assessments indicate that over 70 energetic components are currently fielded. These components contain a wide variety of energetic materials and initiator/detonator technologies. This large number of items and materials makes surveillance activities difficult with current assets (people, funding, technology). This project has focused on development of a new, modular device, containing integrated diagnostics. Additionally, the developed device will incorporate a well-characterized initiation sequence, utilizing the CTH modeling code with new capabilities for thin pulse description, allowing perturbations to the design to be readily incorporated. Our first two years have focused on developing the individual aspects of the modular device. Specifically, we have developed a through bulkhead initiator (TBI) platform, chip-slapper technology, and a miniature waveguide sensor for the energetic material. We have also developed new methods for using experimental data within Sandia's modeling code. During the last year of the project, we have integrated the waveguide device into the TBI platform and demonstrated its performance. A mesoscale model for thin-pulse initiation of hexanitrostilbene (HNS) has been developed. The developed device will significantly reduce the surveillance burden by streamlining the types of devices and energetic materials (EM) that are fielded through its modular design. In addition, the in-situ diagnostics have the potential to eliminate costly dismantlement for EM analysis. Finally, costs of device modifications should be streamlined through the inclusion of the thin-pulse initiation model development.

Summary of Accomplishments

During the first year, a test bed was developed for testing TBI concepts, providing limits on the physical geometry of the device. The device utilized Sandia-developed slapper technology, aimed at increasing safety of the unit.

Modeling work focused on collecting data from the literature on equations of state (EOS) for HNS and any other initiation information. In addition, collection of gradient density information for model inclusion was begun. Work on the in-situ monitoring device consisted of testing various optical sampling options, including UV-visible (UV/VIS), near-infrared (NIR) and infrared (IR) spectroscopy.

During the second year, initial testing of the TBI design was performed. In addition, the optical sampling method was down-selected and attenuated total reflectance (ATR) was chosen as a viable option for inclusion into the chip slapper design. Waveguide devices were fabricated and tested. Triaminotrinitrobenzene (TATB) testing continued and although no detonation was achieved, literature and experimental evidence indicated areas of refinement. Modeling work consisted of collecting data for HNS EOS development (gas gun and compaction data). Experimental density information (focused ion beam [FIB] milling) was processed and methods were developed for translating the information into data usable by the modeling code.

The third year saw impressive progress in the modeling effort. EOS data from the literature and from experimental data enabled the development of initial mesoscale models for HNS. Significant refinement in the in-situ optical device was made as well. Specifically, a "proof of concept" design was developed in which the in-situ monitoring device was placed and tested for optical throughput. Additionally, a larger, 6-kV control display unit (CDU) device was developed and used for testing the insensitive high explosive (IHE).

Significance

Currently fielded energetic components contain a wide variety of energetic materials and initiator/detonator technologies. The developed device will significantly reduce the surveillance burden by streamlining the types and EM materials that are fielded through its modular design. In addition, the in-situ diagnostics have the potential to eliminate costly dismantlement for EM analysis. New mesoscale models for HNS can now be used to understand output characteristics.

Active Polymer Composites for Detecting Abnormal Thermal and Optical Environments

105951
Year 3 of 3
Principal Investigator: J. A. Zimmerman

Project Purpose

Our goal is to develop new active polymer devices (APDs) for sensing and responding to abnormal thermal and optical environments. Heat activated shape memory polymers (SMPs) enable the storage of temporary shapes during a thermomechanical cycle. Newly discovered optically induced SMPs can alternate between different shapes and colors, presenting possibilities for light detection and actuation. Our objective is to exploit the capabilities of SMPs by combining them with piezoelectric materials to create self-powered heat and light triggered actuators capable of performing work and generating an electrical signal to verify the actuation event. We anticipate making needed advancements in polymer synthesis, polymer characterization, and the formulation of high-fidelity models capable of predicting the thermomechanical response of SMPs and the electrothermomechanical response of piezoelectric materials such as PZT (lead zirconate titanate).

Summary of Accomplishments

We constructed a demonstration APD using the principle of a mechanical trigger, i.e., the (slow) response of an SMP induces a large, fast deformation of the piezoelectric material. We used foam versions of SMPs, and performed targeted characterization experiments to maximize both the recovery force available and the amount of deformation. A successful actuator demonstration with piezoelectric and switch responses was conducted.

We improved our constitutive model for shape memory polyurethane (monolith) materials, as testing showed that its prediction of free recovery was good at temperatures $< T_g$, but poor for temperatures $> T_g$. This discrepancy is due to our model only using one relaxation time. We modified the model to include a spectrum of relaxation times, and applied it to simulate tests of a tBA-co-PEGDMA SMP. Our results showed that the modified model improved the agreement of recovery rate with experimental data.

We completed formulation of a large-deformation model for piezoelectric materials, and verified it with simulations of polarized beam bending. Using both our SMP and piezoelectric models, we simulated a composite SMP/PZT beam. Our simulation revealed a very small magnitude electric field, a result consistent with our inability to observe measurable electric currents in our experiments of laminated PZT strips. We also simulated the bending of a thin piezoelectric strip as a cantilever beam with an applied concentrated load at the free end. This simulation shows an induced voltage of 3.61 V, in agreement with deflection experiments.

We synthesized polymers that display a mechanochromic response, i.e., a color change occurs due to application and/or release of a mechanical load. We have used a combination of modeling efforts, crystallographic, and spectroscopic techniques to better understand the mechanisms leading to stress relief in these polymer systems. This mechanochromic response of spiropyrans has potential in applications such as material stress detection and tamper sensing.

Significance

We have gained a tremendous amount of fundamental knowledge on the synthesis, properties and behavior of both heat activated SMPs and mechanochromic polymers, thereby providing a foundation for internal and industrial engineering applications. We have also defined compatibility issues relevant to the design of APDs. We have developed sophisticated models of SMPs and piezoelectric materials, and the capability for coupled simulations.

Refereed Communications

M.A. Rodriguez, G. O'Bryan, W.J. Andrzejewski, and J.R. McElhanon, "2-(E)-[1-(2-Hydroxyethyl)-3,3-dimethyl-3H-indol-1-ium-2-yl]vinyl-6-hydroxymethyl-4-nitrophenolate dihydrate," *Acta Crystallographica Section E*, vol. E69, p. 01906-01907, 2009.

L. Domeier, A. Nissen, S. Goods, and L. Whinnery, "Thermomechanical Characterization of Thermoset Urethane Shape Memory Polymer Foams," to be published in the *Journal of Applied Polymer Science*.

Optical Gaseous Atmosphere Sensing and Monitoring Using Surface Plasmon Resonance Spectroscopy and Custom Optic Coatings

105953
Year 3 of 3
Principal Investigator: S. M. Thornberg

Project Purpose

The gaseous environment surrounding all component materials can adversely impact their useful life and reliability by inducing deleterious aging processes (e.g., corrosion, oxidation, cracking, hydrolysis). The availability of an effective capability to measure, on demand, the chemical composition of internal atmospheres within both the weapon and specific components is a critical aspect of two relatively new stockpile transformation activities underway within the Integrated Stockpile Evaluation (ISE) program: (1) re-initiation of component surveillance, and (2) development of an embedded evaluation technology toolset to predict age-related state-of-health in future common adaptable system architecture (CASA) weapon systems. Of note, knowledge of the general weapon chemistry (e.g., from Pantex core surveillance) only provides a semiquantitative indicator of the “normalcy” of the environment, but does not identify whether specific aging mechanisms are occurring or their extent.

We propose to develop a novel set of miniaturized fiber optic sensors using the emerging phenomenology of surface plasmon resonance spectroscopy (SPRS) as the base technology. Studies have shown that SPRS is very sensitive, and theoretically by using customized optical coatings, can be very selective. Of prime importance, an SPRS-based technology has the potential to eliminate the “Achilles heel” of sensors: calibration and reliability. Calibration can be performed externally using chemometric techniques and reliability improvements are derived from the inherent physics and design simplicity. Properly miniaturized, the technology can be used to routinely analyze gas composition in stockpile weapons and components and also properly function (effective, compatible, no adverse effect on safety/performance) in a CASA embedded evaluation application. This work is appropriate for LDRD because the multicoated SPRS-based fiber optics needed to characterize our atmospheric chemistry do not exist and are not being developed anywhere. The ultimate project objective is to advance the technology to a validated proof-of-concept level.

Summary of Accomplishments

We successfully developed and tested single-ended fiber optic gas phase surface plasmon resonance (SPR) sensors for detection of several contaminant gases of interest to state-of-health monitoring in trace concentrations (low parts-per-million). These contaminant gases include H_2, H_2S, and moisture. Mathematical models were developed to simulate the response of a fiber optic-based SPR sensor and the model results generated compare favorably to experimental data collected. Several SPR supporting metals were modeled for testing including H_2 sensing using Pd films, H_2S sensing using Ag films, and H_2O sensing using SiO_2 films on an Au film. Data illustrate that different metals allow variation in the spectral response to various analytes allowing the manufacture of a three region SPR sensor that is sensitive to all three analytes using the single fiber and experimental system. It has been demonstrated that the H_2 response is unchanged after an extended interval of exposure to H_2S and that moisture can be detected at low frost points (–70 °C) after repeated exposure to H_2 and prolonged exposure to H_2S. Thus, simplified fiber optic SPR geometry using a single-ended fiber has been demonstrated and shown to have multiple responses to several chemical vapors that can be present due to aging effects in sealed systems.

Significance

This suite of effective environmental chemistry sensor technologies will address existing needs within Sandia including two specific stockpile transformation needs: embedded evaluation and common adaptable system architecture. DOD also needs state-of-health prediction for their prognostic health monitoring system, which is required in all their new major systems. A third potential application is for emerging DHS-related real-time chemical detection schemes (e.g., chemical intrusion threats).

Horizon: Next-Generation Architecture for a Small Dynamically Reconfigurable Weapon System

105954
Year 3 of 3
Principal Investigator: B. J. McMurtrey

Project Purpose

There is a need to transform the way we maintain and upgrade the nuclear weapon stockpile by reducing the cost and time required for enhancements, while maintaining or improving the current safety, reliability, and security standards. Our solution involves creating a reconfigurable controller core surrounded by digitally controlled configurable analog interfaces to any external or internal nuclear weapon input/output. The small controller core will be real-time partially reconfigurable so the different weapon processes such as the delivery platform interface, use control, safety, arming, fusing, firing, and telemetry can share the hardware across the time domain. This configuration is optimal because, in current systems, most weapon functions tend to execute for relatively short amounts of time during the different stages of the weapons lifetime.

Summary of Accomplishments

We have developed a dynamic reconfigurable hardware controller that is real-time and partially reconfigurable. We have also created a new design paradigm for targeting this advanced hardware. No current software tools exist to facilitate implementing a digital system with time-swapped hardware functional modules. By extending the principles of high-level object-oriented programming, such as inheritance and polymorphism, we have developed an entirely different methodology and tool flow for modeling and simulating digital systems. Our tools allow modeling of the reconfigurable system in Java, a powerful object oriented language. The tools provide a simulation environment that can cycle-accurately model the partially reconfigurable hardware behavior. Then our tools automatically partition hardware resources, create partial hardware bitstreams, and generate a configuration controller that will determine which reconfigurable modules will utilize the logic resources at any given time.

Finally, we merged our hardware and software in a capstone case study, showcasing the feasibility of the system as well as the advantages and disadvantages of our architecture. In this case study, we implemented a complex weapon electrical system utilizing our simulation tools. Then we utilized our tools to implement this system in our reconfigurable hardware platform.

Significance

This responsive weapon will provide dynamic, generic hardware that can be qualified to very strict environmental standards and then used in any nuclear weapons (NW) platform with only the new software functional control blocks needing to be qualified. Since new upgrades and modifications are done solely by changing software control blocks, they can quickly be designed, tested, qualified, and introduced into the stockpile.

Multilayer Coextrusion Techniques for Developing High Energy Density Organic Devices

105964
Year 3 of 3
Principal Investigator: L. A. Mondy

Project Purpose

Advancements in nuclear weapons design target reduction of volume and mass, such that devices with additional capability, increased safety, and enhanced surety may be incorporated. Within the firing set, capacitor technology is driving towards higher energy densities at reduced weight, leading to the development of components such as the gel-Mylar capacitor and the proposed micro-firing set. Through the science-based engineering approach proposed in this project, a multilayer coextrusion process can be developed to enable a new firing set capacitor with more than an 8× increase in energy density, while retaining radiation tolerance and a nuclear safety weaklink. Addressing the technical obstacles to yielding a prototype multilayer coextruded capacitor including layer-to-layer adhesion, viscosity mismatch between molten polymers, and filler-related issues will expand the applicability of polymeric multilayer coextruded composites beyond nuclear weapons components to other arenas such as optical devices, sensors, and barrier materials. Increasing our understanding of filled systems will be required to meet the technical objective of this work, but will be broadly applicable to other Sandia technologies. Therefore, the development of this skip-generation architecture has not only the potential to transform the stockpile, but also impact many other Sandia programs.

Summary of Accomplishments

We developed and demonstrated a coextrusion capability for filled polymers. The polymers were filled with a variety of additives to enhance the dielectric constant or the conductance, depending on the desired properties. We created a new conductive polymer composite material consisting of solid nickel particles and a low-melting eutectic incorporated into a polymer matrix. Unlike other conductive polymers on the market, this blend is melt processable and extrudable. By coextruding this conductive polymer with a barium titanate filled polymer, we created alternating conductive and dielectric layers, and, hence, a capacitor. We also developed numerical models to help determine the material and processing parameters that impact processing and layer stability. The processing experience and the new science-based engineering tools developed in this project allow the improved processing of filled polymers and will allow the expanded applicability of multilayer coextrusion processing.

Significance

The science-based engineering proposed in this project will expand applicability of multilayer processing to a suite of applications including capacitors, optical devices, membranes, barrier materials, and sensors. The improved processing of filled polymers will also impact a variety of components. Therefore, this work impacts areas including nuclear weapons, nonproliferation, defense systems, and homeland security.

Refereed Communications

R.A. Mrozek, P.J. Cole, and J.L. Lenhart, "Enhanced Melt Processing of Conductive Polymer Composites Through the Addition of a Low Melting Eutectic Material," to be published in *American Chemical Society Preprints*.

Determination and Optimization of Spatial Samples for Distributed Measurements

117843
Year 2 of 3
Principal Investigator: H. D. Tran

Project Purpose

When measuring or inspecting products for acceptance, inspection criteria typically require a single value; however, this single value is not representative of the way that the measurement is taken. For example, a form specification on a machined part, such as circularity or roundness, gives a single value for maximum acceptable deviation of the radius of a part. The inspection of this radius, however, will typically require multiple measurements. There are no accepted standards for determining how many measurements to take, nor for assessing confidence or risk based on the number of measurements and the evaluation of these measurements versus the acceptance criteria. We will develop a standard method for determining the number of measurements, together with the spatial distribution of measurements. This method will also assess the associated risks for false acceptance and false rejection. This method will be developed for dimensional inspection; however, the fundamental method should easily be extensible to other measurement domains which have spatial distribution, such as temperature distribution.

We have chosen the discrete wavelet transform (DWT) as the appropriate orthogonal transform that can use computer model-based geometry, to determine optimal sampling locations. We will then apply the inverse transform to reconstruct measured geometry, and compare with model geometry for acceptance. We will then perform statistical evaluation to give confidence bounds.

The end result will be both an algorithm and computer software, which would use, as input, bounded geometry and acceptance criteria. The output would be measurement point locations. After the measurements are made, the data would be used to reconstruct the measured geometry, and statistical evaluations would also be performed for acceptance. The object is to have this general method adopted as an internationally recognized standard practice.

The general method crosses many disciplines, and therefore, supports broad manufacturing initiatives that impact NW product realization.

Summary of Accomplishments

Working with our university partner, we developed a generalized algorithm (WCI, or wavelet curve interpolation) for lines and curves based on the discrete wavelet transform. This algorithm also generates interpolation between measurement points and assigns confidence bounds to the measured curve. The algorithm is generalizable to surfaces and volumes, since it is based on orthogonal function decomposition. We have tested this algorithm both on simulated data and on experimental data for a typical machined aluminum surface. Experimental results agree with expectations.

A key unanticipated result is that the WCI method also gives confidence bounds.

We have drafted a manuscript for these results, and submitted the manuscript to a leading international journal.

We have identified a case study based on an actual production component. Because there is no accepted standard for sampling strategy, we can see where our methodology is applicable. The result would ensure better communication of intent in design and better confidence in production results. Work with case studies is ongoing, and expected to continue through FY 2010.

We have started informal communications with national technical standards committees. We presented preliminary results and conclusions at the next (for lines and curves) interagency manufacturing operations group (IMOG) meeting, a working group of multiple Department of Energy contractors. We have placed the topic of the need for a sampling standard on the agenda for the next dimensional metrology committee (NCSLI Committee 148).

Significance

This research will result in a new standard practice for inspection. This standard will prescribe how to measure and analyze against specifications. This method will provide manufacturers with greater confidence that their product meets specifications, and eliminate superfluous inspections. This benefits both the economical and reliable manufacture of stockpile components, and also advances DOE's goal for scientific discovery and innovation.

Intrinsically Secure Communications through Adaptive Beamforming

117844
Year 2 of 3
Principal Investigator: M. A. Forman

Project Purpose

The purpose of the project is to demonstrate a full-duplex 60-GHz system that uses cognitive-radio enhancements, channel-impulse estimation, and multidimensional constellations to generate shared secret data between two nodes. This shared secret data can be used as symmetric cryptographic keys or hopping sequences for secure communications. Work will focus on the implementation of the system at millimeter waves using theory developed in the first two years.

Summary of Accomplishments

The creation of a generalized system for generating symmetric cryptographic keys using multiple metrics over multiple domains has been formalized. A complete object-oriented ray-tracing code has been developed in Matlab to simulate a dynamic physical environment. Several software radios, the universal software radio peripherals (USRP), have been purchased. Millimeter hardware has been purchased, channel-impulse estimation code has been developed, and a half-duplex system has been tested in FY 2009.

This work has had two publications accepted, and an invention disclosure (SD 11358) is being drafted into a patent application.

Significance

This work extends the state of the art in symmetric key generation using the channel as a keying variable. Cognitive enhancements allow a system to analyze and adapt to the state of the channel, including mitigating intentional and unintentional jamming, identifying degenerate and periodic channel states, and using multidimensional constellation to extract data from the channel. This work will be of use to physical security applications and containers.

Refereed Communications

M.A. Forman and D. Young, “A Generalized Scheme for the Creation of Shared Secret Keys Through Uncorrelated Reciprocal Channels in Multiple Domains,” in *Proceedings of the 18th IEEE International Conference on Computer Communications and Networks*, March 2009.

Advanced Cathode and Electrolyte for Thermal Batteries

117845
Year 2 of 3
Principal Investigator: D. Ingersoll

Project Purpose

We propose to develop a high-voltage cathode and electrolyte for thermal batteries, the main power supply used in all nuclear weapons and many smart conventional weapons. The materials used in today's weapon systems were developed 20–30 years ago and generate only 2 V per cell, as compared to the >3 V per cell proposed here (a >150% increase). The new materials developed will allow modernization of thermal batteries resulting in lower production cost/time and improved performance through increased reliability and decreased size and weight. Furthermore, the reduced size and weight have the added potential for increasing weapon system mission range and payload.

To meet this goal, questions of both an applied and fundamental nature will be addressed, such as the thermodynamic stability of the novel materials at high temperature and in the presence of high concentrations of ligands; reversibility of the redox process and its functional dependence on temperature; the electrochemical stability of the electrolyte; and the nature of the charge transfer process. These issues will be investigated using a suite of synthetic, electrochemical, spectroscopic, and in-situ spectroelectrochemical methods. Included is the development of new methods of characterization, such as in-situ neutron diffraction, which can then be applied to other energy storage needs.

The fundamental and high-risk nature of this work is at odds with the demands associated with the cost/time constraints and low-risk approach typically associated with specific programmatic system objectives. Furthermore, this activity has the potential for impacting all future weapon system power supplies. As such, this activity is more appropriate as an LDRD project rather than a programmatic one.

Summary of Accomplishments

We have successfully completed the in-situ neutron diffraction experiment and monitored the phase transformations of the cathode as well as the anode. We have completed initial predictive modeling of materials properties, focusing on the charge transfer behavior (ionic and electronic) and structural transition characteristics. We have developed a new hydrothermal synthetic route for preparation of the doped and undoped iron phosphate and have prepared sufficient quantities of materials for model validation. We have developed "semi-soft" synthetic routes for the early transition element oxide solid ion conductors and have completed preliminary evaluation. We have noted a correlation between the optical characteristics of these materials and the coordination environment. We have demonstrated a thermally stable lithium-ion battery (200 °C) using a thermally stable binder and separator and cast electrodes. We have demonstrated continued stability and operation of the phosphate in contact with the electrolyte up to 125 °C. This thermally stable rechargeable battery has potential to fulfill the need of high-temperature operation for oil drilling applications. We have developed a new class of ionic liquids that serve the dual roles of electrolyte and cathode. Although not suited for thermal battery applications for technical reasons, these materials have the potential for use in flow batteries for stationary applications.

Significance

This project focuses principally on applying advanced science and technology to advanced battery development for national nuclear and defense needs. However, a part of this work has now reached a level of maturity sufficient to continue development in support of US energy security needs. While this ancillary work is still in its infancy (estimated to be TRL 2), energy security needs are sufficient to continue development of these technologies in support of US electric utility grid and oil drilling applications.

MEMS-Enabled Integrated Optical Circuits for Nuclear Weapons Applications

117846
Year 2 of 3
Principal Investigator: G. N. Nielson

Project Purpose

Microelectromechanical systems (MEMS)-enabled integrated optical circuits have the potential to significantly impact a number of nuclear weapon components (such as discriminators and encryption systems), particularly as steps are taken toward further optical control of weapons. To date, only very preliminary work in MEMS-enabled integrated optical circuits has been done. This project is intended to expand that initial work, raise the TRL level of current devices, and explore the potential benefit to nuclear weapon components. The primary challenges are, first, creating a fabrication process that compatibly incorporates optical waveguides, MEMS, and germanium photodiodes, and second, applying appropriate design principles to achieve the optical and mechanical performance desired.

It is anticipated that the MEMS-enabled integrated circuits will provide a unique set of performance characteristics. Chips can be fabricated requiring only optical inputs and outputs with the optical input signals controlling the resulting optical outputs. No additional electrical power or signal inputs are required. The chips will handle high optical power levels (up to a few watts at least — free space optical MEMS can handle hundreds of milliwatts at best). The optical isolation between optical paths is incredibly high, thus crosstalk is virtually nonexistent and, with the light confined in waveguides, there is no stray light going in unintended directions. Logic can be implemented in the optical circuit to provide a number of results, including enforcing sequence without requiring a clocking mechanism or external application specific integrated circuit (ASIC).

Summary of Accomplishments

We have fabricated and tested the first prototype devices that combined MEMS with waveguides and we have studied various possible techniques and designs to combine germanium photodiodes with the waveguides in this device. While we have learned a significant amount from the first prototype devices, the testing was not successful at demonstrating optical switching. Most of the fabricated devices buckled due to residual stress. The intact devices were tested and did mechanically displace as desired. However, the waveguides were almost completely opaque, thus optical switching could not be observed with these prototypes. Due to these results, we have conducted significant structure and process redesign work for the second prototype devices. We have redesigned the structure to make the second prototype much less sensitive to residual stress. In addition, the new process flow uses larger features and is therefore easier to fabricate. The optical loss in the MEMS device waveguides was extremely high. We have tracked this problem to silicon carbide nanocrystals that formed in the surface of the silicon waveguide core material. We have performed a design of experiments of twenty different process variations to identify a process that eliminates these nanocrystals and provides low-loss waveguides compatible with the MEMS process. We have now identified a process for low-loss waveguides that is compatible with MEMS processing (this is a key accomplishment). We have also nearly completed the second-generation process flow development. We encountered many challenges in the process but have found solutions to move forward. We expect fabricated devices available for testing within a month. We have explored various options for creating the germanium photodiodes. Our goal with the germanium photodiodes is a simple, functional device that is compatible with our current waveguide/MEMS.

Significance

This project will advance the state of the art in integrated optical circuits and will lead to new capabilities in optical circuit technology. The expected performance characteristics are well suited to the needs of nuclear weapon systems, providing significant benefit to Sandia's nuclear weapons mission. Other applications that may benefit include quantum computing, telecommunications, parallel computing, and secure data transmission.

3D Integration Technology for Highly Secure, Mixed Signal, Reconfigurable Systems

117847
Year 2 of 3
Principal Investigator: S. L. Shinde

Project Purpose

This project addresses Sandia's needs for increased functionality in reduced volume. Integration of dissimilar device technology using 3D integration incorporates diverse architectures. Interconnect density increases by orders of magnitudes. Current approaches using board stacking drive substantial development, complexity, and cost, but the reliability is poor. Current approaches also have security vulnerabilities. Considerable advantage is obtained by combining functions into a single solution utilizing vertical die stacking. One avenue of this technology utilizes surface activated bonding (SAB) and is the basis for this research. Stacking addresses the described problems by drastically increasing the number of interchip interconnections while reducing complexity, cost, and improving reliability. Stacked elements preclude probing of the circuitry, significantly improving system security.

The bonding of dissimilar materials has been practiced in laboratories. Through-wafer-via technology with high aspect ratios also represents a risk. We will utilize the full range of Sandia's Microsystems and Engineering Sciences Applications (MESA) fabrication capabilities. The thermal stability of large numbers of vias will be modeled. As via density increases, we envisage compounded problems with small coefficient of thermal expansion (CTE) mismatches. We will establish the limits of via density, aspect ratios, and materials issues, through detailed modeling.

We propose to develop surface-activated bonding and silicon through-wafer-via technologies. We will deliver 3D integrated test structures that demonstrate both technologies utilizing the full capabilities of the new MESA complex. Phase 1 concentrates on die-to-wafer, wafer-to-wafer SAB using a science-based approach to understand surface activation for nonpackaged components and wafers. This will enable covalent bonding at temperatures near 50 °C. We are developing low-temperature deposited interface layers and will investigate surface activation techniques compatible with dissimilar materials. Phase 2 involves SAB of structures with metal interconnects. Concurrently, we will develop silicon through-wafer-via technology as part of the front-end device fabrication process. Finally, Phase 3 will deliver fully-functional 3D prototypes that demonstrate the integration technology to technology readiness level (TRL) 3.

Summary of Accomplishments

Significant progress was made in FY 2009 against all our stated milestones.

Wafer to wafer bonding using both surface activation and metal to metal bonding techniques was demonstrated at temperatures below 100 °C and 200 °C respectively. In addition the design for a test vehicle with structures compatible with both wafer to wafer and die to wafer was completed.

We completed development of the complete process module for creating front-end-of-line (FEOL) through-silicon vias (TSVs) in our silicon fabrication facility. This was enabled by Bosch etching of high-aspect-ratio holes, creating a thin dielectric layer on them for electrical isolation, filling them with sacrificial Si, carrying out front-end processing, and removing the sacrificial Si by etching followed by deposition of tungsten to create the interconnects and polishing the top to create a surface for back-end processing. We are now in the process of measuring the isolation of these vias by thinning the wafers and accessing the vias from the back-side.

We have also designed a test vehicle with memory devices and stacking compatible interconnects that will allow us to test the effects of front-end-of-the-line (FEOL)-TSV processing on these devices.

We carried out extensive modeling activities to simulate the thermomechanical behavior of test structures undergoing the temperature variation in a fabrication sequence. We carried out stress measurements on blank thin films of all the materials present in the test structures to generate materials properties data needed for our simulation. The simulation has already revealed areas of stress concentration in the structure. The simulation thus not only identifies stress concentration areas in existing designs, but also will provide design guidelines for mitigating their effect on reliability of these structures.

In addition to internal presentations, we have presented one invited talk, and will be presenting two talks at an upcoming international conference.

Significance

This work addresses needs for bonding dissimilar materials and low-temperature packaging to enable new complex microsystems. Die stacking is an enabler for a variety of new system architectural and security options utilizing cross-cutting technologies. Success with this scientific and engineering challenge could benefit NW and national security applications and would also have potential commercial interest.

Creating a Smart Fast-Neutron Calibration Source

117849
Year 2 of 3
Principal Investigator: S. Mrowka

Project Purpose

In most surveillance activities, measurement of neutron generator (NG) performance is constrained by unwieldy physical spaces. In these instances, in-situ calibration of solid-state neutron generator monitors (NGMs) is degraded because the standard reference neutron detector, the lead probe, cannot be directly used to calibrate the NGM. Instead, indirect processes involving calculations of correction factors using secondary transfer standards, radiation transport simulations and engineering analysis are necessary; each introducing uncertainties that degrade the final calibration precision of the NGM.

We are pursuing development of a special fast-neutron reference source that can self-report its neutron yield and neutron rate either via sensors embedded inside or in very close proximity outside the sealed neutron tube. The internal sensors directly measure alpha particles ejected from the hydride target during the D + T fusion reaction, providing a "first principles" quantitative gauge of neutrons produce. External sensors can detect neutrons directly.

Modifying the tube design for an internal sensor requires R&D to: a) identify sensors capable of withstanding the harsh processing and functional environments associated with tube manufacturing and operation; b) develop an alpha particle transport and detection efficiency model; and c) design a sensor mounting scheme.

External (plastic scintillation) sensors would not require tube modification and will be the focus of this year's work.

This reference neutron source would see application throughout the nuclear weapons complex (NWC) in cases where the controlatron and lead probe are currently used. In stockpile surveillance and joint test assembly (JTA) activities, this instrument will provide a new calibration capability allowing more precise calibration of NGMs used to assess neutron generator functional performance, producing more accurate neutron generator life predictions. In neutron tube and neutron generator production activities the smart fast neutron reference source will address quantification of margin and uncertainty (QMU) and Lean Six Sigma production goals by providing a self-consistent calibration capability within war reserve (WR) functional test equipment.

Summary of Accomplishments

- Completed fiber detector evaluation
- Performed single fiber tests
- Constructed and tested 48 channel fiber array
- Demonstrated feasibility of reducing neutron measurement uncertainty at low count rates, important for end-of-life determination.

Significance

A smart, fast-neutron reference source capable of directly reporting neutron yield will support DOE Defense Program goals to bolster our ability to perform stockpile stewardship. The source will benefit the nuclear weapons mission by providing a unique tool for calibrating and assessing the performance of neutron measurement systems in integrated stockpile evaluation and neutron generator production activities, thus improving confidence in our stockpile performance estimates.

Microresonators for Advanced RF Systems

117851
Year 2 of 3
Principal Investigator: C. D. Nordquist

Project Purpose

As radiofrequency (RF) systems are transformed to reduce the number of piece parts and improve reliability, reliable high-Q miniature resonators become a need that commercial suppliers cannot meet. These resonators must have high Q for reduced phase noise, be integrated with radiofrequency integrated circuits (RFICs) for reduced parasitics, and be more reliable than other components in the system. Commercial devices are large, don't integrate well into a chip-and-wire environment, and are designed for high-volume applications so specific designs for low-volume applications incur high nonrecurring expenses and unit costs. To address these needs, we are exploring acoustic aluminum nitride (AlN) resonators for realizing high-Q resonators for highly integrated RF systems.

AlN contour-mode microresonator technology is an enabling technology, with the potential for Q>1500 in a microscale device that can be integrated using chip-and-wire approaches. This technology allows batch microfabrication of different designs of microresonators meeting a variety of requirements on a single wafer. While some demonstrations have been completed in this technology, the temperature stability and failure mechanisms of these devices must be understood and addressed. Additionally, the devices must be packaged to allow intimate integration with other technologies such as GaAs or Si RFICs.

The purpose of this project is to understand and address several of these factors limiting the maturity of this technology. Specifically, the project will develop wafer-scale packaging, improve the environmental stability of the technology, and obtain an early understanding of the device failure mechanisms. Wafer level packaging will protect the devices in a controlled microenvironment, allowing high-yield integration into higher level systems and testing in a controlled ambient. Improving the environmental stability of the device will allow its use in a broad range of system environments. Understanding the failure mechanisms will enable improvements to the device design and technology in the future.

Summary of Accomplishments

In FY 2009, we have identified a failure mechanism caused by contamination, demonstrated hermetic packages using wafer-scale bonding, and measured the electrical performance of the packaging interfaces. These accomplishments will provide the foundation for meeting the primary project goal of advancing the microresonator technology in the remaining year.

In the area of failure modes, a 100 ppm drift in resonator frequency was measured over a 50 day storage test. Further testing in a contaminated vacuum system and modeling verified that this drift was due to contamination absorbed from room air. This work verified that clean hermetic packaging is a key element to achieving reliable devices and understanding all of the device failure mechanisms.

In the area of wafer scale packaging, we fabricated large area leak test structures, enabling rapid characterization of the integrity of the wafer-bonded packages during process development. We compared the strength and sealing of Au-Au and AuGe-Au bonding approaches, and identified AuGe-Au bonding as the most promising path. We demonstrated hermetic AuGe-Au bonded packages that survive further processing such as dicing and thinning to 100-µm thickness. We demonstrated the lid fabrication process using deep silicon etching. We are currently addressing yield and cleanliness issues and are transferring this packaging process to microresonator devices. We expect hermetic thin microresonator packages, with integrated leak check capability, by the end of CY 2009.

To enable the characterization of the small microresonator packages, we have designed and fabricated four different pressure sensors using the microresonator process. Three of these sensors have been characterized from <1 mTorr to atmospheric pressure, and show consistently measurable changes over these pressure variations. Approaches have been developed to allow extraction of the sensor response using autoprober measurements, allowing nondestructive electrical characterization of all of the packages on a wafer.

Significance

By generating the knowledge base and technical expertise to deliver miniature custom RF resonator components, this project has the potential to transform RF systems by reducing system volume and improving performance. Two areas that would benefit are fuzing radar and telemetry. Additionally, the technologies and knowledge developed by this project may also be extended to other investment areas and systems such as digital clock references, analog filtering, and miniature power electronics.

Novel Foam Encapsulation Materials and Processes

117853
Year 2 of 3
Principal Investigator: L. A. Mondy

Project Purpose

Foam encapsulation provides protection from shock, vibration, and thermal influences for a wide variety of electromechanical weapon components. Because the encapsulation occurs near the end of the manufacturing process, expensive components are at risk if the encapsulation is flawed. Processing of encapsulants in complex electromechanical components has been a challenge in previous weapons systems and there are advocates of eliminating foam. This may not be an option for many current and future components because foam is a strong but lightweight material that provides a good compromise between the conflicting design needs of structural stability and electronic function. Instead, we will design novel foams, based on modern concepts such as nanoparticle stabilized interfaces and hybrid/stacked reaction chemistries, which will mitigate previous difficulties such as density gradients, voids, residual stresses, and cracking. At the heart of the new process are both new materials and chemistries, as well a two-stage process where the foam is produced from its precursors and subsequently injected in the mold. The decoupling of foaming and filling will decrease voids, as pressure driven flow fills interstitial spaces more easily, decrease density gradients that occur due to in situ foaming, and reduce residual stresses to near zero. In addition, it will allow us to perform quality assurance on the foam for cell size and density variations, before it is injected into the mold. In the development of new processes, there are risks; we will mitigate risk by taking a multipronged approach examining a variety of processes and chemistries, and by always providing metrics to demonstrate quantitatively how our new process is an improvement over previous processes. We have brought together a multidisciplinary team of experts in polymer chemistry, foam processing, foam engineering and multiphase modeling that are both creative and pragmatic and have a history of successfully developing new processes and chemistries.

Summary of Accomplishments

Our strategy was to create a shear-stable foam system that has sufficient initial polymer network support to prevent drainage, cell coarsening and collapse, but is still amenable to processing until a later transition to a solid material. We used various constituents to produce stable foam formulations based on a chemically blown system and added special building blocks to provide partial early gelation for enhanced foam stability. We compared properties (Tg, thermal expansion, compressive strength, homogeneity and cell structure, and density) of our new foams to those of foams currently in the stockpile.

We also created noncurable systems for fundamental foam stability measurements, probing the roles of various stabilizing agents such as surfactants, particles, and chemical gelling agents. We used rheological measurements combined with bubble size analysis of foam cells to develop a rheological diagnostic tool to examine cell coarsening and provide evidence that we can successfully slow cell coarsening rates using chemical stabilization means. We also explored the ability of particles to stabilize a polymeric foam. Using noncurable foams in processing tests, we demonstrated that stable foams could survive the shear during the pressure fill of a quality assurance mold, originally developed by the Kansas City Plant for epoxy foams.

To begin development of a model for chemically blown foams (and before our final foam formulation has been selected), we studied a polyurethane, which is used throughout the complex and is an appropriate analog to our new foams. We developed a homogenized foam model where the foam material density changes with time as the exothermic reactions progress and the viscosity depends on the current gas fraction, extent of polymerization, and temperature. The parameters were populated with infrared spectroscopy (IR) data for the curing reaction, foam rise experiments for the gas evolution rate, and dynamic viscosity measurements.

Significance

These new materials will better insulate nuclear weapon components from shock and vibration and will not exhibit residual stresses that can damage sensitive electronic components; therefore they will enable nuclear weapons that are safer, more reliable, more easily transportable, and more resistant to aging. Because processing of these new materials will be more easily controlled than current foams, this work will improve yield, reduce cost, and minimize potential significant finding investigations (SFIs).

Refereed Communications

J.H. Aubert, M.C. Celina, J.M. Kropka, L.A. Mondy, and R.R. Rao, "Improved Foam Materials Through Characterization of Foam Stability," to be published in *Polymer Preprints*.

L.A. Mondy, R.R. Rao, H. Moffat, D. Adolf, and M.C. Celina, "Structural Epoxy Foams," *Chapter 16 of Epoxy Polymers: New Materials and Innovations*, J.P. Pascault and R. Williams, Eds., Wiley-VCH Verlag GmbH & Co.

The Development of a Mechanical Weaklink Prototype for NW Systems

124643
Year 2 of 2
Principal Investigator: J. L. Dohner

Project Purpose

Thermal weaklinks, having been developed and integrated into a number of nuclear weapon (NW) systems, play an important role in controlling failures that could result in a loss of assured safety (LOAS). In contrast, mechanical weaklinks do not exist in any NW system, even though there are a number of credible mechanical insults that could also produce a LOAS. This lack of mechanical weaklink presence is due to the difficulty of finding a material that will satisfy reliability design constraints as well as or better than existing materials residing within a detonation-critical component while having the added property that its structure is predictably altered under a definable set of abnormal insults resulting in irreversible component failure. In this work, we propose to overcome this problem by building a material that will have desirable reliability and safety characteristics using mesoscale manufacturing technology.

FY 2009 work is guided by the results from an FY 2007 feasibility study which identified a detonation critical element for weaklink material replacement and by FY 2008 work which developed a weaklink material and optimized the identified detonation critical component for weaklink acceptance. We will work to integrate the developed weaklink material into the identified component to produce a prototype, reliable detonation critical component that irreversibly fails in defined abnormal environments. Predictable failure will be validated through the use of experimental environmental analysis. Margins of safety and resulting stronglink design criteria will be determined through the use of numerical analysis.

The result of this work will be a reliable, safe prototype component. Considering the ubiquity of this component in the stockpile, if implemented, we expect it to significantly enhance stockpile safety.

Summary of Accomplishments

A prototype component using meso manufactured material was developed and tested to prove the weaklink concept. Initial subcomponent testing was performed on this manufactured material. Results were analyzed to determine both safety and reliability statistics. These statistics were positive, proving the concept at the material level. Subcomponent results were then used to design a final prototype. Function testing was performed on a set of three prototypes. This testing was also successful, proving the weaklink concept. This work brought the technology readiness level of this concept from a NW safety TR1 to a NW safety TR4, allowing for the discussion of this concept as part of a 6.1 safety theme in future stockpile life extension programs.

Significance

The proposed weaklink would be part of a detonation critical component and has the potential to improve the safety of nearly every present and future weapon system. With this concept at TR4, it can be included in the development of a weapon safety theme.

Embeddable Optical Current Monitors for High-Current Signal Confirmation

130791
Year 1 of 2
Principal Investigator: M. J. Cich

Project Purpose

Monitoring of high-current pulsed signals is of great interest for a number of nuclear weapon (NW) applications including signal confirmation in joint test assemblies (JTAs) as well as built-in-test and state-of-health monitoring for advanced firing sets. Also, nuclear weapon design requires the ability to generate, transmit and control high-current pulses. Measurement of these current pulses is required during development, production at the Kansas City Plant (KCP), and ongoing surveillance at the Weapons Evaluation Test Laboratory (WETL). Development of a truly embedded current sensor would support the B61 and W88 shelf life extension programs (SLEPs) and future weapon development.

Current-voltage transformers (CVTs) are now typically used to measure current signals but consume considerable power and are subject to electromagnetic interference (EMI). CVTs are also difficult to implement and integrate with cable systems for testing and limits application.

Recent work on magneto-optical current sensors has shown great promise for improving performance as well as gaining advantages of EMI-immunity and low power consumption. Our team has recently developed optical current sensors using bismuth-doped iron garnets in a two-pass reflective geometry, demonstrating sensing of current pulses with 150-ns rise times and peak currents ranging from 500 A to 3 kA, limited by the range of the capacitor-discharge unit used for testing. However, in order to make these current sensors truly embeddable and functional for the largest number of applications, another order-of-magnitude reduction in size is required. The tradeoff with reducing sensor size is reduced sensitivity which is proportional to the optical path length through the magneto-optical material.

We propose to develop novel magneto-optical current sensors which employ control over domain motion and location to reduce sensor size but maintain sensitivity and reproducibility. This approach should reduce sensor size to the order of 1 mm^3 which will enable truly embeddable, nonintrusive current sensing in the kA range for NW applications.

Summary of Accomplishments

Excellent progress has been made toward our goals. Highlights of our technical results include the following:

1. Electromagnetic simulations of standard and novel notch cables which show limited and enhanced magnetic field lines, respectively, for current monitoring. Our custom notch designs should increase the B-field through the sensor by several orders of magnitude.
2. Built capability to perform local domain characterization on rare-earth iron garnet films including imaging, Mueller matrix characterization and power diffraction analysis. The Mueller matrices for the two domain types and the domain interface have been directly measured, which will help assess sensor performance.
3. Began effort to deposit and characterize SmCo magnetic films on bismuth iron-garnet films to enable local magnetic control of domain structures.
4. Investigating typical applications, cable geometries, and developing custom cables with enhanced B-field.
5. A conference paper has been submitted and accepted at the SPIE Optics + Photonics Conference in San Diego, CA in August 2009.

Significance

This embeddable optical current monitoring technology would benefit several NW applications such as built-in joint test assembly (JTA) end-event confirmation, built-in-test and state-of-health monitoring in advanced firesets and benefit nuclear design through surveillance at WETL, development and production at KCP.

Faraday Microshields and Novel Electromagnetic Isolation Structures

130792
Year 1 of 2
Principal Investigator: K. A. Peterson

Project Purpose

Isolation requirements for advanced radiofrequency (RF) modules are presently dependent on via-fence enclosures. This approach provides up to 100 db isolation between radiofrequency integrated circuits (RFICs), but the 150 dB isolation required in radar applications is beyond reach. Furthermore, via-fence shielding and associated cavities add significant cost to the overall RF module due to the number of layers needed and additional processing steps. New techniques promise improved isolation and density with better producibility at lower cost using low-loss materials. The need for via fences and cavities can be eliminated by coating RFIC-based circuits with polymer and then overcoating the polymer with a conductive layer. This unconventional approach should provide an ideal Faraday "microcage" at the integrated circuit (IC) level with extremely high electromagnetic isolation/shielding. The approach should also enhance ruggedness/reliability by strengthening solder and wire bonded attachments. The stability of the encapsulation in the presence of high thermal dissipation will be critical. A variety of conductive materials and application processes will be evaluated. An RFIC will be designed specifically for chip-scale Faraday packaging using ball grid arrays. Another technique will create a layered structure for RFICs mounted directly to packages and heat sinks and wire bonded. Additional techniques using novel board-level approaches for sidewall metallization will also be investigated.

Summary of Accomplishments

Accomplishments this year include the design, refinement, fabrication, and testing of a test board for measurement of performance and isolation. This is a test board that can be used both as a radiofrequency generator and as a receiver. The materials study has pointed to foamed polymers as a technique for achieving low dielectric constants. Polystyrene has been prototyped for its low dielectric constant and other foams will be considered for their closed-cell properties and manufacturability. Performance tests indicate that the dielectric affects the frequency and loss, but the addition of the shield has a minimal further effect. Additional test vehicles have been designed to look at the effects with actual RFICs and effects of heating — expected for high-power devices. A new technique for providing maximum isolation in the board itself has been demonstrated. The technique, previously thought to be impossible, provides solid walls of metal in place of via fences. This technique has also been used to isolate input/output pins and to fabricate lids for baseline measurements. By minimizing the leakage of the board, the isolation provided by microencapsulation of devices will also benefit. These accomplishments ease the second year's work by providing a good baseline and initial good measurements for performance. Isolation measurements will also be accomplished this fiscal year.

Significance

This project will create new capability in reliable, inexpensive, producible solutions for nuclear weapons (NW) mission needs (arming, fuzing and firing [AF&F] and more). Commercial off-the-shelf (COTS)-based communication microtransceivers should also benefit from this work by eliminating the need for bulky plastic-encapsulated packaging. This work will also continue to investigate RF properties of encapsulants at frequencies of interest for other programs.

Field and Charge Penetration by Lightning Burnthrough

130793
Year 1 of 3
Principal Investigator: L. K. Warne

Project Purpose

The continuing current component of the lightning environment is capable of breaching metal barriers. However the breach takes the form of a small hole (typically a centimeter) which is surrounded by a hot plasma. Because lightning is made up of large amplitude return strokes separated by these continuing current intervals it is not known whether such a breach will leave interior cables or other components in proximity to the hole vulnerable. One valuable measurement was made in the early 1990s on a cable behind a burnthrough hole subjected to a return stroke, which yielded relatively low levels of induced voltage and current. But it is not known whether the setup in this measurement captured extreme levels, or what physical principles were at work to prevent more extreme levels from being observed.

We propose in this project to examine both theoretically and experimentally the physical principles at work in the transfer of field and charge through the hole. The goal is to provide a rigorous basis for levels of induced voltages and currents. Such an understanding will allow a more realistic assessment of this physical phenomenon.

Summary of Accomplishments

In FY 2009 we conducted a series of experiments of short circuit current and open circuit voltage behind a burnthrough hole. Initial short circuit current measurements agreed with those from the older tests conducted in the 1990s, however it was identified in these that continuing current intervals between return strokes were more representative of nominal rather than extreme durations of lightning continuing current. In addition, high-speed, time-correlated photography was added in these new experiments, to enable tracking of the burnthrough events with the electrical penetrations. These records indicated that a significant burnthrough hole in the conductive barrier had not yet formed with nominal intervals of continuing current when the second return stoke hit. Because of this, extreme intervals between return strokes were also included in these experiments. These yielded higher levels of collected interior currents and faster rise rates, however voltage levels were no larger than those observed in the older tests.

Indirect coupling levels were predicted for both the electric field, generated by an approaching discharge channel, as well as the magnetic field, generated by return stroke currents attached to the edge of the burnthrough hole. Experiments were also conducted using lower-level sources to validate these calculations. When the most extreme levels of lightning current time rate of change are used in these models, voltage limits are produced that appear to be below standard insulation strengths.

Initial calculations on direct coupling through the hole were also carried out. Electrical breakdown thresholds along electric field lines through the hole to the interior cable and to the surrounding enclosure barrier in ambient air have been calculated. These initial estimates indicate breakdown to the barrier rather than to the interior, in agreement with experimental observations. Finally the return stroke plasma conductivity has been estimated and initial current conduction calculations to the interior performed.

Significance

Opinions about the significance of lightning burnthrough have varied between two extremes (from complete reliance on the referenced test, to a position that safety can no longer be assured). The understanding, as well as models, of the energy transfer process to be developed in this project will provide a quantitative basis on which to make assessments about this penetration, which is relevant for many existing systems.

Considerable progress has been made this year on gaining an understanding of the penetration mechanisms involved in coupling to interior components through burnthrough holes. Presentations have been made throughout the year to the responsible organizations at Sandia. There has been considerable interest from these groups in the results from the first year of the project.

MEMS-Based Nonvolatile Memory Technology

130794
Year 1 of 3
Principal Investigator: M. S. Baker

Project Purpose

Electrical nonvolatile memory (NVM) technologies are currently used for several purposes in nuclear weapons systems. Each purpose has different requirements for the number of bits stored, the speed and power required to read and write, duration of storage without power, erasing/rewriting without a trace of previous storage (lack of remanence), and radiation hardness. The perfect NVM technology does not exist, so compromises are made in system design and operation.

We propose to create a microelectromechanical system (MEMS)-based NVM that would enable new system designs. Data would be represented by the position of a buckled beam, e.g., up or down for 1 or 0, respectively. Electrodes above and below would electrostatically actuate each beam and capacitively sense the position. We believe that this scheme has inherent advantages in radiation hardness, duration of storage, and completely erasing previous data. The focus areas include fabrication of the beam structure, design and integration of the sense/drive electronics, and materials reliability studies.

The fabrication thrust has high risk. While we will build upon several years of improved understanding of stress in polysilicon microbeams, we need to make significant advancements in order to achieve reliable buckling across the entire wafer. Further, in order to achieve low voltage actuation and sensing, we will need very small thicknesses and gaps (on the order of 100 nm). The combination of extremely thin structures and complex residual stresses is formidable.

An integral part of the project will include a materials reliability effort. The performance of the nonvolatile memory device is intimately tied to the elastic mechanical response of the dual-state buckled beam. Creep and fatigue degradation of the structural silicon layer are two potential failure modes over the multidecade lifetime of the component. To address these issues, we will rely on a combination of analytical materials models and long-term testing.

Summary of Accomplishments

The FY 2009 milestones can be categorized into three groups: Design and analysis, fabrication, and materials reliability. We have either met or are on schedule to meet all of our FY 2009 milestones. The first milestone was to model the buckled beam behavior and actuation voltage as a function of beam geometry and residual stress to map out the available design space for a successful buckled beam memory element. This analysis has been completed using the commercial finite element analysis software ANSYS, which is capable of performing fully coupled structural-electrostatic simulations required for predicting actuation voltages.

The bulk of the work in FY 2009 has focused on developing two new silicon fabrication processes for creating the nonvolatile memory beam with a controlled level of residual stress. The first process, called the vertical buckling or out-of-plane process, has been demonstrated in a short loop with successful beam buckling. The second process, called the in-plane buckling or silicon on insulator (SOI) process, is currently in fabrication. These two processes offer different methods of stress control and process complexity in order to minimize the fabrication risk associated with controlling residual stress in the polysilicon beam while also maintaining the necessary feature size control.

A study has been performed to address risks related to the polysilicon material reliability, including material creep, fatigue, and wear. Based on data available in the literature, the polysilicon beams are not expected to experience fatigue failure, as the stress present in the beams is below any measured fatigue limit. To evaluate the risk due to material creep, a theoretical deformation mechanism map was derived for polysilicon with a 0.1-µm grain size using governing equations for the various creep mechanisms. Even at very high stress and temperature, the creep rates are below 10^{-20}/s, resulting in an infinitesimal strain over 30 years.

Significance

This project ties to Sandia's national security mission in the area of nuclear weapons technology development. The advantages provided by this new memory technology would enable new system architectures that would have advantages over existing solutions and would enhance our future weapon system safety, security and use control.

Novel Dielectrics with Engineered Thermal Weaklink

130797
Year 1 of 3
Principal Investigator: S. M. Dirk

Project Purpose

The nuclear safety criteria for a thermal weaklink is that it must fail predictably and irreversibly. We propose to engineer a dielectric system that has a known, predictable failure mechanism built into the polymer backbone that will fail predictably in a designed manner at a designed temperature. At the failure point, the dielectric will be transformed permanently to a conducting polymer with conductivity of an amorphous metal, significantly altering the capacitor's ability to store the necessary charge. In addition, it is projected that under normal environment operation the proposed polymer will provide a significant current leakage path, in effect creating a robust/intrinsic bleed path (*in situ* bleeder-resistor) for removing stored charge when power is removed.

Summary of Accomplishments

Key technical accomplishments for FY 2009 have included a demonstration of switching from a good dielectric to a poor dielectric at controlled temperatures. Furthermore, we have completed a study evaluating how temperature effects the formation of conjugated polymers as a function of leaving group stability. Clearly, judicious choice of leaving group, and moreover, leaving group stability control the temperature at which the dielectric material switches to a conductive polymer. Finally, we have electrically characterized one of our synthesized materials. Our synthesized material has a 100% improvement in the dielectric constant when compared to Mylar. The dissipation factor of both Mylar and our synthesized polymer are very similar.

Significance

Development of a polymer dielectric designed to fail in a predictable manner at a designed temperature would allow for the deployment of a "first principles" thermal weaklink which would greatly improve the safety of the nuclear weapons stockpile.

Signal Processing Techniques for Communication Security

130798
Year 1 of 3
Principal Investigator: R. J. Punnoose

Project Purpose

Wireless communication can enable new logistics and tracking applications for many diverse applications.

The goal of this project is to use time-reversal electromagnetics to provide inherent wireless security at the physical layer by focusing the communication signal at the receiver. This technique has the potential to provide lower probability of intercept/lower probability of detection (LPI/LPD) characteristics to radio communication independent of any spread-spectrum modulation.

The focusing ability of an antenna depends on its size and is limited by diffraction. The Rayleigh diffraction limit makes it impractical to achieve narrow focus for our intended applications since large antennas would be required. Time-reversal techniques have the following properties: a) physical objects in the environment are beneficially used to create a large virtual aperture; b) increased focusing ability; c) no need for knowledge of receiver position; d) no need for line-of-sight.

The object of this project is to a) characterize the focusing ability with respect to the number of antennas and spacing and with respect to the physical objects in the environment, b) selectively detect and reject hostile signals using the time reversal techniques c) simultaneously focus the signal at a desired location and null the signal at undesired locations.

Summary of Accomplishments

In FY 2009, several techniques were investigated for creating channel models of cluttered environments. The time-reversal technique is dependent on the physical environment and thus requires detailed transient electromagnetic simulation. The finite difference time domain (FDTD) method is most suited for providing an adequate simulation environment. Commercial FDTD tools were examined for suitability and were found to be wanting in their ability to create arbitrary clutter objects. We implemented an FDTD simulation environment where arbitrary objects can be placed. To reduce computational complexity, a 2D simulation model was used. This allows for rapid experimentation with time-reversal concepts and algorithmic ideas. Although this will not model a specific 3D scenario, it will give statistical results and will identify the important clutter parameters and their effect on the time-reversal performance

In FY 2009, we managed to extract channel parameters from FDTD simulation and apply it to create a time-reversed signal for focusing. We also experimented with several techniques for nulling the signal at specific locations.

Significance

This work, if successful, will add another dimension of security to wireless communication applications.

Solid State Neutron Sources

130799
Year 1 of 3
Principal Investigator: J. M. Elizondo-Decanini

Project Purpose

The primary goal of the proposed work is to develop neutron sources using solid state technology, including all elements of the neutron production process. The first year primary milestone was to demonstrate the physics behind the proposed ideas using a scaled-down prototype. Successful demonstration of the project ideas will open the door for the application of solid state and microelectromechanical system (MEMS) technology to produce neutron sources en masse and inexpensively.

Summary of Accomplishments

We successfully demonstrated more than twice the expected operating voltage in a device significantly scaled down from present technology: 1) demonstrated ion beam production, 2) with ~10 times the anticipated current, and 3) with pulse lengths in the tens of microseconds, 4) demonstrated neutron production with a nonsealed prototype (neutron calibrations and redundant demonstrations are in progress).

Ahead of schedule, we demonstrated the use of MEMS technology to produce the basic elements of a neutron source. Given the geometry and the scale of the device, this represents a significant development for mass production of inexpensive neutron generators.

Significance

The proposed technology uses integrated solid state and MEMS architectures for the production of neutrons. This allows the sources to be disposable and/or easily replaceable, thus providing flexibility. It provides a new design opportunity for future devices where neutron sources are required, such as agile portable and large arrays for homeland security monitors, programmable rugged sources, microsized medical applications, and replacement of present sources.

Understanding and Predicting Metallic Whisker Growth and its Effect on Reliability

130800
Year 1 of 3
Principal Investigator: D. F. Susan

Project Purpose

Tin whiskers are conductive tin filaments that grow from tin-plated surfaces, such as surface finishes on electronic packages. The phenomenon of tin whiskering has become a major concern in recent years due to requirements for lead-free soldering and surface finishes in commercial electronics. At Sandia, tin whiskers are a reliability concern due to increased use of commercial off-the-shelf (COTS) parts and possible future lead-free requirements in high-reliability microelectronics. In general, pure tin finishes are more prone to whisker growth than their Sn-Pb counterparts and high profile failures due to whisker formation (causing short circuits) in space applications have been documented. Despite the long history of tin whisker research and the recently renewed interest in this topic, a basic understanding of whisker growth is required to develop suitable quantitative modeling and prediction methodologies.

It is proposed that, through a combination of carefully designed experiments and computational modeling, an understanding be developed of the underlying mechanisms that control the nucleation and growth of tin whiskers. Experimental work will include the effects of critical variables such as tin microstructure, grain orientation, and temperature on the propensity for tin whisker formation. Electron backscatter diffraction (EBSD) will be used to determine the role of tin grain orientation on whisker development. The focused ion beam transmission electron microscopy (FIB/TEM) technique will be used to extract samples directly from the root of tin whiskers in order to study the nanoscale structure associated with tin whisker growth. Concurrently, computational modeling, which is based on molecular dynamics techniques for describing stress-driven mass transport processes, will be developed to predict transport mechanisms feeding whisker development. Understanding the mechanism may enable prediction of when whiskers will grow and, ultimately, this knowledge will allow for control of whiskers and elimination of the problem in long-term, high-reliability applications.

Summary of Accomplishments

In the first year of this project, tin whiskers were successfully grown from as-deposited (no applied stress) tin coatings on copper substrates. The best results have been from alkaline tin plating baths. The results from methane-sulfonate baths have been less successful with no observed whiskers.

Scanning electron microscopy (SEM) characterization is ongoing, with observation of tin whiskers soon after plating and as a function of time afterward. The whiskers continue to grow and new whiskers nucleate for several weeks after plating. It is apparent that long “prototype” whiskers are fairly rare. However, many other small nodules or short whiskers are observed. Most importantly, taken together these many small whiskers generate significant new surface area and volume “pushed up” from the surface. The strain relief mechanism is presumed to be volumetric in nature. Techniques are being developed to measure these quantities. The goal is to measure the nucleation site density and the other quantities as a function of both temperature and applied strain. The whisker mechanism likely involves recrystallization followed by a grain growth stage in the form of whiskers. Recently, dynamic recrystallization has been put forward as a whisker growth mechanism and some of our results may provide support for this theory.

So far, SEM has been successfully applied to whisker characterization. We have also applied the FIB technique for cross-sectioning through whiskers. There have been difficulties with ensuring thermal “grounding” of whiskers to prevent melting under the electron beam. These techniques are currently being developed. EBSD has been used to successfully determine the crystallographic growth direction. Based on analysis of 40 whiskers, this newly developed technique has shown that the <100>, <001>, and <101> directions (tetragonal Sn crystal structure), are the preferred growth directions for tin whiskers.

Significance

This proposed work exercises Sandia’s unique materials characterization capabilities in a challenging way and will maintain our expertise. Tin whiskering is of increasing concern for NW, satellites, and homeland security applications. As such, it is a very relevant research field for Sandia, considering our emphasis on high reliability microelectronics, the shift toward COTS parts, possible future Pb-free requirements, and the shift of the supplier base to Pb-free processes. Furthermore, it will be possible to apply the techniques and modeling tools developed in this work to other, yet unforeseen, materials problems involving thin films, diffusion, and residual stress.

Tin whisker growth is a serious problem which has caused past failures of high-value electronics and it is especially critical with regard to high-reliability electronics required for NW. The underlying motivation for research is the move toward Pb-free COTS parts and likely future requirements for Pb-free electronics, which will bring the issue of tin whiskers even more into the spotlight. This complex problem is an opportunity for Sandia to make significant scientific contributions in the areas of diffusion, nucleation and growth, and stress-relief mechanisms. Despite the resurgence of interest, there are still few landmark studies and there is no generally accepted theory for whisker growth. Our “bottom-up” approach to analyzing tin whiskers could represent a major leap forward in understanding this unusual phenomenon, and forms the foundation for meaningful plating/soldering process design and quantification of margin and uncertainty (QMU) assessment. The goals are to be able to predict and, ultimately, eliminate whisker growth in long-term high reliability applications.

Refereed Communications

P.T. Vianco and J.A. Rejent, “Dynamic Recrystallization (DRX) as the Mechanism for Sn Whisker Development, Part I: A Model,” *Journal of Electronic Materials*, vol. 38, pp. 1815-1825, September 2009.

P.T. Vianco and J.A. Rejent, “Dynamic Recrystallization (DRX) as the Mechanism for Sn Whisker Development. Part II: Experimental Study,” *Journal of Electronic Materials*, vol. 38, pp. 1826-1837, September 2009.

Vapor Phase Lubrication for Advanced Surety Components

130801
Year 1 of 3
Principal Investigator: M. T. Dugger

Project Purpose

Future weapon architectures will employ surety components with smaller dimensions than legacy components. These may use materials ranging from engineering alloys to silicon. Materials selected for manufacturability, strength, etc., frequently exhibit poor friction and wear properties, necessitating lubricants. Conventional solid lubricants oxidize, increasing friction and wear and uncertainty in performance with age. Depositing lubricants uniformly without damage is difficult with current methods and impossible with shrinking component dimensions. Recent alternatives such as impingement MoS_2 and diamond-like carbon have met current life extension program requirements, but will be difficult to deposit uniformly with controlled chemistry and adhesion on smaller parts without damaging them. The elimination of hazardous solvents has created a critical need for new stainless steel bearing lubricants.

The goal of this project is to develop a completely new paradigm for surety component lubrication known as vapor phase lubrication, or VPL, that will provide a low friction film of molecular dimensions that is self-healing, and that forms automatically during sliding on small parts of complex shape. The underlying scientific discovery has already been demonstrated and reported by the principal investigator. VPL is based on a reaction between gas phase molecules and the surface that forms a lubricant film only at contact locations. This approach has shown a 10,000 fold increase in operating life of silicon micromachines without failure, and recent experiments indicate that VPL is also effective on stainless steel. The use of VPL in weapon components requires understanding the reaction mechanisms, optimizing vapor chemistry for different substrates, developing vapor delivery strategies compatible with weapon components, investigating aging of the resulting film, and determining the compatibility of the vapor with other component materials. Significant development, with relatively high risk, is required to mature VPL for the range of weapon operating temperatures required and to create vapor delivery approaches.

Summary of Accomplishments

Recent work has shown that as contact pressure is increased, a higher concentration of pentanol vapor is required to prevent wear. At sufficiently high vapor pressure, wear is prevented without polymerization and deposition of reaction product. Therefore, accumulation of reaction product, which was feared to eventually degrade device frictional behavior and electrical contact resistance, is not required for effective lubrication. Quantitative head space gas analysis has been developed to understand the vapor amounts and composition in a closed system. The analysis method results in the expected linear relationship between absolute vapor quantity and sample volume determined by gas chromatography for small volumes, and has ppm sensitivity for 0.3 mL sample volume.

Many different epoxy resins have been synthesized and loaded with pentanol to investigate controlled release. Several building blocks were incorporated that will ultimately influence vapor phase equilibrium concentration. Of these, multiple matrix materials that show an ability to release pentanol have been identified. Several routes to accomplish on-demand delivery have also been evaluated. A bisammonium salt has been synthesized and evaluated with thermogravimetric analysis (TGA). The sample produced the desired olefin, but degraded soon after olefin delivery, prompting modification of the counter ion to lower delivery temperature.

Extended duration operational (mechanical life) testing has shown that VPL dramatically reduces wear and debris generation in both crystalline and polycrystalline silicon microelectromechanical systems (MEMS). Test methods and devices have been established to determine effects of VPL on both friction coefficients as well as adhesion energies in MEMS devices. Nine electrical contact stronglink (ECS) prototype units are being modified to allow the same unit to be tested in dry followed by VPL environments. The test methodology consists of measuring minimum operating time, minimum operating voltage, electrical contact resistance, and visual inspection of contact surfaces following life testing.

Significance

The proposed approach will free designers from accommodating lubricant thickness in dimensional tolerances, avoid the need to apply lubricants to small parts of complex shape, and result in a simpler, more reliable product at reduced cost. The result will be improved yield and reduced variability, thereby improving our ability to quantify margins and uncertainties. Application of VPL to complex devices would be applicable to mechanisms for defense systems and commercial applications as well.

New Safety Architectures Enabled Through the Use of Advanced Technologies

138705
Year 1 of 1
Principal Investigator: E. Wilson

Project Purpose

Enhanced Nuclear Detonation Safety (ENDS) was created more than 30 years ago and has been implemented using electrical isolation using barriers, stronglinks and weaklinks. All of the systems fielded since the development of ENDS have similar high-level architectures. System barriers are based on standing off unintended energy transfer between exclusion regions using isolating stronglinks that utilize robust mechanical discriminators. Disadvantages in current nuclear safety implementations include the high cost due in part to rugged mechanical stronglinks and the lack of fail-safe mechanisms for critical abnormal environments such as mechanical shock. In addition, large volume and mass allocations have been needed to attempt to meet the stringent requirements for isolation of unintended energy based architectures.

Recently developed ideas offer potential options to rethink how we achieve nuclear safety. These new ideas, however, cannot be inserted into existing safety architectures as a one for one replacement. A fresh implementation of the ENDS approach is needed to create opportunities for these ideas.

Summary of Accomplishments

We have demonstrated that it is possible to cut 304 stainless steel with deposited pentaerythritol tetranitrate (PETN). The minimum geometry of PETN that would cut 0.13 mm (0.005 in.) thick steel was 0.75 µm wide and 140 µm thick. Future work on explosive cutting should consider geometry, mask design, confinement, detonation wave collision, different explosive materials, and the free volume into which the cut expands.

Recommendations for future work include investigating mask designs that will allow a continuous ring of explosive to be deposited. For future work, a continuous ring with a consistent width could be used. Mask designs that could take advantage of detonation wave interactions and the resulting mach stem at colliding waves could potentially enhance the precision of a cut. Investigating other materials that have a higher output than PETN could potentially lead to more efficient cutting as well. Improvements on confinement of the explosive on the sides of the deposited film could enhance propagation and energy transfer into the metal to be cut.

We have also demonstrated through notional designs that SMA (subminiature version A connector) technology could be used to increase safety margin while also reducing the complexity of the design. The implementation of SMA technology into a stronglink to make it inherently locked should also be explored further in advanced development efforts. SMAs have already been utilized in current stronglinks (in a capture application), could enhance nuclear safety without significantly affecting reliability. Additionally, further evaluation is required to assess the impact of radiation exposure to nitinol in weapon applications.

Significance

Currently, our stronglinks rely on the robustness of their discriminator/drive mechanism to ensure that the energy coupler does not become enabled. A large amount of work is applied to the discriminator/drive mechanisms so they meet abnormal mechanical, electrical, and thermal environments. Success would provide simpler and lower cost ENDS architectures that could be developed and manufactured in less time, while improving safety.

Advanced Tritium Storage Science

138804
Year 1 of 1
Principal Investigator: D. F. Cowgill

Project Purpose

Helium created in tritium storage materials limits their useful life. New storage materials are being researched that either retain little helium or sequester it in slowly aging bubbles. However, material selection is often limited by slow tritium extraction kinetics. Research on materials that satisfy the needs for both helium control and rapid tritium extraction is ongoing; however, since tritium-based experiments exploring the aging behavior of these characteristics are extremely complex and require long shelf-life studies, progress will remain very tedious if it relies solely on aging studies. This project explored a new method for generating insoluble gas bubbles in storage materials – one that holds potential for evaluating bubble evolution in a tritium-free environment. The approach generates hydrogen gas bubbles in storage hydrides by pulse heating the material with a transient too rapid for the hydrogen to escape through the surface. The super-saturated hydrogen accumulates in small bubbles whose spacing is determined by hydrogen diffusion during the transient. Repeating the process should force these surrogate bubbles to follow the same evolutionary behavior experienced by helium bubbles in the tritide; i.e., the same bubble interaction physics, mechanics of inter-bubble fracture, and fracture network percolation. The technique holds promise for screening prospective tritium storage materials and for further testing of our bubble evolution models. The project also examined a means of fabricating nanodimensional storage material capable of low helium retention and a reactive gas scheme for rapidly extracting hydrogen (tritium) from the storage material.

Summary of Accomplishments

Several needs for the development of advanced tritium storage materials were explored. First, we examined the possibility of creating hydrogen bubbles in hydrided materials as surrogate structures for the study of naturally occurring helium bubbles in tritides. We showed that bubbles can be created by rapid hydride decomposition using thermal pulses generated with both joule and laser heating techniques. Joule heating created large bubbles throughout bulk foil ribbons in sufficient quantity to be examined by nuclear magnetic resonance (NMR) techniques. Hydrogen NMR of the ribbons showed the room temperature spin-lattice relaxation is modified from the solid hydride characteristic by rapid hydrogen transport between the hydride and gaseous bubble phases, providing information on bubble volumes and internal bubble surface areas. The shorter thermal pulses generated by laser heating created, in the near-surface region, the much smaller bubbles characteristic of helium bubbles in metal tritides. In a separate effort, we produced nanodimensional storage material in the form of metal hydride nanowires from electrodeposition of the metal into ion tracks created in a dissolvable polycarbonate mold. Wire diameters as small as 10 nanometers were generated in quantities large enough to permit measurements of hydride formation. Lastly, we examined the rate and efficiency of gaseous hydrogen generation from the easily controllable exothermic gas-solid reaction. We found the reaction rate and degree of completion depend on the quantities of species used and the physical characteristics of the solid reactant. When coupled with a solid reactant satisfying the helium control requirement, this approach can provide a new means of generating gaseous helium-free tritium.

Significance

The three advances expand the potential approaches for tritium storage. They enhance the list of material candidates and provide a new means for evaluating aging effects that minimizes the need for complex, long-term tritium experiments. The new surrogate bubble tool will also be valuable for enhancing the fidelity of our current tritide aging model through additional tests of current assumptions and evaluations of fundamental model parameters. This model supports planned tritium experiments aimed at comparing early helium bubble development in new storage materials and provides guidance and testing to new storage concepts and material development. The potential for rapid, controlled tritium extraction by gas-solid tritide reaction will allow the use of atypical storage materials. These advances may also prove useful for creating new advanced hydrogen storage materials for commercial applications. Their continued development will complement and provide new directions to the Sandia-managed Metal Hydride Center of Excellence.

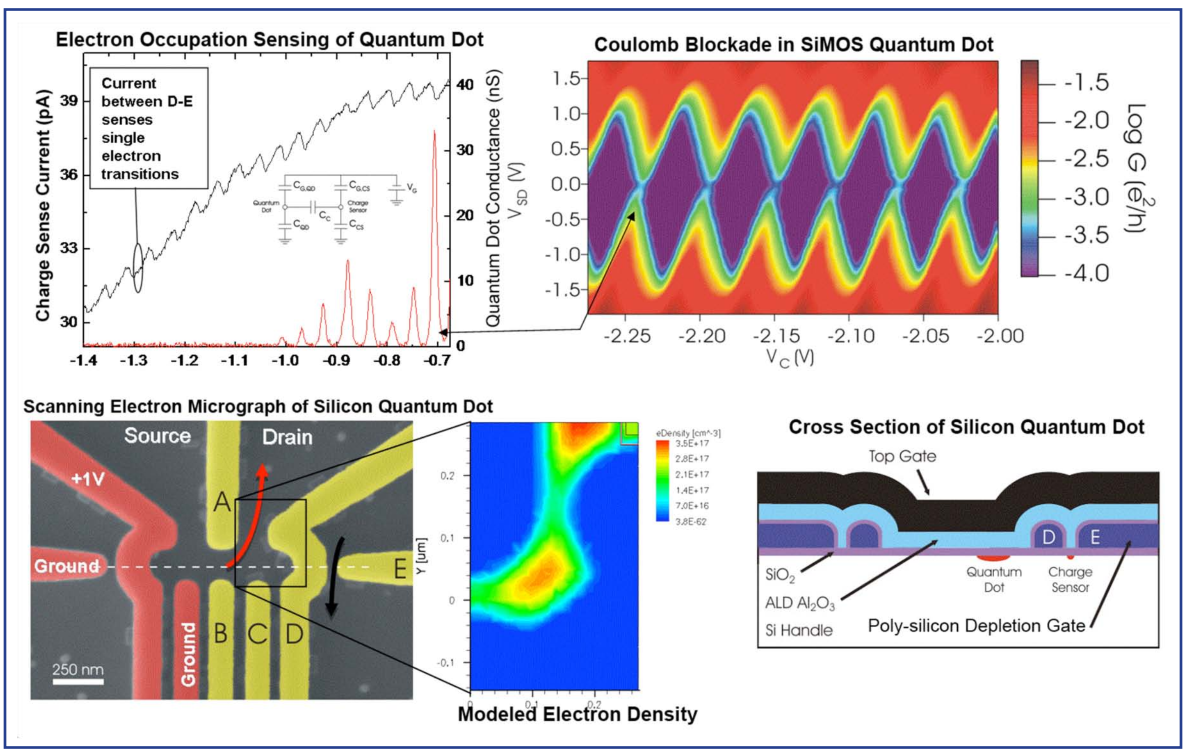
GRAND CHALLENGES INVESTMENT AREA

Grand challenge projects are designed to address scientific challenges and urgent national security issues that are broad in scope and potentially game-changing in their impact. As such, these projects require the assembly of often large, always interdisciplinary teams of scientists and engineers, and are commonly funded at an annual level of from $1M–$5M. Examples come from areas such as quantum computing, sensor architectures for moment-to-moment surveillance of the environment, nanoscience applications in high-power laser technologies, molecular immunology studies at single-cell resolution, and computational approaches to the discovery of clandestine terrorist networks.

Quantum Information Science and Technology

Project 119352

Potentially capable of solving problems that are intractable for current computers, quantum computers are viewed as a key adjunct to classical computers, particularly in the realm of data searching, cryptanalysis, certain optimization problems, secure communications, and in quantum theory itself. The first step in engineering such a device is the realization of physical quantum bits (qubits), and it would be highly desirable were this to be accomplished in silicon, thereby rendering integration with classical computer circuitry far easier, as well as optimizing a quantum property of electrons known as spin decoherence time (a limiting factor for qubits previously developed in gallium arsenide). In this project, quantum bits are being pursued through the use of silicon double quantum dots and the electrostatic confinement of single (or a small number of) electrons, whose quantum property of spin serves to represent the different states of the bit. The quantum circuit must also be designed to perform error correction. Additionally, a cryogenic (functional at 4 K) classical-quantum interface circuit has been developed, and a qubit modeling capability is operational and is being used to guide further design.

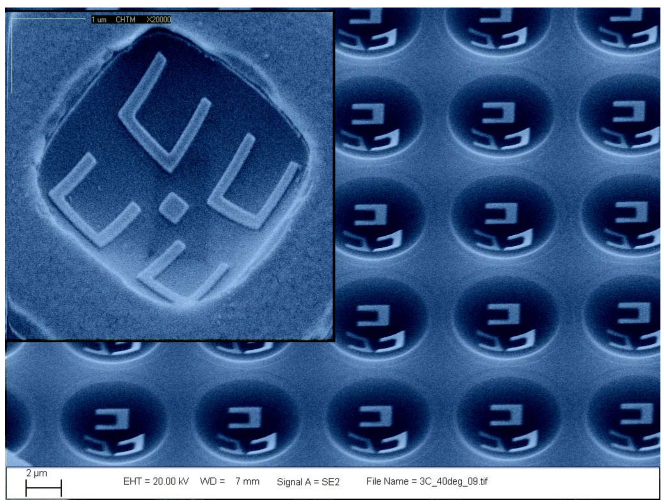


A collection of results for the pictured (in electron micrograph and cross-sectional drawing) dual silicon quantum dot qubit.

Metamaterial Science and Technology

Project 131302

Artificially constructed materials not found in nature, metamaterials represent a new frontier in materials science, in the sense that materials can be designed and created — through micro- and nanofabrication — with particular purposes in mind. To operate in this novel realm requires integration of many functionalities, from design and simulation, to synthesis, fabrication, and characterization. This project is conducting just such ground-breaking research, with particular emphasis on materials that are optically active in several ways, for example as refractive lenses, photon funnels, and as cloaking devices, in which virtual invisibility is the goal. Using a layered approach, where each layer is composed of a two-dimensional array of nanostructures, the project is seeking to manipulate long-wavelength infrared (LWIR) in a low-loss fashion. The project is developing new fabrication processes as well as new methodologies to analyze its fabricated metamaterials.



Colorized scanning electron micrographs of newly fabricated infrared metamaterials.

GRAND CHALLENGES INVESTMENT AREA

Highly Pixelated Hypertemporal Sensors for Global Awareness

95211
Year 4 of 4
Principal Investigator: R. R. Kay

Project Purpose

This project was organized into four sub-teams: system engineering, silicon circuits, packaging, and opto-electronic high speed data interconnect. Each team worked independently to complete milestones and demonstrations throughout the project in support of a single integrated concept.

The final demonstration of the use of through-silicon-vias to provide electrical interconnect between vertically integrated silicon signal processing layers was unable to reach completion in FY 2008, due to delays in getting materials from a third-party vendor. In collaboration with Ziptronix, our partner in the 3D integration concept, a decision was made to use Chartered Semiconductor, in alliance with Tezzeron Inc., to fabricate complementary metal oxide semiconductor (CMOS) wafers with integrated through-silicon-vias. The designs were provided to Tezzeron, after their participation in a critical design review, in early March, 2008. Fabrication was to have begun immediately following design receipt by Charted Semiconductor. Unfortunately this did not occur due to circumstances beyond the control of Sandia. Wafer fabrication delayed the final assembly of the 3D test vehicle by Ziptonix and Sandia beyond the end of the FY 2008.

In order to complete this integrated packaging test vehicle demonstration, the project team requested and received approval for an extension into FY 2009 in order to complete assembly and test of this packaging test vehicle. Completion of the packaging test vehicle would represent the validation of the overall assembly architecture for signal processing rich, very large area focal plane arrays.

Summary of Accomplishments

The project achieved numerous accomplishments over its life. Some of the most notable are the following:

- Development of a remote sensing system evaluation software environment. This tool allows modeling of earth background scenes as observed from an orbital platform. The structured scene is rendered onto the focal plane array pixels by including effects of optical system blur and instrument line-of-sight jitter, creating a time varying signal per pixel. Transient targets of interest can be superimposed upon this background such that evaluation of target detection in the presence of background can be evaluated.
- Focal plane array architectural definition to support 2K x 2K pixels sampled at 10,000 samples per second per pixel with high frequency information of interest.
- Demonstration of this circuit architecture by fabrication and test of an integrated circuit (chip) which demonstrates the overall performance and functionality. The test chip has been evaluated and undergone a second iteration. Functionality of the circuit architecture has been demonstrated.
- Development of a tiled, layered integration architecture which allows assembly of a large (up to 80 millimeters per side) focal plane array from smaller more easily produced tiles (15–20 millimeters per side). The tiles are abutted with only a 10 micrometer gap, allowing a seamless coverage of the focal plane field of view.

- Completion of a “phase I” packaging and integration device that demonstrates electrical and mechanical interfacing of a 4 x 4 grid of 15 mm on a side silicon tiles to a silicon motherboard. The device demonstrated the feasibility of the assembly processes required to implement the integration architecture.
- Design and tapeout of 2-layer CMOS active circuitry to mimic the pixel and digital signal processing layers of the focal plane array architecture, as well as a silicon motherboard for CMOS tile integration.

Significance

The results of this Grand Challenge LDRD project will have benefit to many future remote sensing missions. The technologies being developed will enable improved performance over the current state-of-the-art focal plane arrays, a path to implement complex and advanced pixel architectures; reduced size, weight and power for space flight missions, and direct application to advance other non-focal plane array circuits.

Network Discovery, Characterization and Prediction

119351
Year 2 of 3
Principal Investigator: W. P. Kegelmeyer

Project Purpose

Many of the most pressing threats to our national security are enabled by networks of proliferators, terrorists, hackers, financiers and recruiters. We may preempt individual attacks, but if the network survives, the threat remains. Under this Grand Challenge project we will discover the means to identify and analyze these networks, creating unprecedented decision-support capabilities for Sandia and the Nation.

The project will combine aspects of data fusion, advanced visualization, novel analysis techniques and predictive simulation. We will be building upon world-class capabilities already at Sandia in technical analysis, information visualization, high performance graph analysis, and prediction. The project will encompass six directorates combining application expertise, mathematics, high performance computing, knowledge management, and human factors. We will use a spiral management model in which we iteratively bundle the fruits of our research into prototypes for analyst use and feedback.

The challenges associated with discovering, characterizing and predicting adversarial networks are enormous, and will require research and development across a broad range of areas. We will,

- develop advanced methods for fusing heterogeneous data coming from cyber events, intelligence reports, communication links, financial transactions and more;
- invent new techniques for predicting network behavior with and without interventions;
- create scalable exploration and analysis environments that allow an analyst to work with orders of magnitude more information than before, and gain insights orders of magnitude faster; and
- perform fundamental research in the quantification of uncertainty for the intelligence domain.

This fundamental, high-risk research will result in specific Sandia capabilities, but will also broaden and deepen expertise in informatics. As more and more of our Laboratory missions focus on knowledge processing, the capabilities resulting from the project will provide the foundation for many future undertakings.

Summary of Accomplishments

- We built and repeatedly demonstrated our first prototype, harvesting and delivering advances in newly researched informatics algorithms and visualization methods, addressing four cyber forensics use cases formally elicited from Sandia analysts.
- We engaged in and documented many efforts to evaluate the effectiveness of our research and prototypes from the analyst perspective. As an example, we have identified significant user interface issues in the first prototype, and provided documentation on those issues in time to tackle them in the user interface of Prototype 2.
- We have completed parallel implementations of two basic tensor algorithms (PARAFAC and Tucker).
- For graph characterization, we have developed scalable graph metrics such as vertex betweenness, degree distribution, degree-degree correlation, assortativity, clustering coefficient and pseudo-diameter, and implemented engines for descriptive, correlative, contingency, order and multi-correlative stats, and for principal components analysis. Further, in the first half of FY 2009 we parallelized five of those six engines.

- We have conducted predictive analysis of social learning networks. Analysis of co-evolving games and sub-state proliferation is underway. One insight stemming from this work is that the “predictability” of a network can possibly be assessed in advance of, and separate from, any concrete prediction. This assessment can recommend observables upon which to best base predictions, or to advise that prediction might not be possible with the data at hand.
- We designed and delivered P2, a prototype for making sense of documents that has, among other features, the novel capability to uncover links between pairs of entities that are never mentioned in the same document.
- In a novel demonstration of running an informatics application on a high-performance computer, we performed real-time pairwise similarity calculations on Red Storm to permit interactive clustering of large corpora of multilingual documents, and visualization of those clusters.

Significance

We see significant applied impacts in several national security mission areas, especially cyber security and nonproliferation analysis. Our focus on cyber security in the first prototype has proved prescient, as the US government has shown a marked acceleration of attention to cyber security in just the past year. Similarly, the intelligence community is increasingly interested in advanced informatics to support counterproliferation and technology surprise analyses.

Informatics projects at Sandia have been, up to now, small and largely disjoint. This Grand Challenge project coalesces that work, leveraging it to connect with new research in areas where Sandia can establish a leadership position and make a difference to the nation’s “big data” challenges; it provides a unifying programmatic focus that defines a sustainable science and technology research area.

The project’s work is relevant to a range of Sandia programs. For example, capabilities demonstrated in our first prototype are already relevant to cyber security applications. Complex data problems exist in remote sensing, energy systems, stockpile stewardship, and numerous other national-scale problems. Further, there are large data problems encountered by decision-makers in energy, critical infrastructures, transportation, and national defense. We see the NGC developing capabilities that can be leveraged across multiple problem areas.

In sum, the Network Grand Challenge project is creating a unique capability to answer currently unanswerable questions. In the future, we see that capability being applied beyond the field intelligence element (FIE); our advances are likely to be pertinent anywhere the data is so complex or so voluminous as to defy its effective use.

Quantum Information Science and Technology

119352
Year 2 of 3
Principal Investigator: M. S. Carroll

Project Purpose

The vision for this Grand Challenge project is to develop the quantum equivalent of a scalable classical transistor which may eventually realize the full potential of quantum computation (QC).

To achieve this vision, the focused goal for this program is to generate the computer engineering design for a self-sustaining error corrected logical quantum bit (qubit) and demonstrate the critical hardware element necessary to build it, a silicon qubit scalable to a logical qubit.

The current limitations to realizing a logical qubit are the following:

- Non-solid-state approaches appear intractably large for integration and scaling to a logical qubit
- Decoherence times of other non-silicon solid-state approaches appear to be intractably short (e.g., GaAs & Josephson junctions)
- Physically realizable fault-tolerant architectures that address the realities of integrating quantum circuitry with classical control do not exist
- Demonstration of physical qubits in silicon remain elusive

To address these fundamental limitations we propose to:

1. Develop scalable silicon quantum circuit hardware by implementing a recently successful GaAs qubit geometry in silicon. Demonstration of Si qubit hardware with long decoherence time will represent a world first and will be a critical step towards viable quantum circuitry.
2. Develop an efficient fault-tolerant architecture to utilize the Si qubits with the guiding goal of implementing a self-sustaining error corrected logical qubit. This computer engineering design, supported by critical hardware experiments for a model validation, will be a differentiating capability to assess the silicon approach and to provide direction for hardware development.

Summary of Accomplishments

The project has met or exceeded the milestones and made significant contributions that are increasingly being recognized by the outside community.
Specific accomplishments are as follows:

<u>Si dual quantum dot (DQD) qubit</u>

- Front-end/back-end process steps characterized and improved to yield first disorder free quantum dot behavior (one paper published, one paper at review and approval stage, and invited talks presented)
- Samples of front/back-end platform supplied to outside users in QC community (National Institute of Standards and Technology [NIST], Princeton University, Lawrence Berkeley National Laboratory [LBNL])
- Valley splitting measurements completed (paper in progress)

Second-generation DQD qubit

- Donor implanted device fabrication in progress
- Geiger mode single ion detection paper (paper published)
- SiGe growth on strained silicon on oxide completed and tests in progress

Classical-quantum interface

- Individual CMOS7 (complementary metal oxide semiconductor 7) cryogenic circuit elements tested at 4 K (invited talk and paper in progress)
- Digital read-out and current amplifier designed and demonstrated at 4 K (2 invited talks, 1 paper published, and paper in progress)
- Initial electronics constraints for logical qubit (paper in progress)

Qubit modeling

- 3D finite elements capacitance model developed and used to verify disorder-free dot (paper at review and approval stage)
- 3D technology computer aided design (TCAD) (Synopsis: Sentaurus) model developed and used to identify significant DQD design guidance
- Design of exchange interaction in double quantum dot (paper submitted to Physical Review Letters)

Logical qubit

- Developed physical layer model for Si double quantum dot qubit: native gate set, error models, and electronics constraints for double quantum dot logical qubit (error corrected memory)
- Monte Carlo threshold analysis of Bacon-Shor logical qubit using physical layer model (paper submitted)

Communication
20 invited talks, 7 papers published, 1 accepted, 4 submitted, 2 at review and approval stage

Significance

Quantum information science and technology impacts national security in the areas of secure communications, novel sensing and information processing. Certain algorithms, which are intractable on traditional classical computers, can be efficiently solved using a quantum computer. These problems include exact quantum simulations, optimization problems, and unstructured searches of large databases. Efficient solutions to these problems could lead to breakthroughs important to DOE, DHS and national security.

Refereed Communications

L.A. Tracy, et al., "The Observation of Percolation-Induced Two-Dimensional Metal-Insulator Transition in a Si MOSFET," *Physical Review B*, vol. 79, p. 235307, June 2009.

R. Rahman, et al., "Atomistic Simulations of Adiabatic Coherent Electron Transport in Triple Donor Systems," *Physical Review B*, vol. 80, p. 035302, July 2009.

Eric Nordberg, et al., "Enhancement Mode Double Top Gated MOS Nanostructures with Tunable Lateral Geometry," to be published in *Physical Review B*.

Metamaterial Science and Technology

131302
Year 1 of 3
Principal Investigator: M. B. Sinclair

Project Purpose

Metamaterials form a new class of artificial electromagnetic materials that have the potential to enable a wide range of revolutionary new optical devices and profoundly impact National Security applications. For example, theoretical designs for electromagnetic structures capable of rendering objects invisible at chosen frequencies have recently been proposed and validated using radiofrequency (RF) metamaterials. However, progress toward practical implementation of metamaterials, particularly at infrared and visible frequencies, has been hampered by high absorption losses of the metallic structures used in most metamaterials. The goal of this project is to create low-loss infrared metamaterials through a comprehensive approach using new geometries, material sets, and nanofabrication techniques. Achievement of this goal will also represent a first step toward increasing bandwidth and providing tunability. This effort leverages Sandia's extensive capabilities in nanomaterials, nanophotonics, electromagnetic theory and modeling, high performance computing, materials science, electromagnetic characterization, and micro/nano fabrication. This project will demonstrate low-loss, three-dimensional infrared metamaterials that manipulate electromagnetic waves in a volumetric manner. Such metamaterials are expected to impact a broad range of Sandia missions. The ability to control the 3D paths of optical rays using these metamaterials also relaxes the constraints of normal optics and will enable other novel devices such as super-light, thin and fast lenses and concentrators. They will provide the capability to arbitrarily engineer key optical material properties, to enable new optical designs and devices which can dramatically lower the size, weight, and power (SWaP) in nonproliferation and defense applications. Furthermore, this capability might also enable spin-off programs in RF metamaterials for high-impact national security applications. The exploding international research in this technologically disruptive area also mandates a leadership position in this field.

Summary of Accomplishments

We have made substantial technical progress toward our goal of developing useful infrared metamaterials. We have fabricated several different metal-based metamaterials to exercise the complete design/fabricate/characterize cycle. To analyze the results, we have constructed detailed split ring circuit models, and have developed parameter retrieval code for both isotropic and bi-anisotropic metamaterial. We have also used these metamaterials to perform first ever measurement of infrared metamaterials using time domain spectroscopy techniques. To investigate the dielectric resonator approach to low-loss metamaterials, we have developed an advanced effective media theory for cubic lattices of one-phase and two-phase spheres. In addition, we have fabricated and are testing dielectric sphere based metamaterials in the radiofrequency spectral range. Furthermore, we have performed the first ever high performance computing simulation of a finite metamaterial structure (a five layer dielectric sphere metamaterial) to investigate negative refraction, boundary layer effects, surface waves, and scattering in metamaterials. To investigate polaritonic metamaterials, we have fabricated 2-dimensional metamaterials from epitaxial silicon carbide thin films, and we have begun to synthesize and characterize the infrared properties of other polaritonic materials. For metamaterial theory, we have begun an examination of losses and scaling associated with best case designs of metallic metamaterials in an effort to understand and place fundamental limits on achievable levels of transparency with these structures. For advanced three-dimensional fabrication of metamaterials, we have begun to develop polymers, polymer foams, and sol-gel fluorides that exhibit low-loss in the thermal infrared and can be used as matrix materials. We have also developed a new approach to the fabrication of three-dimensional metamaterials through directional evaporation. For phase sensitive characterization of metamaterials, we have developed a tandem interferometer system and have initiated development of an ultrafast laser based time domain spectroscopy system.

Significance

Our key R&D accomplishments will be of great benefit to the general S&T community in several ways. First, we will quantitatively establish the theoretical limits of metamaterial performance in a number of key areas, including transparency. This understanding will help to close the “hype gap” and will assist researchers to determine which applications can truly benefit from metamaterial technology. Although our project is primarily focused the development of useful metamaterials for application in the thermal infrared, we believe that many of the insights that we developed will be applicable across spectral ranges, from the visible to the RF, and thus be of use to a wide audience. In the infrared, we will demonstrate the use of new material sets and fabrication techniques for the production of advanced 3D metamaterials that approach theoretical performance limits. Our high performance computing efforts will demonstrate new computational methods that can be used to extend electromagnetic modeling to extremely large problems. Such a capability would be applicable to a wide range of electromagnetic design and simulation problems, and would be relevant over a wide range of frequencies. We will also demonstrate advanced phase-sensitive infrared characterization tools that can be used for a wide variety of investigations. In addition, our R&D accomplishments will provide the capability to arbitrarily engineer key optical material properties, to enable new optical devices with dramatically lower size, weight, and power requirements. Such devices have the potential to impact a broad spectrum of national security, nonproliferation and defense missions.

Refereed Communications

D.J. Shelton, D.W. Peters, M.B. Sinclair, I. Brener, L.K. Warne, L.I. Basilio, K.R. Coffey, and G.D. Boreman, “Effect of Thin Oxide Layers on Resonant Frequency and Amplitude in Infrared Metamaterials,” to be published in *Applied Physics Letters*.

Reimagining Liquid Transportation Fuels: Sunshine to Petrol

131303
Year 1 of 3
Principal Investigator: J. E. Miller

Project Purpose

The purpose of this project is to develop a technological solution to two of the most daunting problems facing humankind: energy security and climate change. Our vision is captured in one deceptively simple chemical equation:

Solar Energy + xCO_2+ $(x+1)H_2O \rightarrow C_xH_{x+2}$ (liquid fuel) + $(1.5x+.5)O_2$

Practical implementation of this equation seems far-fetched since it effectively describes the use of solar energy to reverse combustion. However, it also describes photosynthesis and, as such, summarizes the biomass approach to fuels production. Regrettably, photosynthesis and consequently the biofuels approach have a very low sunlight-to-hydrocarbon conversion efficiency and suffer from a number of other shortcomings. Thus, developing an alternative approach that more-directly and -efficiently produces a liquid fuel is desirable. The development of a process that sustainably and cost effectively reenergizes thermodynamically spent feedstocks to create reactive fuel intermediates would be an unparalleled achievement and is the key challenge that must be surmounted to solve the intertwined problems of accelerating energy demand and climate change. We propose that the direct thermochemical conversion of CO_2 and H_2O to CO and H_2, which are the universal building blocks for synthetic fuels, should serve as the basis for this revolutionary process. To realize this concept, we are addressing and solving the complex chemical, materials science, and engineering problems associated with thermochemical heat engines and the crucial metal-oxide working-materials deployed therein.

Summary of Accomplishments

Accomplishments for each of the principal focus areas are the following:

Materials

- Evaluated density functional theory (DFT) functionals for metal substituted ferrites; path forward identified for modeling most materials of interest.
- Developed computational method to predict iron solubility in yttria-stabilized zirconia (YSZ); Demonstrated and characterized thermally driven iron oxide transformations and migration in and out of YSZ substrates via in-situ x-ray diffraction, microscopy, etc.
- Developed procedures for analyzing and imaging YSZ samples by low energy electron diffraction (LEED) and low energy electron microscopy (LEEM); expanded ultrahigh vacuum capabilities.
- Collected kinetic data for model materials in stagnation flow reactor (SFR); correlated results with presence of spinel phase; developed first-generation kinetic model of redox materials.
- Collected kinetic data for CO_2 and H_2O splitting over ceria/zirconia monoliths.
- Evaluated metal oxide volatility as function of temperature and steam exposure to guide operations and prioritize materials; experimentally evaluated iron loss from model materials; constructed materials durability apparatus.

Reactors

- Updated solar test facility including controls and data acquisition; mounted counter-rotating-ring receiver/reactor/recuperator (CR5) and began operations.
- Developed and mounted second-generation CR5 rings.

- Developed simplified apparatus for characterizing heat transport within CR5.
- Identified and fabricated three promising monolithic structures; developed new technique for fabrication.
- Developed and implemented a 2D, two-phase model of CR5.

Systems:

- Established a baseline architecture in Aspen that includes water gas shift, separations, and methanol synthesis; assembled an Aspen flow sheet to represent the CR5.
- Performed a comparative analysis of methanol production via two different pathways: ($CO + H_2O$) and ($CO_2 + H_2$); established break-even price for CO or H_2.
- Identified major cost drivers for complete sunshine to petrol (S2P) system.
- Demonstrated new CO_2 absorbers with capacities > 1.5 mmol/g.

Significance

The availability and price of transportation fuels is coupled to economic and national security as are the effects of climate change. Our results are being applied to improve materials and designs critical to ultimate viability of our approach to solar fuels. Additionally, our results help identify key factors that drive durability and cost to help focus our efforts and others joining the field. Development of a carbon-neutral technology to domestically produce fuels and reduce our reliance on imported oil supports DOE's strategic Energy and Environment goals.

Refereed Communications

R.B. Diver, J.E. Miller, M.D. Allendorf, N.P. Siegel, and R.E. Hogan, "Solar Thermochemical Water-Splitting Ferrite-Cycle Heat Engines," *Journal of Solar Energy Engineering* , vol. 30, p. 041001-1, November 2008.

M.D. Allendorf, R.B. Diver, N.P. Siegel, and J.E. Miller, "Two-Step Water Splitting Using Mixed-Metal Ferrites: Thermodynamic Analysis and Characterization of Synthesized Materials," *Energy and Fuels*, vol. 22, pp. 4115-4124, November 2008.

Featureless Tagging Tracking and Locating

131305
Year 1 of 3
Principal Investigator: K. C. Branch

Project Purpose

Tagging, tracking, and locating (TTL) materials, assets, and personnel of high importance are integral to several national security and defense missions. Existing TTL systems enable these missions within certain constraints. However, they do not provide the entire set of capabilities that are required for many TTL missions. Existing TTL systems necessarily trade between geographic range, persistence, geolocation precision, physical size, or some combination thereof.

What has yet to be created is a TTL system that provides broad-area coverage and a featureless capability. Broad-area coverage provides the ability to cover large geographical regions, continuously 24 hours a day, 7 days a week, and locating with a single interrogator's reception. The featureless capability provides a tag that is extremely difficult for an adversary to detect, both electronically and physically. The combination of small size, low power, complex waveforms, precision location, and signaling architectures has never been attempted and presents a number of distinct technical challenges.

Our concept centers around a dual-mode (beacon and synthetic aperture radar [SAR]) tag. We have identified three research pillars that require technology advances in order to achieve our goals. I.) We will create and develop new featureless signaling waveforms, detection and geolocation algorithms, and develop a novel tag architecture resulting in an innovative dual-mode broad-area featureless TTL capability. II.) We will make technical advances in MEMS acoustic microresonator delay elements, and III.) We will develop antenna technologies required to obtain a tag that is very small.

The impact on national security of a physically and electronically featureless TTL system capable of continuous persistence across a city, country, and eventually the globe, providing near instantaneous geolocation would be a tremendous tool to benefit our national security.

Summary of Accomplishments

The first year of this project has included the development of credible concepts of operation as well as point validation of component hardware used to form a development testbed.

Highlights from each pillar include the following:

- (I) Microresonators have been scaled using optical (mass producible) lithography to frequencies as high as 9 GHz.
- (II) Completed assessment of SAR-tags in impaired environments.
- (II) Completed link analysis between featureless tag concept and proposed or existing detection infrastructure.
- (II) Developed new techniques for single platform geolocation for beacon tags with order of magnitude angle-of-arrival (AOA) accuracy improvement.
- (II) Developed a novel featureless waveform method for near-coherent integration of wide band waveforms.
- (III) Investigated: 1. fundamentals of electrically small antennas, 2. tunable antennas, 3. smart (adaptive) antennas.

(III) Completed a design of a placement insensitive antenna that radiates in presence of ground plane, regardless of orientation.

(All) Progress/accomplishments have been documented in 3 papers, 9 presentations, and 4 invention disclosures.

Our system approach is driven by both technology advances and future applications. For example, our external advisory board (EAB) feedback has influenced our decision to prototype/test early and often rather than wait untill our final project year. In parallel, our market research analysis encompassed both tag and component technologies (microresonators and antennas). The EAB and market research findings are finalized in reports.

Significance

A December 2004 Defense Science Board study "Transition to and from Hostilities" states that "current U.S. intelligence, surveillance, and reconnaissance (ISR) capabilities are inadequate for many tasks that emerge in asymmetric warfare" and that a "Manhattan Project of scale and intensity" is needed to develop these capabilities. Advancements in any of the three proposed technology pillars could mitigate these national security issues.

Quantitative Study of Rectangular Waveguide Behavior in the THz

135792
Year 1 of 1
Principal Investigator: M. C. Wanke

Project Purpose

This project will quantify the behavior of microfabricated terahertz (THz) rectangular waveguides on a configurable, robust semiconductor-based platform. These waveguides are an enabling technology for coupling THz radiation directly from or to lasers, mixers, detectors, antennas, and other devices. Traditional waveguides fabricated on semiconductor platforms such as dielectric guides in the infrared or co-planar waveguides in the microwave regions, suffer high absorption and radiative losses in the THz. The former leads to very short propagation lengths, while the latter will lead to unwanted radiation modes and/or crosstalk in integrated devices. We will exploit the initial developments of THz micromachined rectangular waveguides developed under the THz Grand Challenge project (completed in FY 2008), but instead of focusing on THz transceivers, we will quantify the propagation loss, dispersion and far-field radiation patterns of the waveguides. Clearly demonstrating the performance of micromachined waveguides and THz QCLs integrated with waveguide structures will be valuable to the broader THz community as well as address interests of the National Aeronautics and Space Administration (NASA) and the Defense Advanced Research Projects Agency (DARPA) who are seeking THz local oscillators and THz integrated circuits respectively.

Summary of Accomplishments

During the nine-month duration of this project, we measured far-field beam patterns of empty rectangular waveguides, measured the propagation loss versus length of the waveguides, lowered built-in stress in integrated laser/waveguide devices improving processing yield and measured improved performance and beampatterns from lasers integrated with the rectangular waveguides. In the process of measuring beampatterns, we learned how sensitive the measurements were to feedback, which can probably explain many of the unexplained features found in beampatterns in the literature. We wrote one International Society for Optical Engineering (SPIE) proceedings paper and are close to submitting a second paper with the loss versus frequency results.

Significance

This project addresses the DOE’s scientific discovery and innovation strategic goals, by exploring an underdeveloped frequency range of the electromagnetic spectrum while advancing the underlying knowledge base and Sandia’s capabilities in radiofrequency (RF) design, THz technologies, and novel micro-manufacturing capabilities. These capabilities will help open up new areas of technology for both commercial enterprise and national security interests, such as chemical sensing and portal monitoring.

Host Suppression and Bioinformatics for Sequence-Based Characterization of Unknown Pathogens

137012
Year 1 of 1
Principal Investigator: T. W. Lane

Project Purpose

Bioweapons and emerging infectious diseases pose formidable and growing threats to our national security. While modern DNA assays can identify known pathogens quickly, identifying unknown pathogens currently depends upon slow, classical microbiological methods of isolation and culture that can take weeks to produce actionable information.

The goal of this project is to develop technologies that will provide culture-independent characterization of an unknown biological threat through nucleic acid (NA) sequence analysis and bioinformatics processing and interpretation of the resulting data. The key to technical success in this project is to develop molecular biology methods that reliably, effectively and controllably enriches for pathogen specific nucleic acid sequences in a complex background of host nucleic acids. These enriched nucleic acids could then be subjected to ultrahigh-throughput sequencing (UHTS) for rapid analysis. The resulting dataset will be fed into a bioinformatics pipeline designed to accommodate the unique nature of UHTS data and to derive maximal predictive value. The project plan defines a set of nine-month milestones to assess candidate nucleic acid preparation and enrichment methods resulting in the development and demonstration of the optimal technology. In addition we will design and test a bioinformatics pipeline capable of handling the large and unique datasets from UHTS and provide useful interpretation of such data along with a measure of the uncertainty associated with its predictions Proposed project milestones are as follows:

Milestone 1. Develop and demonstrate molecular biology protocols that are able to selectively enrich/suppress NA fragments specific to a pathogen or to the host response to a pathogen.

Milestone 2. Develop a design for a bioinformatics pipeline that will efficiently assemble and annotate short nucleic acid sequence reads, predict functional and phylogenetic characteristics of the pathogen and quantify the uncertainty associated with its predictions.

Summary of Accomplishments

We prepared T4 bacteriophage stocks as a surrogate pathogen and human genomic DNA as host. We designed T4- and human-specific DNA probes for blots, optimized conditions and determined that this method is not sensitive enough. We designed T4- and human-specific primer/probe sets for quantitative polymerase chain reaction (qPCR), and optimized reaction conditions and cycling parameters. We devised a strategy for normalization of host background in a mock clinical sample of mixed host and pathogen DNA. We analyzed the digestion profile of the T4 genome and human chromosome 20, and identified enzymes to use to convert a mixed sample into a population of DNA fragments of the desired size range.

The feasibility of performing DNA manipulations using a microfluidic platform was tested. A thin, nanoporous, negatively charged membrane was photopolymerized within a microchannel, serving as a “filter” or “trap” against which DNA could be trapped, e.g., for enzymatic or hybridization reactions. The DNA trap could be coupled to a microchannel for electrophoretic sieving for online analysis of product size. Additionally, microliter-sized droplets placed on hydrophobic surfaces were also evaluated for sample delivery and manipulation as a method for processing DNA samples in an automated device. Droplets containing genomic DNA of various fragment lengths were translated along an electrode array.

Algorithms and data pipelines were evaluated leading to development of capability for short reads analysis and contig assembly. Real and simulated sequencing data was used for in silico experiments that helped identify technical challenges in bioinformatics of UHTS data analysis. Experiments included assembling 20 million paired-end bacterial short reads and identifying an unknown viral pathogen in a simulated mixture of viral and human short reads. State-of-the-art hardware platforms were obtained and evaluated for handling large volumes of sequencing data. This bioinformatics platform can be suitably modified to answer metagenomic questions in complex microbiome studies.

Significance

This proposal allows Sandia to address a problem of interest to the Department of Homeland Security Chem/Bio Science & Technology Directorate, the Defense Threat Reduction Agency's Transformational Medical Technologies Initiative and Transformational Countermeasures Technology Initiative, and also to the National Institute of Allergy and Infectious Diseases. The strategic plans for all three call for new efforts to address unknown biological agents, and Sandia can be at the forefront of these activities.

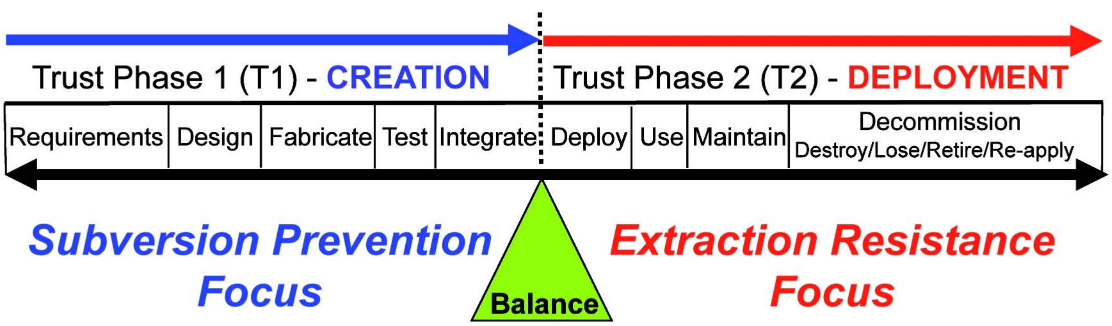
SENIORS' COUNCIL INVESTMENT AREA

This investment area supports a diversity of research projects under the national security umbrella, which are deemed worthy of funding under the auspices of the Seniors' Council, a cadre of Sandia senior scientists. There is no per se restriction on the topical area of the research proposal, so projects generally fall into several different scientific areas, whose only link is the common thread of the Laboratories' national security mission.

Infrastructure for Nondestructive, Real-Time Fingerprinting of Integrated Circuits

Project 139146

Deployed information processing systems are constantly in danger of subversion by adversaries or by counterfeiters seeking financial gain. Although fabrication in a trusted foundry initially protects such components, they are, during deployment, subject to subversion by substitution; that is, counterfeit data or other information can be substituted for the actual information in such systems. One obvious method of mitigating such subversion is a robust method of hardware authentication. Physical unclonable functions (PUFs) provide a mechanism for accomplishing this goal. Subtle chip-to-chip variations that occur during manufacturing can be exploited by PUFs. This short project has prototyped field programmable gate array (FPGA)-based PUFs interrogated through the JTAG interface, and implemented and analyzed fuzzy extraction with error correcting codes (ECCs) to remove noise from a PUF output. It developed and analyzed the "list infrastructure" required to detect and prevent insertion of, or playback of, maliciously fabricated authentication data. The outcomes of this project are applicable to cyber security in any fielded information-processing device that collects and processes data in a nonsecure environment

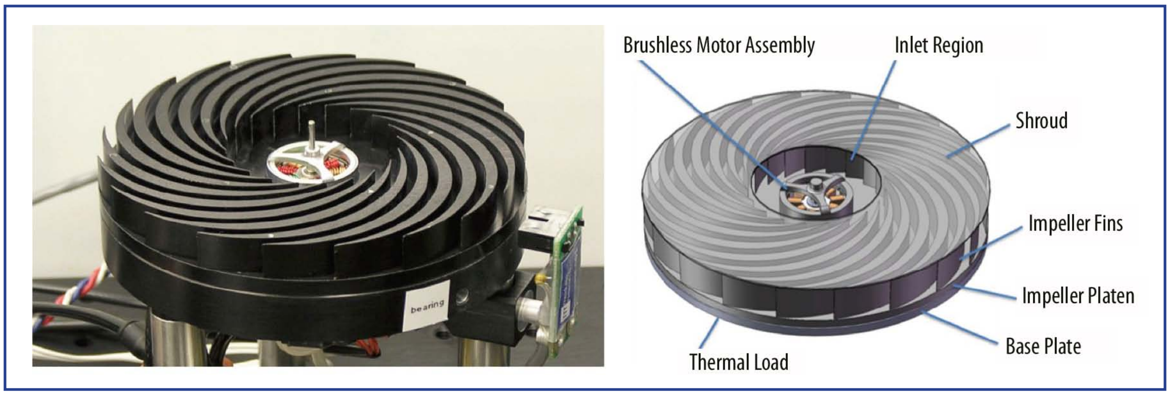


Simplified Threat Model

A Fundamentally New Approach to Air Cooling

Project 135192

Although air-cooled heat exchangers constitute a technology area of fundamental importance, device architecture and performance have changed little during the past 40 years. This project has developed a new design for such exchangers whose impact in dissipating heat and saving energy is likely to be felt in a broad cross-section of technology. Key among these, the electronics industry is facing a roadblock along the growth curve of Moore's Law (i.e., increasing central processing unit [CPU] clock speed accomplished by increasing on-chip transistor density). The issue is adequate heat dissipation from these chips — which this project addresses. In the energy sector, electrical power consumption is determined in part by the performance of air-cooled heat exchangers in a wide variety of energy consuming devices. The largest opportunities for decreased energy consumption as a result of this project's successes are in applications such as air conditioning, heat pump systems, refrigeration equipment, and computer server farms.



Photograph (left) and drawing (right) of the new heat-exchanger design developed in this project

SENIORS' COUNCIL INVESTMENT AREA

Feasibility Investigation of a Quantifiable and Objective Approach to Organizational Performance Enhancement

129145
Year 2 of 2
Principal Investigator: A. J. Scholand

Project Purpose

The project is aimed at developing advanced algorithms that identify and characterize the nature of working relationships by processing archival artifacts generated by computer-mediated communication systems. These relationships will be aggregated into a directed graph of affective relations between individuals. The accuracy of the characterization algorithms will be assessed by performing various types of social network analysis on the graph, and comparing the results to survey-elicited responses from the participants. The development of these algorithms will innovate in the integration of concepts of cognitive attention and complexity limits, the sustainability of strong and weak interpersonal ties, and computational linguistic analysis to provide important insight into the richly layered and textured nature of workgroup relationships. Investigations into appropriate linguistic dimensions to analyze will be conducted in part by researchers at the University of Texas. We anticipate that the dynamic network resulting from the application of these algorithms will represent facets of information relevant to interpersonal dynamics, aspects of distributed cognition and group work, and the development of organizational power and control. Anticipated benefits include quantitatively based sociotechnical efficiency improvements and expertise in successfully executing work between groups of individuals where information is developed, shared, and acted upon in an operational context.

Summary of Accomplishments

Communication negotiates meaning out of the events around us. This communication is also richly layered with information about the relative social, psychological, and emotional connections that situate us within a community. We developed a new methodology, social language network analysis (SLNA) to make these structures accessible for analysis, and demonstrated how the application of SLNA to a real world knowledge-intensive collaborative work communication corpus highlights and makes explicit important components of organizational functioning, such as information exchange and evaluation (a function of perceived expertise) and social support.

Significance

By providing a means to better comprehend interpersonal and social dimensions of collaborative technical work that will ultimately improve the execution of that work, the research contributes to the DOE Science Strategic Goal in the DOE Strategic Plan. In addition, the efficiency improvements made possible by this research tie directly to NNSA's vision for complex transformation as well as to DOD mission effectiveness by improving force cohesion and efficiency.

Laser Detection

129299
Year 2 of 2
Principal Investigator: L. R. Thorne

Project Purpose

A large number of laser applications critical to US national security have been developed and currently are in active use, for example, laser energy is used as a carrier for point-to-point communication. Conversely, development of this and other laser-based technologies by other entities pose potential national security threats to the US. Although extremely challenging technologically, the ability to remotely detect the geographical origin, propagation path and other characteristics of laser emissions is an important part of mitigating laser-based security threats. Our approach is to identify atomic and molecular species that interact with specific laser wavelengths and produce resonance fluorescence emission which can be detected remotely. Initial efforts were successful and model calculations indicate the feasibility of two different but related approaches. We now seek to take the next logical step in developing this technology, specifically to conduct a pathfinder experiment to demonstrate proof of concept.

Summary of Accomplishments

We have further refined the two detection methodologies that were identified in the initial phases of this study by estimating several important optical and other properties of the materials involved. We have also designed an experimental layout that will permit evaluation of long-lived laser-induced and resonant, two-photon fluorescence. The design emphasizes precise control over the test atmosphere, background illumination, and sensitive fluorescence detection. We have also made additional refinements in our signal generation and detection model to more realistically estimate the detected signal strengths.

Significance

We believe that success of this research will have a significant impact on Sandia's ability to detect and diagnose laser energy propagating in the atmosphere for a variety of DOE and DOD applications including, for example, laser-based communications, laser threat warning space systems and directed-energy programs. This capability would clearly benefit Sandia's missions in military applications and space systems.

Land-Surface Studies With an Imaging Neutron Detector

130419
Year 2 of 2
Principal Investigator: N. Mascarenhas

Project Purpose

Water, whether in liquid or solid form, plays a central role in land-surface processes directly important to society and to our general understanding of global scale processes. However, instrumentation for measuring key land-surface variables such as soil water content, snow depth and biomass are lacking, particularly at a scale intermediate between invasive point measurements and kilometer scale remote sensing images. We propose to investigate the possibility of using a neutron scatter camera developed for imaging hidden nuclear materials to measure land surface water or biomass. The premise of the technique is that the hydrogen contained in water strongly attenuates fluxes of naturally occurring cosmic ray neutrons. The technique is passive, noninvasive, nondestructive and operates at a scale of 10-100 m^2, which is unattainable by other instruments.

Summary of Accomplishments

A directional neutron detector was used to characterize the response of ambient neutrons in the 0.5–10 MeV range to water located on or above the land surface. Ambient neutron intensity near the land surface responds strongly to the presence of water, suggesting the possibility of an indirect method for monitoring soil water content, snow water equivalent depth, or canopy intercepted water. For environmental measurements the major advantage of measuring neutrons with the scatter camera is the limited (60°) field of view that can be obtained, which allows observations to be conducted at a previously unattainable spatial scales. This work is intended to provide new measurements of directional fluxes which can be used in the design of new instruments for passively and noninvasively observing land-surface water. Through measurements and neutron transport modeling we have demonstrated that such a technique is feasible.

Significance

One of DOE's principle goals is to ensure a reliable, affordable, and environmentally sound energy supply for our nation. The demands placed on available energy and water supplies coupled with the complex interdependencies relating these resources could threaten the continuity of energy supply in the future. The proposed project will develop tools and techniques that will be beneficial to accurately understanding the availability of water for energy production and a myriad of other uses.

Plasmonic Enhanced Ultrafast Photoconductive Switch

130420
Year 2 of 2
Principal Investigator: E. A. Shaner

Project Purpose

The goal of this work is to investigate plasmonic coupling to ultrafast material towards development of ultrafast photoconductive switches with ground-breaking performance. Modern photoconductive switches are based on technology that is over twenty years old where all improvements to date have been on the material side of the problem. This project aims to attack the issue from a different standpoint by addressing the internal conversion efficiency of the switch. In ultrafast optoelectronics, the speed of the device is derived from sub-picosecond recombination times, an inherent property of the material. While this enables ultrafast operation, at the same time, it limits carrier collection efficiency. By applying plasmonic coupling concepts, we believe we can change this situation by forcing enhanced carrier generation at the interfaces between the metal electrodes and the semiconductor. The end result should be an improved carrier collection efficiency that will lead to larger photocurrents. If successful, this work will improve the output power of photomixing antennas as well as pulsed terahertz systems.

Summary of Accomplishments

We fabricated optoelectronic switches that are fully integrated with broadband spiral antennas. The switches are designed to concentrate radiation at 780 nm wavelength onto a central slot where efficient ultrafast carrier collection can occur. Many plasmonic designs were simulated, fabricated, and tested to arrive at the final implementation which still awaits optoelectronic testing.

Significance

Terahertz spectroscopy has been shown to identify fingerprints of key explosive materials. While research is still ongoing in this area, the capability to register molecular fingerprints, as opposed to atomic signatures, is unique to this frequency range. As such, terahertz spectroscopy may play a vital role in DHS prevention efforts.

Unintended Consequences of Climate Mitigation

135039
Year 1 of 2
Principal Investigator: P. V. Brady

Project Purpose

Traditional strategies for mitigating climate change envision carbon taxes, or cap and trade protocols, to force greater conservation ("demand reduction"), and/or increased reliance on renewables and nuclear power. Newer approaches emphasize geoengineering solutions such as: terrestrial biomass storage (e.g., locking up carbon by growing trees, or converting biomass into inert soil carbon), carbon capture followed by sequestration (CC/S), ocean fertilization, and albedo modification (e.g. pumping SO_2 into the atmosphere to form sunlight-reflecting aerosols), among others. These strategies have the potential to trigger other global, often climate-affecting, processes. For example, reforestation produces methane, an even more potent greenhouse gas than CO_2. Introducing SO_2 into the atmosphere could diminish the Earth's ozone layer. Ocean fertilization might rob nearby fisheries of nutrients, or lead to oxygen-free "dead zones." Meanwhile, engineering the climate by simply decreasing the burning of fossil fuels would incur stark decreases in gross domestic product (GDP) – part of the reason for looking at geoengineering efforts in the first place.

While climate mitigation schemes have received ample attention in the technical literature, the unintended consequences have received only marginal consideration. Yet, because the fear of unintended consequences looms so large, it is the uncertainty in the collateral damage of side-effects that may prevent climate mitigation. We believe that quantifying the nature and potential impact of the unintended consequences of climate engineering strategies is the critical step to actually deploying global climate mitigation. We therefore propose to: 1. Identify the most important side effects of each carbon mitigation scheme; 2. Quantitatively assess their likelihood, magnitude, and impact, and 3. Determine the mixture of climate mitigation strategies that maximizes impact while minimizing collateral damage.

Summary of Accomplishments

This was a late start project in FY 2009. Accomplishments include the following:

1. Identified primary unintended consequences of principal climate mitigation schemes. The work focused on planetary albedo modification, carbon capture/sequestration, ocean fertilization, and biochar because these schemes appear to be both: a. able to materially impact climate over decadal time spans and b. financially plausible.
2. Assembled preliminary economic analyses of mitigation implementation outlays.

Significance

Climate change has the potential to prompt multiple new national security challenges by, for example, undermining existing water supplies, disrupting agricultural production, and prompting unexpected migrations. By better understanding the economic factors and uncertainties that underlie and potentially limit mitigation of climate change the proposed work might better allow the Nation to respond to these national security challenges.

Authentication for High-Exposure Cyber Systems

135040
Year 1 of 1
Principal Investigator: L. G. Pierson

Project Purpose

This project proposes to examine a technical approach to enable progress on authentication, which is the most fundamental security primitive that underpins all cyber security protections. Current internet authentication techniques require the protection of one or more secret keys along with algorithms/computations designed to prove possession of the secret without actually revealing it (so that the authentication process can be exercised multiple times without generating and qualifying a new secret).

This project seeks "authentication without secret keys," which is even more difficult than "authentication (of messages) without secrecy (of messages)" that has been studied in the literature since Gus Simmons' landmark efforts. The reason to strive for authentication without secret keys is that protecting secrets (even small ones only kept in a small corner of a component or device) is much harder than protecting the integrity of information that is not secret (an integret).

Protecting a secret requires physical barriers or encryption with yet another secret key. Protecting an integret requires comparison with multiple copies held in a manner that makes it hard to modify the copies.

All message authentication schemes in use today require protection of a small secret against extraction by an adversary over some portion of the life cycle. This project seeks to refine an authentication approach by eliminating the need to protect a small secret from extraction by an adversary, while accomplishing robust authentication of internet transactions. The resulting method will be examined for suitability for authentication of components, data, programs, network transactions, and/or individuals).

The successful development of authentication without secret keys will enable far more tractable system security engineering for high-exposure, high-consequence systems by eliminating the need for brittle protection mechanisms to protect secret keys (such as are now protected in smart cards, etc.).

Summary of Accomplishments

Secret-keeping in authentication systems leads to brittleness in the sense that extraction or discovery of these secrets by an adversary leads to catastrophic failure of the authentication system, because the adversary then has sufficient information to spoof the authentication.

This work has shown that authentication systems that do not use secrets are possible, but appear to be difficult to implement in terms of data volume that must be processed. In particular, investigation of methods that leverage the use of physically unclonable functions (PUFs) to generate easily identifiable characteristics should be high priority. While the measurement of these PUFs can be regarded as a hard-to-extract secret, with proper design the secret may be made less brittle than conventional authentication secrets generated and held by other means.

This work has outlined an approach to developing metrics for authentication system brittleness that looks promising, but needs refinement and improvement by application to analysis of real systems. We believe that metrics that identify which portions of the life cycle rely on secret-keeping, augmented with metrics for the exposure of authentication components to the adversary during each phase of the life cycle will enable more robust analysis of these systems, and will enable comparison of resilience of different authentication schemes against these kinds of failures.

This study recommends future research into authentication systems that do not depend on secrets. Such research should be well-grounded in knowledge of current authentication systems and PUF techniques, and have relatively concrete ideas regarding how to differentiate a real-time measurement of a hard-to-clone characteristic from a playback. These techniques show great promise for chip verification (assurance against wholesale substitution or counterfeiting), chip-to-chip authentication (for component binding and configuration control in high-assurance systems), as well as for authentication of messages, network transactions, and individuals.

Significance

Our national cyber infrastructure is vulnerable to multiple adversaries as evidenced by daily cyber attacks reported in the public literature. This work will serve to reduce the R&D risk by examining feasibility of an authentication concept that could greatly improve our ability to apply attribution and deterrence concepts to protection of DOE and other national cyber infrastructure (which has proven to be extremely difficult without improved authentication tools).

Molecule-Based Approach for Computing Chemical Reaction Rates in Upper Atmosphere Hypersonic Flows

135041
Year 1 of 1
Principal Investigator: M. A. Gallis

Project Purpose

Modeling chemical and ionization reactions at the extreme conditions of hypersonic flows in the upper atmosphere is an important but unsolved problem. Given the paucity of measurements at these nonequilibrium conditions, current reaction-rate models are based, at best, on extrapolations of measured low-temperature equilibrium rates, and at worst, on estimations from radiation data. When used in Navier-Stokes codes, these models lead to unknown and potentially large errors in hypersonic flow predictions. For a chemical reaction rate model to be valid and reliable for nonequilibrium flows, it is of paramount importance that the model depend only on molecular level processes and not rely on equilibrium information. Unlike Navier-Stokes codes, which require chemical reaction rate models as inputs, the direct simulation Monte Carlo (DSMC) method deals with individual molecules and their collisions and thus can simulate chemical reactions at a more fundamental level. In particular, from specified molecular level processes, DSMC can compute chemical reaction rates even for highly nonequilibrium hypersonic flows. We propose to develop a DSMC-based approach for determining chemical reaction rates from molecular processes that can be used to develop nonequilibrium reaction rate models for important chemical reactions in upper atmosphere hypersonic flows.

Summary of Accomplishments

This project applied a recently proposed approach for the DSMC method to calculate chemical reaction rates for high-temperature atmospheric species. The new DSMC model reproduces measured equilibrium reaction rates without using any macroscopic reaction rate information. Since it uses only molecular properties, the new model is inherently able to predict reaction rates for arbitrary nonequilibrium conditions. DSMC nonequilibrium reaction rates are compared to Park's phenomenological nonequilibrium reaction rate model, the predominant model for hypersonic flow field calculations. For near-equilibrium conditions, Park's model is in good agreement with the DSMC-calculated reaction rates. For far-from-equilibrium conditions, corresponding to a typical shock layer, the difference between the two models can exceed 10 orders of magnitude. The DSMC predictions are also found to be in very good agreement with measured and calculated nonequilibrium reaction rates. Extensions of the model to reactions typically found in combustion flows and ionizing reactions are also found to be in very good agreement with available measurements, offering strong evidence that this is a viable and reliable technique to predict chemical reaction rates.

Significance

This project supports DOE's strategic goal of providing world-class science to address mission needs. Predicting reentry vehicle signatures requires accurate knowledge of the production of radiating species, such as nitric oxide, during upper atmospheric flight. This DSMC-based approach offers the possibility of accurate computations of the nonequilibrium, high-temperature chemical reactions and their rates needed by DOE and DOD to make such predictions.

Refereed Communications

M.A. Gallis, R.B. Bond, and J.R. Torczynski, "A Kinetic-Theory Approach for Computing Chemical Reaction Rates in Upper Atmosphere Hypersonic Flows," to be published in the *Journal of Chemical Physics*.

Technologies for Autonomous Satellite Capture

135042
Year 1 of 1
Principal Investigator: D. G. Wilson

Project Purpose

A critical need for our nation and DOD/DOE is to achieve and maintain space dominance. Currently, the US lags behind other nations in critical technological advances in the area of autonomous space capabilities. A window of opportunity exists for Sandia to invest in this technological area for significant benefit of Sandia mission needs that include these critical technologies: autonomous spacecraft guidance and control capture algorithms, real-time-vision-based automated pose estimation, long-range acquisition sensors, and intelligent docking mechanisms.

Current DOD missions deal with autonomous rendezvous/capture of cooperative satellites only. A more difficult problem where Sandia can provide unique capabilities and gain a competitive advantage is to solve the autonomous rendezvous/capture of uncooperative targets, such as tumbling or hostile satellites in orbit. The capture of uncooperative satellites is significantly more complex but could provide huge benefits for defensive military missions and commercial rescue/repair missions. Our proposed solution will leverage and extend unique Sandia technologies (exergy-based control & real-time-vision-based pose estimation) to provide core, critical needs. In addition, the successful development of this core technology could be used, in-turn, as a standalone payload to support evasive defensive maneuvers for satellites. Applications also exist in a wide range of other Sandia mission areas including Defense Systems and Assessments (autonomous unmanned aerial vehicle [UAV] flight systems, ultraprecision weapon delivery, robotic systems), Homeland Security and Defense (rapidly deployable 3D video motion detection systems, remotely operated weapon systems), and Energy Resources and Nonproliferation (real-time 3D sensing, feedback, and control of wind turbine blades, real-time solar concentrator alignment).

Summary of Accomplishments

- Developed exergy/entropy based control algorithms for both relative translation motion and rotation motion maneuver.
- Developed computationally efficient vision-based self-calibration techniques developed for real-time implementations.
- Self-calibration developments documented in a draft journal paper

Significance

This research project will help overcome current limitations involving national security of critical space assets by enabling new science and technology in a 2–5 year timeframe from the new capabilities for in-space servicing. Our approach is founded on scientific principles that are tightly integrated into modeling and simulation and information technology. Our successful development and proof-of-concept experimental and simulation results will benefit both DOE and DOD sponsors. These unique self-calibration capabilities provide the core mathematical framework needed to solve many of the 3D sensing and perception challenges in space robotics applications, and may have broader impact in other applications.

A Fundamentally New Approach to Air Cooling

135192
Year 1 of 1
Principal Investigator: J. P. Koplow

Project Purpose

Although air-cooled heat exchangers constitute a technology area of fundamental importance, device architecture (a fan mounted in close proximity to a finned metal heat sink) and performance have changed little during the last 40 years. Lack of progress in this area reflects the fact that the intrinsic performance limitations of air-cooled heat exchangers stem directly from fundamental physical effects: 1) boundary layer formation at the surface of the finned heat exchanger, and 2) in the case of small devices used in electronics, the very low mechanical efficiency of small, high-speed turbo machinery. The serious problem of heat sink fouling remains unresolved as well.

The goal of this project is to demonstrate the feasibility of a fundamentally new device architecture invented at Sandia to simultaneously address all of the above problems. The work conducted under this project will entail detailed heat transfer measurements on a prototype device, and numerous practical aspects of device development described below. Such proof of concept work will be required to obtain support for a much larger effort for full-scale device development and optimization (computational fluid dynamics and laboratory testing).

From an economic standpoint, the most important applications of air-cooling technology are throughout the electronics and energy sectors. In the electronics industry, continued progress along the growth curve of Moore's Law (i.e., central processing unit [CPU] clock speed and very large scale integration [VLSI] transistor density) can only be realized if the "thermal brick wall" problem that confronts the current generation of CPU technology can be addressed. In the energy sector, electrical power consumption is determined in part by the performance of air-cooled heat exchangers in a wide variety of energy consuming devices. The largest opportunities for decreased energy consumption are in applications such as air conditioning, heat pump systems, refrigeration equipment, and computer server farms.

Summary of Accomplishments

We have achieved a breakthrough in air-cooled heat exchanger technology. This technical area is of great importance, but has seen little progress during the past 40 years.

As a baseline for comparison, we use the state-of-the-art air cooled heat exchanger system specified in Defense Advanced Research Projects Agency (DARPA) Broad Agency Announcement (BAA) 08-15 (thermal resistance: 0.20 C/W, power consumption: 100 W, size 1.05 liters). Our first prototype device achieves the same cooling performance (0.20 C/W) but uses a factor of 10 less power (10 W) and is a factor of 4 smaller (0.24 liters).

We have also simultaneously solved the longstanding problems of heat exchanger fouling and fan noise. In addition, we have demonstrated that an air gap distance of order 20 microns, which provides greatly relaxed mechanical tolerances compared to a conventional air bearing, can be used in such a device.

All of this has been accomplished using a simple and elegant device architecture that is well suited for low-cost fabrication (important from the standpoint of large-scale impact). Based on what was learned during this project, we believe that device performance can be improved well beyond the results obtained with the version 1 prototype device.

Significance

The primary areas of impact relevant to the DOE’s national security mission are:

- CPU performance (solving the “thermal brick wall problem” that limits clock speed and VLSI density)
- Operating margin of the nation’s electrical power grid under peak load conditions.
- Reducing the size, weight and power consumption of portable instrumentation and sensors.

Molecular Fountain Based on Kinematic Cooling

135802
Year 1 of 1
Principal Investigator: D. W. Chandler

Project Purpose

The goal of this proposal is to construct a novel molecular fountain apparatus capable of producing dilute samples of molecules at near zero temperatures in well-defined, user-selectable, quantum states. The foundation for this research is the previously developed kinematic cooling technique, which uses a crossed atomic and molecular beam apparatus to generate single rotational level molecular samples moving slowly in the laboratory reference frame. The kinematic cooling technique produces cold molecules from a supersonic molecular beam via single collisions with a supersonic atomic beam. A single collision of an atom with a molecule occurring at the correct energy and relative velocity can bring a small fraction of the molecules to a standstill in the laboratory. We are presently utilizing a crossed molecular beam scattering apparatus that was built 15 years ago to study reactive scattering and although it has allowed us to demonstrate this new technique for making sub 1 Kelvin temperature samples, due to its design cannot be optimized for the kinematic cooling process. The new apparatus proposed here will overcome several problems that exist with the present apparatus. We propose to build a newly design crossed molecular beam scattering apparatus that is optimized for the production of ultracold molecules for injection into a molecular fountain.

Summary of Accomplishments

We built an apparatus for the production of a molecular fountain. This apparatus consisted of two molecular beams crossed at 90 degrees. Scattering from these beams was directed against gravity into a hexapole electric field for guiding the atoms or molecules. The apparatus has been built and is now being tested.

Significance

This work relates to the mission of the DOE Basic Energy Sciences program to remain at the forefront of molecular and atomic science relevant to gas phase chemistry and optical diagnostics. This project offers a new tool for study in this area.

Designer Catalysts for Next Generation Fuel Synthesis

137804
Year 1 of 2
Principal Investigator: S. G. Thoma

Project Purpose

Transition metal sulfides (TMS) such as MoS_2 are workhorse catalysts for upgrading heavy petroleum feedstocks and removing sulfur, nitrogen and other pollutants from fuels. Next generation fuel cycles that will likely rely even more heavily on TMS catalyzed reactions include:

- Reclamation of low-value crude/petroleum-processing-by-products.
- Direct coal liquefaction.
- Hydrogen generation by H_2O & H_2S splitting (photo-oxidation).
- Biofuel production: energy efficient alcohol synthesis from bio-feedstocks via greater catalytic alkali promotion selectivity.

Catalytic sites with different functions occur at the edges and basal planes of the layered TMS sheets. Decreasing catalyst particle size increases the number of active sites per mass and also increases the proximity of the various sites, which is extremely important to both catalyst selectivity (making specific chemical products from feedstock) and activity (catalyst performance and reaction yield). Further, quantum confinement effects have been shown to dramatically enhance the catalytic activity in nanoscale TMS catalysts. The ability to control TMS catalyst growth/structure is therefore fundamental to controlling and enhancing catalyst function for specific applications. The ultimate reduction in TMS scale results in single-layer-TMS (“layer-TMS”), which have previously been identified and demonstrated, though high-yield, scalable syntheses have not.

A new generation of catalysts is needed to make next generation fuels economically viable. In prior work, we developed a synthetic approach to create a family of catalysts that combines single layer, multivalence, quantum confinement effects into a single TMS catalyst platform. Further, because of our ‘bottom-up’ approach, we believe we can also combine dopant promotion and support into one platform and create dopant-TMS combinations not possible by other methods. This will enable making new feedstocks economically viable as well as enhancing recovery from existing feedstocks.

Summary of Accomplishments

FY 2009 Accomplishments include:

- We have taken delivery of a standard industrial Co-doped MoS_2 catalyst that we will use to compare Sandia catalysts to via the hydrodesulfurization (HDS) of dibenzothiophene (DBT)
- Assembly and validation of HDS catalytic testing equipment
- Activation of industrial catalysts and testing using this system
- HDS experiments of Sandia catalysts begun – results indicate the need to remove excess sulfur from post-synthesis material
- Physical and chemical characterization of Sandia catalysts underway, using transmission electron microscopy (TEM), Fourier transform infrared spectroscopy (FTIR), x-ray diffraction (XRD), ultraviolet-visible transmission electron microscopy (UV-VIS), Raman spectroscopy, and magnetic susceptibility.

Results indicate MoS_2 clusters based upon 5 Mo atoms that are self-assembled into larger super-structures.

- Successful scale-up of Sandia catalyst from 5 mL per batch to 3 liters per batch, also improvement of yield from the 5 mL level of 11% to the 3 liter batch level of 51%.

Significance

This project is relevant to the DOE Strategic Plan Strategic Theme 1, Energy Security, Promoting America's energy security through reliable, clean, and affordable energy.

Reduced Order Models for Thermal Analysis

137807
Year 1 of 2
Principal Investigator: D. K. Gartling

Project Purpose

High-fidelity computational models of large, complex systems are now used routinely to verify design and performance. However, there are applications where the high-fidelity model is too large to be used repetitively in a design mode. One such application is the design of a control system that oversees the functioning of the complex, high-fidelity system model. Examples include control systems for manufacturing processes such as brazing and annealing furnaces as well as control systems for the thermal management of optical systems. In this case a reduced order model is needed that represents the overall behavior of the system with a relatively few degrees of freedom. Such models are routinely used in solid mechanics where modal analysis has reached a high state of refinement. The same techniques have not been applied or developed for thermal problems though the theory is very similar for standard conduction problems. One major difficulty with the development of reduced order models for thermal analysis is the need to include the very nonlinear effects of enclosure radiation in many applications. This proposal is directed toward the development and testing of numerical algorithms that would allow reduced order models to be generated for general conduction/radiation problems.

Summary of Accomplishments

Reduced order models (ROM) may be constructed by either of two general methods, modal analysis or proper orthogonal decomposition (POD). Because the reduced order model of interest represents a multiphysics application, a necessary prerequisite is the ability to construct and solve a fully coupled representation of the thermal conduction and enclosure radiation problem. A parallel version of a fully coupled solver has been implemented and tested in a finite element code. This task proved more time consuming than anticipated as the solver interface was not designed for the dense matrix structure found in the radiation equation set. The fully coupled, parallel solution capability is noteworthy in itself as the convergence properties of this system are far superior to the segregated methods typically used.

Both ROM algorithms rely on the solution of a generalized or standard eigenvalue problem. Again, the current finite element solver interface does not allow direct connection with the Sandia eigensolver in the Sandia developed Trilinos solver library. An open source software package (ARPACK) was obtained and is currently being interfaced with the conduction/radiation code. Testing of the modal and POD methods for reduced order model construction will begin in the near future.

Significance

The development of advanced simulation methods is crucial to Sandia's mission in national security. The reduced order modeling proposed here has the potential to immediately impact design, analysis and optimization of complex thermal systems, particularly satellite systems. Most importantly, the ROM will allow thermal control systems to be rapidly designed and evaluated. An additional benefit would be to enable rapid quantifying margin and uncertainty analyses on weapon components.

Infrastructure for Nondestructive, Real-Time Fingerprinting of Integrated Circuits

139146
Year 1 of 1
Principal Investigator: T. M. Bauer

Project Purpose

This project seeks to augment the trustworthiness of deployed information processing systems by advancing the state of the art for authentication of microelectronics components to protect against subversion by substitution.

Trusted foundry processing of microelectronics protects against subversion only during the fabrication phase of a product life cycle. During the deployment phase of a product life cycle, it can be difficult to demonstrate authenticity even for components from a trusted foundry. Some deployed information processing hardware relies on physical system protection to maintain trustworthiness. An alternative to physical system protection is to employ robustly authenticated hardware. Physically unclonable functions (PUFs) can be leveraged to increase trust by hardening systems against subversion through instantiation of counterfeit components. PUFs are derived from random physical characteristics of the system from which they are sourced, which makes a PUF output difficult to predict. The random PUF output can subsequently be used for authentication.

A survey of the open literature shows that microelectronics are a rich source of PUFs because subtle variations in fabrication processes result in subtle variations in physical and operational properties of fabricated devices. Accordingly, PUFs extracted from microelectronics are of interest to cyber security. In principle, PUFs employ a challenge-response protocol, however, the full details of the implementation are poorly defined. For instance, while the open literature describes circuits that can be exploited for PUFs, the integration of PUF output into repeatable, rapid response authentication remains to be fully described. Furthermore, there is no trusted third party certification authority that certifies PUF challenge-response authentication data. With this project, we will investigate the infrastructure required to facilitate implementation of PUF-based systems and handling of PUF-based data. We envision that the result of our investigation will be applicable to widely deployed commercially manufactured integrated circuits (ICs) and systems such as field programmable gate arrays (FPGAs).

Summary of Accomplishments

To protect against the threat of substitution of subverted or counterfeit information processing hardware, we developed the infrastructure required to leverage PUF technology for robust authentication of ICs. Our key accomplishments:

1. We analyzed circuit PUFs in the open literature and prototyped FPGA-based circuit PUFs to achieve a random bit stream. We measured and analyzed the inter- and intradevice variability associated with these circuits and demonstrated improvements to interdevice variability through circuit selection and circuit layout.
2. We developed and analyzed fuzzy extraction algorithms with error correcting codes (ECCs) to extract random, reproducible bit streams from a PUF output. Through fuzzy extraction of PUF data, we determined the bit error probability of various ECCs with and without concatenation.
3. We interfaced a PUF output to an RSA (Rivest,Shamir and Adleman algorithm) key generation utility to produce key pairs for use in public key infrastructures (PKIs) and verified key uniqueness between devices. We used the key pairs to create certificates issued by a third party and to generate self-signed certificates.

4. For authentication, PUFs implementation results in a random bit stream that is tied to a specific IC. The integrity of IC-PUF association determines the robustness of the authentication, so the integrity of the list infrastructure that maintains the IC-PUF association becomes critically important. To evolve list infrastructure, we developed and analyzed efficient protection mechanisms to detect and prevent vulnerabilities. We analyzed many list infrastructure implementations and documented advantages and disadvantages associated with each implementation.
5. Using a PUF that has low intradevice variation and high interdevice variation reduces the overhead associated with bit generation, fuzzy extraction, and error correction. Accordingly, we considered IC materials and fabrication processes that can be leveraged to maximize interdevice variation while minimizing intradevice variation.

Significance

One of the most challenging tasks associated with imparting trustworthiness to deployed information processing systems is the assurance against substitution of counterfeit components. We seek to augment the trustworthiness of deployed information processing systems by advancing the state of the art for authentication of microelectronics components to protect against subversion by substitution. We envision these efforts to evolve to enable a low-cost "JTAG-accessible (Joint Test Action Group-accessible)" function block that can be universally inserted into almost any digital and/or mixed signal IC (using industry standard interfaces requiring no additional I/O pads or pins), enabling the tracking of individual components through the assembly and deployment phases of the life cycle.

The technology developed through our research provides a foundation for implementing new protection measures for integrated circuits that enable detection (and thus deterrence) against component substitution, which improves the trustworthiness of even widely deployed hardware.

The Theory of Diversity and Redundancy in Information System Security

139352
Year 1 of 2
Principal Investigator: M. D. Torgerson

Project Purpose

Because complete verification of realistic computer software and hardware is usually infeasible, new approaches are needed to address the present and future dangers of malicious intrusion into information systems. Both accidental flaws and deliberate subversions can create vulnerabilities for attackers to exploit. This project proposes to investigate new aspects and combinations of diversity and redundancy to bolster security.

In this context, diversity is the practice of applying differing implementation techniques to do the same task in different settings. Redundancy uses multiple implementations of the same functionality to arrive at a decision. Various aspects of the notion of combining diversity and redundancy have been explored by the computer security community, such as replicated hardware, threshold cryptography, Byzantine fault tolerant protocols, and multiple operating systems. Depending on the technique, the research has seen varying degrees of success.

To mitigate the effect of an unknown implementation error (as opposed to random physical failures), one may replicate diverse implementations, all passing the required functional tests but not sharing the same implementation induced vulnerabilities. The output may be combined and/or voted upon to produce a final "answer." If done sensibly, this may dramatically reduce the probability of a damaging attack. Of course, the reduction will depend strongly on the degree of diversity achieved.

We feel that there is a spectrum based on the complexity of the underlying system for which replication and diversity may be appropriately applied. For simple systems and information flow models, these ideas are intuitively viable and have been shown useful in certain circumstances. On the other end of the spectrum, they are computationally untenable and impossible to synchronize. Our research will delineate this spectrum and develop the theory behind measuring diversity in order to create a "diversity distance" between implementations.

Summary of Accomplishments

This project began in May 2009. We have completed the bulk of our literature search. We have begun a draft compilation of results surrounding fault tolerant methods of diversity, redundancy and replication. With that foundation, we are beginning to transition to modeling adversarial manipulations in the face of diversity, redundancy, and replication.

Significance

Threats against information security are well known and adversely affect DOE as well as the nation at large. If this work is successful, it will provide the theoretical underpinnings necessary to advance, in a scientific way, the notions of diversity and redundancy. The theory to be developed by this project may enable the design of real-time detection and mitigation of the exploitation of unknown and residual vulnerabilities in our information processing systems.

High-Efficiency (> 50%) PV Cells

139353
Year 1 of 1
Principal Investigator: G. N. Nielson

Project Purpose

The theoretical maximum efficiency of PV conversion of solar power is 86.8%, however, commercially available PV cells are from 6% to, at best, 20% efficient. We have identified a method that we believe will allow significant improvements in efficiency, with the potential of reaching efficiencies above 50%. We propose a design and analysis effort around these ideas with the goal of creating a strong analytical basis for these new concepts and an optimized design.

The PV structure we propose takes advantage of microsystem concepts that have been developed in other technology areas (i.e., microelectromechanical systems [MEMS]). The structure is a novel multijunction cell comprised of materials that are selected to create the optimal bandgap spread across the solar spectrum. The structure is a stack of several independently wired PV cells (as opposed to the monolithically grown, series connected multijunction cells). These PV cells do not need to be lattice matched so PV materials can be selected based on optimized bandgap values. The cells are very thin (on the order of a few microns) and absorb the wavelengths of light that the cells are particularly well suited to absorbing and converting to electricity while allowing the remaining wavelengths of light to pass through to the next cell. Low-Q optical cavities surrounding the individual cells are designed to enhance this effect at the band edge where conversion efficiency is the highest but absorption is lowest. The lateral extent of these cells is also small, on the order of 100 µm. This brings significant benefits, such as more-efficient and lower-cost optics for light collecting, better thermal management, and simpler methods for optical tracking of the sun. These benefits are important in achieving high efficiencies. Furthermore, the small lateral extent enables parallel self-assembly concepts allowing large-scale, low-cost assembly of the cells into modules.

Summary of Accomplishments

During the course of this project, we have analyzed a number of aspects of the microsystem enabled PV system concept. We have analyzed the micro-optics for the concentration of the sunlight, the spread of the bandgaps across the solar spectrum, new concepts for trapping light of the desired wavelength within the appropriate solar cells, and how to efficiently connect individual junctions to collect power from the cells. The results of the simulations we performed indicated that these techniques will lead to increased efficiency and/or reduced costs for PV systems.

For the optical concentration, we were able to develop designs for the micro-optics that allows for simple, millimeter-scale displacements to allow for tracking over a range of ± 10 degrees at 100× concentration. Furthermore, this optical system provides normal illumination of the PV cells, allowing the antireflective (AR) coatings to operate in an optimal arrangement.

We explored new methods of increasing optical path lengths of the light within the PV cells in a manner that would allow stacked cells to operate efficiently. The simulation and analysis of this method indicated improved performance relative to simple AR coatings.

We analyzed new methods of combining cells to improve system efficiency. This analysis indicated that improved efficiency can be realized by individually contacting the cells. Additional benefits, such as shade tolerance, were also indicated.

We analyzed what bandgaps should be used in a multijunction PV cell without the constraint of lattice matched materials. This analysis indicated that lattice matching requirements are a significant constraint to improved operational efficiency.

Significance

This project is focused on the development of a new method of PV energy production with unique characteristics that current technologies do not have. This technique has the potential to exceed 50% efficiency. This would provide a much higher amount of power per area than any other PV technique. This would be a revolutionary new source of energy for satellites, remote military operations, and the electric grid. All of these applications are key to the mission of DOE.

Uncertainty Quantification for Large-Scale Ocean Circulation Predictions

139867
Year 1 of 2
Principal Investigator: C. Safta

Project Purpose

The amount of anthropogenic greenhouse gases in the atmosphere is likely to continue increasing for decades, if not centuries, and is believed to play a major part in shaping the future earth climate. One remarkable prediction from climate models is that global climate phenomena potentially exhibit discontinuous behavior under forcing from various parameters. Specifically, consider the meridional overturning circulation (MOC), which is one of the most discussed environmental phenomena under danger of collapsing as a result of increased greenhouse gas concentrations. The MOC plays an extremely important role in the northward heat transport in the Atlantic Ocean and its weakening or collapse would cause major climatic change and, consequently, economic disruptions at both regional and global scales.

It is therefore self-evident that the assessment of fidelity of such high-consequence predictions as MOC weakening or collapse, is of crucial importance. Because of limited observations and the difficulties associated with high-resolution modeling, the current state of predictive power is quite restricted, necessitating the need to account for uncertainty in climate models and associated model parameters. In order to enhance the state of the art in the assessment of predictability of climate models, we propose to use advanced spectral uncertainty quantification (UQ) methods to efficiently and accurately propagate the uncertainty in climate model parameters to model outputs. These methodologies will be coupled with advanced methods for discontinuity detection in order to capture bifurcation in the model behavior with respect to parameters. Our approach relies on an efficient representation of uncertain quantities using spectral expansions of random variables/fields. We will use methods requiring the least number of samples to achieve a given degree of accuracy in the quantification of uncertainty in model outputs.

Summary of Accomplishments

1. Established a surrogate model for the meridional overturning circulation and developed a Bayesian inference methodology to identify and construct stochastic representations of discontinuities in the climate model observations; the methodology is robust with respect to data and model parameters uncertainties.
2. A domain mapping utility based on the Rosenblatt transformation was developed to connect the irregular parameter domains on either side of the discontinuity to rectangular computational spaces with uniform probability distributions. This allows an efficient spectral representation of the climate model output in terms of Legendre polynomials.

Significance

An improved treatment of uncertainty within various climate models will allow us to tackle the propagation of uncertainty across interfaces with other models and lead to a consistent treatment of uncertainty propagation between climate and socio-economic models. This will be very beneficial for Sandia's role in the modeling community and will have long term impact on energy and national security considerations.

Automated Verification of Concurrent Systems

140640
Year 1 of 1
Principal Investigator: D. Bueno

Project Purpose

Software systems are only increasing in complexity. Due to the limitations of Moore's law, developing more-efficient software must mean developing more parallel software. No longer do software developers benefit so much from new hardware releases. Developing parallel and asynchronous software systems represents a paradigm shift in the way programmers must think. There is a large body of evidence suggesting this paradigm is much more difficult to reason about than sequential programs. DOE must meet this complexity in a deliberate fashion, in order to ensure critical systems continue to function according to specification.

A promising approach for these problems is model checking. Model checking is a method for formally verifying a variety of safety and security properties of concurrent system models with high expected code coverage, and thus higher confidence of correctness. Model checkers can reliably discover more errors and vulnerabilities than traditional testing. Moreover, each discovered error is reproducible; model checkers are able to output a trace of system states exposing the failure.

Our work intends to explore how to make model checking practicable, concentrating on automated extraction of models from source code. It is a known fact of theoretical computer science that verifying properties of arbitrary source code is impossible. Therefore, generating a checkable model of necessity loses some information. Losing too much information would make the model unusable, and thus we intend to explore how to generate useful and rich models from source code, and when it makes sense to do so. If we are able consistently to generate useful models, we will enjoy being able to check a variety of important safety and security properties, with high expected code coverage.

Summary of Accomplishments

We discovered heuristics that can help determine when model checking would be likely to succeed for software. These allow those interested in investigating model checking to make relatively quick and easy decisions regarding how useful model checking ought to be for their task. This is valuable, because model checking is not widely practiced (yet) when it makes sense to.

1. Model checking is useful for checking distributed properties of a distributed system. A distributed system has multiple, independent, communicating processes; each process may have complicated individual behavior. Model checking is useful when that individual behavior can be abstracted away, leaving only the distributed behavior.
2. Model checking is useful when the number of processes is small (for example, less than 7).
3. Model checking is useful when it is relatively easy to write a test harness that can exercise the model, similar to what must be done when writing unit tests.

We identified hurdles to automated model extraction. Model extraction would provide easy-to-construct models for checking. However, for arbitrary software, this problem is difficult. We identified where the difficult parts lie, so that follow-on work can be concentrated appropriately.

1. Pointers and recursive types are difficulties, as expected.
2. Extricating the distributed behavior from the rest of a system is quite difficult, and likely needs user guidance.
3. We initially attempted to translate an abstract syntax tree into the model checking language. We ought to have been using a lower-level, typed representation (such as the low level virtual machine [LLVM]) intermediate representation).

Significance

Our overarching goal is to make formal methods usable by software developers who are not formal methods experts, because formal methods in general are able to bring more rigor to the software development life cycle. This work attempts to mitigate the risk that automated model generation will produce models which simply are not practical. If we can delineate the scope over which these formal methods can have success, we can properly apply them and reap the benefits.

Uncertainty Quantification of US Southwest Climate from IPCC Projections

140641
Year 1 of 2
Principal Investigator: M. B. Boslough

Project Purpose

The Intergovernmental Panel on Climate Change (IPCC) Fourth Assessment Report (2007) made extensive use of coordinated simulations by 18 international modeling groups using a variety of coupled general circulation models (GCMs) with different numerics, algorithms, resolutions, physics models, and parameterizations. These simulations span the 20th century and provide forecasts for various carbon emissions scenarios in the 21st century. All the output from this panoply of models is made available to researchers on an archive maintained by the Program for Climate Model Diagnosis and Intercomparison (PCMDI) at Lawrence Livermore National Laboratory.

There is significant variability among these models which contributes to uncertainty in the degree of future global climate change. The results of these models were aggregated into best estimates and uncertainties by the IPCC, whose Summary for Policymakers (SPM) focused primarily on global averages such as radiative forcing, sea level rise, and mean global surface temperature as the most important metrics for quantifying climate change. We believe such global aggregations are inadequate because climate is like many nonlinear dynamic physical systems for which temporal and spatial fluctuations can be proportionately much greater on local and regional scales. Climate change is likely to continue manifesting itself in the most sensitive regions before serious global consequences are experienced.

We propose a project that focuses on metrics associated with regional climate change. The first region we have chosen to address in this study is the US Southwest, because it is important to the US economy and national security, it is the region we live in and are familiar with, and it is particularly vulnerable to climate disruptions. Proposed regional metrics for climate change span sustainability measures of water, energy, health, agriculture, and biodiversity, and include risks associated with extreme weather events and irreversible cascading chains of events associated with “tipping points.”

Summary of Accomplishments

We have collected and reviewed literature in the field of uncertainty quantification and climate — a task that will continue throughout the project. We have downloaded and examined archived data from ensemble climate change simulations. We have analyzed and plotted data and have begun developing a statistical framework for intercomparison of data sets. We have identified the US Southwest and the North Slope of Alaska as two regions of interest for our project. We have learned that that the North Slope of Alaska is three times as sensitive to initial conditions as is the US Southwest but have not yet determined the significance of this observation. We have begun building a collaboration between Sandia and the University of New Mexico (UNM) and now have our contract in place with a UNM meteorologist. We have identified the need for dynamically visualizing spatially varying data to allow users and analysts to see spatial trends and how those trends may change over time. The benefit lies in the additional insight and understanding that can be gained over looking at static maps and/or line graphs over time. We have constructed templates that make use of Google Earth to visualize state-level resolution.

Significance

The US cannot afford to be surprised by regional climate change either within or outside our national boundaries. In regions of the Earth — such as the African Sahel — climate change has already led to agricultural collapse and chaos. Other regions — such as the Arctic — are changing very rapidly in a way that will have enormous impact on society and national security. Economic and national security considerations require the range of possible change be assessed within US territory.

Quantitative Laboratory Measurements of Biogeochemical Processes Controlling Biogenic Calcite Carbon Sequestration

140764
Year 1 of 2
Principal Investigator: T. W. Lane

Project Purpose

This project is designed to address shortcomings in our understanding of biogenic calcite deposition and dissolution, and provide to climate modelers improvements in the accuracy and uncertainty of key parameters. We will focus on producing data from organisms responsible for major biogenic carbon fluxes. A specific group of marine algae referred to as the coccolithophores are considered to be the most productive calcifying organism on earth. A focus of the project will be to measure, under thermodynamic conditions found in the deep ocean, the rates of chemical reactions involved in the geochemical processing of coccoliths produced by *Emiliania huxleyi*, using material grown in temperature and pH ranges relevant to modern ocean surface conditions.

We propose a multidisciplinary study linking the underlying coccolithophore physiology of biogenic calcite deposition (coccolith formation) with the rate of biogenic calcite dissolution under oceanographically relevant physiochemical parameters. In this way we will relate the environmentally induced changes in coccolithophore physiology, regulation of the calcification process, and coccolith structure to the environmentally modulated dissolution characteristics of the resulting biogenic calcite. We will culture *E. huxleyi* under different conditions of pCO_2 and seawater chemistry. We will measure the resulting calcification rates and characterize the morphology of the coccoliths by scanning electron microscopy. We will harvest coccoliths from culture grown under various conditions and determine their rate of dissociation under different conditions of pressure and seawater chemistry. We will use and artificial seawater formulation so that we can rigorously control the concentration of the relevant constituents. At the same time we will carry out a digital transcriptomic analysis of culture to correlate specific growth conditions to physiological state and regulation of the calcification process. Digital transcriptomics will be carried out by ultrahigh throughput sequencing of mRNA.

Summary of Accomplishments

We have obtained the coccolithophore *E. huxleyi,* and it is now in culture at Sandia. We have carried out growth curves of the organism at high and low pCO_2 and purified calcium carbonate (biogenic calcite) coccoliths from cells grown under both CO_2 regimes (FY 2009 Milestone 1). We will be analyzing the structure of those coccoliths by scanning electron microscopy prior to the end of this fiscal year (FY 2009 Milestone 2).

We have devised a strategy for carrying out the in situ high pressure measurements of biogenic calcite dissolution. We have carried out low-pressure baseline measurements. We are on schedule to complete design and assembly of the system for the measurement of the dissolution of calcite under high pressure and will be making such measurements by the end of the fiscal year (FY 2009 Milestone 3).

We have worked out the protocol for purifying messenger RNA from *E. huxleyi* and will be producing mRNA for transcriptomic analysis early in FY 2010.

Significance

This project is designed to address the goals of the US Carbon Cycle Science Plan to quantify and understand the uptake of CO_2 in the ocean. This research will help to attribute observed changes in the ocean carbon sink to variations in circulation, biology and chemistry and incorporate improved oceanic flux estimates into climate models.

Developing a Cyber Security Systems Methodology for Analysis of Life Cycle Protections

140766
Year 1 of 1
Principal Investigator: G. W. Richter

Project Purpose

There is a national need for a comprehensive approach to improving trust, reliability, and security of information systems that moves away from conventional approaches that risk being outpaced by adversaries, and which do not address core issues, especially for high-exposure systems. The cyber security community has yet to develop and describe a comprehensive and systematic methodology for cyber security in the broader sense that could be used to inform research and development directions at the Laboratories, the Department of Energy, and beyond. In fact, cyber security is a daunting problem with multiple dimensions, including design/development/deployment life cycle and varying and sometimes conflicting requirements for confidentiality, integrity, and availability of specific information. The technical problem is that this scope is more complex than can be handled by existing cyber system engineering tools and methods.

This study will develop an initial, cost-effective systems engineering methodology for cyber security protections, vulnerabilities, and trade spaces in order to evaluate and compare the reduction in risk factors among optional solution approaches. Instead of attempting to produce a comprehensive threat analysis, analytical concepts from game theory will be employed to incorporate offensive and defensive aspects of multiple adversaries, the trades and payoffs among strategies, and potential adversary decisions into the model. The central hypothesis of this work is that a simplified methodology can be found to make system security engineering tractable and cost effective for dynamic adversarial environments. The initial test of this hypothesis is to subject a simplified methodology incorporating both offensive and defensive aspects to a multiplayer game theoretic analysis to determine what assumptions are required to achieve optimum strategy (i.e., a Nash equilibrium), and then examine the feasibility of satisfying these assumptions.

Summary of Accomplishments

We defined various categories of cyber attacks and quantitatively compared cyber security risks with physical risks within a game-theory framework. By focusing on physical risks which bear key similarities with cyber risks, we were able to show where the impact of cyber attacks is likely to be negligible (or acceptable) and where and how it is truly revolutionary.

We used this game-theory framework to create taxonomies that describe the attributes of physical and nonphysical (cyber) security systems and the interactions among participants in these systems. These taxonomies allow us to better understand various cyber security challenges, solutions, and risks. Using this framework, we examined game-theoretic pay-offs for models of simple scenarios between cyber attackers and defenders.

We generated a high-level list of strategies for approaching cyber security issues which includes both traditional approaches as well as new approaches that are derived from a comparison with physical security solutions.

Significance

This research is expected to develop new metrics and lay the foundation for more robust and cost-effective cyber security system engineering practices, paving the way for improvements in the way DOE and other agencies resolve cyber security equity issues and how resources become allocated to information assurance efforts.

Development, Sensitivity Analysis, and Uncertainty Quantification of High-Fidelity Arctic Sea-Ice Models

141507
Year 1 of 2
Principal Investigator: P. B. Bochev

Project Purpose

The disproportional impact of the accelerating climate change on the Arctic, combined with the strategic and geopolitical importance of this region, call for high-fidelity, predictive sea ice simulations that support science-based policy-making.

To address this need we propose to develop new high-resolution sea ice models and study the sensitivity and the uncertainty in the predictions with respect to variations in the input and model parameters. This task requires sea ice models that (1) include motion and deformation in the plane of the ice and changes in ice thickness due to radiative fluxes from the sun, atmosphere, and ocean, and (2) can handle common physical features of the ice such as cracks and ridges.

To this end, we propose to use an elastic-decohesive constitutive relation and a material point method (MPM). The former incorporates explicit cracking and has better fidelity than the standard viscous-plastic model, while MPM offers benefits over standard Eulerian methods for sea ice by simplifying the ice thickness transport with the use of Lagrangian material points and by providing a natural way to handle the interaction of the sea ice with a coastline using two different particle regions.

A predictive sea ice model involves a large number of material and environmental parameters that are inherently uncertain. We will study the sensitivity of the new sea ice model with respect to these parameters in order to assess their relative importance for the propagation of uncertainties. This will allow us to reduce the dimension of the parameter space in the uncertainty quantification process.

Summary of Accomplishments

We focused on meeting the software and hardware prerequisites for the task with the highest priority — sensitivity analysis of MPM and CICE (a numerical model of sea ice developed at Los Alamos National Laboratory [LANL]). The work involved setting the software and hardware platforms for the studies. Specifically:

- We acquired, built and installed CICE, the LANL sea ice code
- Acquired a representative driving data set from LANL
- Generated a custom build of Dakota for the testing harness
- Identified the main equations from the CICE model
- Worked on cleaning up the current MPM sea ice code
- Investigated variables for use in the Dakota sensitivity study
- Started to identify data sets for use in the study

Significance

Climate change is a significant national security threat. Improving regional sea ice models and understanding their uncertainty will enable more accurate climate predictions. Sandia has the opportunity to provide science-based decision support and mitigation tools that go beyond simulation, in an effort to fully evaluate the global threat of climate change.

STRATEGIC PARTNERSHIPS INVESTMENT AREA

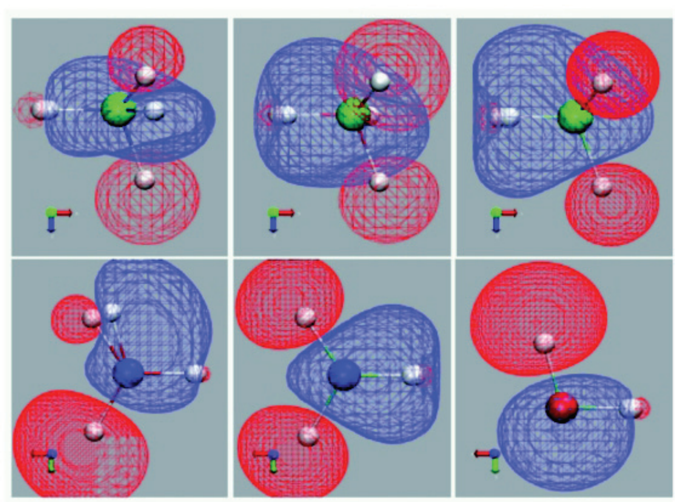
The common defining feature of projects in this investment area (IA) is a strong cooperative research endeavor with one or more academic or corporate partners. Because of Sandia's leadership in the multipartner National Institute for Nano Engineering (NINE), many SP projects are found in the nanotechnology arena. In addition, other projects within this IA, include the Sandia Fellows, and the President Harry S. Truman postdoctoral fellows, awarded annually to two or three recipients. In addition to being a great honor, the Truman is unique in that it supports a three-year initiative to pursue leading-edge research defined by the candidate's own proposal, which must be consonant with Sandia missions but which otherwise provides significant intellectual scope.

Multiscale Schemes for the Predictive Description and Virtual Engineering of Materials

Project 120209

The ability to tailor a material to a set of specifications— such is the upshot and the ultimate goal of the computational studies being pursued in this project. In a plant leaf, for example, special molecular complexes serve as the agents of solar energy transformation. Suppose that nonbiological materials could be designed that could carry out this process, harvesting solar energy even more efficiently and on a larger scale?

Or what if a more-efficient energy storage material, with better phase-transition (solid-liquid) properties could be designed for Sandia's solar tower, which stores solar-thermal energy that is subsequently released from a molten salt. Such problems are amenable to analysis by computational sciences involving advanced atomistic materials simulation techniques such as ab initio molecular dynamics, a relatively new field bridging statistical mechanics and electronic structure theory. In this Truman Fellowship project, the relationship between structure and properties has been investigated for various important materials and their properties using atomistic structure, chemical bonding, quantum, statistical thermodynamic, and statistical considerations. Examples include structure-material property relations for charge transfer rates of polycyclic aromatic hydrocarbons (PAH), methyl-adsorption energies on nanocluster core-shell catalyst candidates, or alchemical forces for molecular frontier orbital eigenvalues.

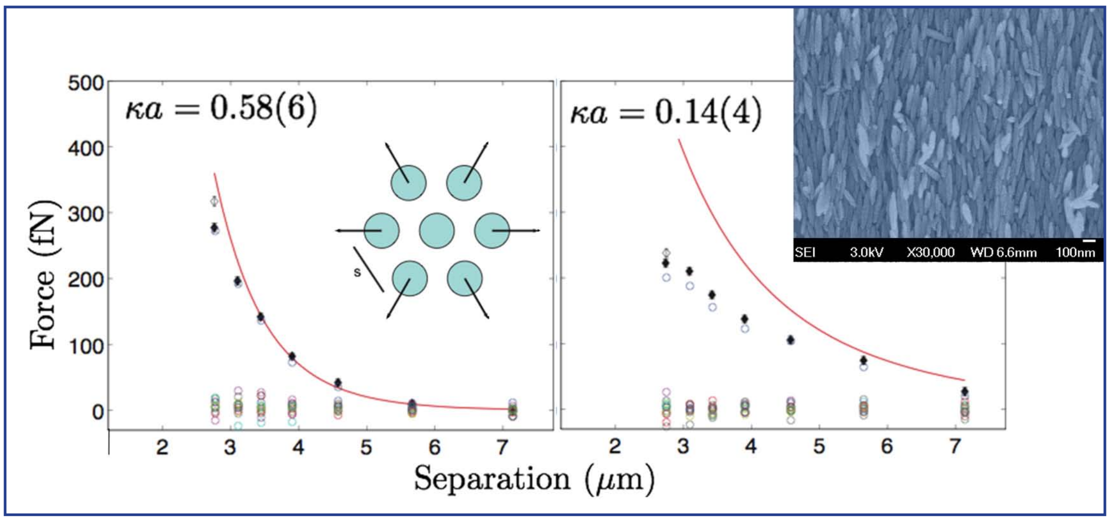


Computational representation of alchemical potential used to compute alchemical forces connecting molecular pairs CH_4/NH_3, CH_4/H_2O, CH_4/HF (left to right top row), and NH_3/H_2O, NH_3/HF, H_2O/HF (left to right bottom row).

Nanoengineering by Optically Directed Self-Assembly

Project 113488

Bringing together a multidisciplinary team from Sandia, Yale University, and the University of Delaware, this NINE project developed novel methods of directed self-assembly of nanomaterials using optical fields, for example, employing laser tweezers, a technology that enables noninvasive optical manipulation of particles, from glass microspheres of ~3 micron diameter to 20-nm gold nanoparticles. Laser tweezers are used to create ordered materials with complex crystal structures or using aspherical building blocks that are free of random defects, thereby enabling realization of novel nanomaterial characteristics such as full photonic bandgaps. These tweezers also allow defects to be systematically engineered into the photonic crystals, which would be impossible with spontaneous self-assembly. The capability for performing nanomanufacturing of particle structures with controlled optical properties has been demonstrated.



Using laser tweezers, this project was able to measure femtonewton resolution forces between colloidal particles(plots). At upper right is a scanning electron micrograph of controlled orientation of nanostructured TiO_2 nanoparticle films (parallel orientation, in this instance) deposited in the presence of an electric field.

STRATEGIC PARTNERSHIPS INVESTMENT AREA

Three-Dimensional Analysis for Nanoscale Materials Science

94814
*Year 4 of 4
Principal Investigator: I. Arslan

Project Purpose

The new era of nanotechnology demands a sophisticated understanding of materials on the nanoscale if it is to continue moving forward. In particular, the two dimensional (2D) transmission electron microscope (TEM) analysis that has been useful for the study of crystals, where the third direction is uniform, is no longer sufficient to characterize the complex, three dimensional (3D) structures that define nanotechnology. To characterize these structures, we have developed the technique of scanning transmission electron microscope (STEM) tomography on the JEOL 2010F microscope at Sandia, California. This relatively new technique allows us to study the size, shape, and distribution of a variety of different nanomaterials in 3D. Using new holder technology, we are now able to rotate the specimen a full 360° (called on-axis tomography), completely removing the “missing wedge” which currently limits resolution and clarity in tomograms today. As these specimens require a needle-shaped geometry, they are perfect to correlate with existing atom probe tomography techniques in use at Sandia. Furthermore, we will take advantage of the simultaneous imaging and spectroscopic capabilities to perform monochromated and un-monochromated electron energy loss spectroscopy (EELS) for a full analysis of the structure-property relationships of materials. Lastly, through external collaborations at other national laboratories and universities, we will use aberration-corrected STEM and EELS for an atomic resolution understanding of intricate materials systems. These techniques are at the forefront of the nanotechnology field, and their applications to fundamental materials science problems at Sandia will therefore have a great impact on many areas of national security, such as next generation energy and gas storage materials.

Summary of Accomplishments

The first completed task was on cobalt-based Fischer–Tropsch systems, which are widely used to convert synthesis gas to clean hydrocarbon fuel. Two Co_3O_4 catalyst systems with different supports were studied. The first system was found to form an interlocking structure with its support with no free surface area. The second catalyst was found to be more selective and this was attributed to its unique nanocage morphology that allows larger surface area for reactions to take place. This is 3D nanoscale information that could not be quantified without the use of STEM tomography.

The second completed task was on GaN/AlN core/shell nanowires, which are important for light emitting diodes, diode lasers, and high electron mobility transistors. The surfaces play an important role in these 1D systems, and the only way to analyze the surfaces and bulk simultaneously is by using STEM tomography. While the defects seen in the 2D images appeared to be bulk defects, the 3D reconstructions revealed that the defects are actually just on the surface of the nanowires.

The third completed task revolved more around technique development. It correlated electron tomography (ET) and atom-probe tomography (APT), which are both 3D techniques on the nanoscale. ET provides larger scale morphological information while APT provides smaller scale chemical information in 3D. Correlating

*This 36-month project spanned four fiscal years.

these two techniques can yield a level of materials understanding that has never been reached before. This first correlation has allowed us to quantify the artifacts in both techniques, understand the evaporation process in APT, determine the optimal reconstruction parameters for both techniques, and evaluate the quality of the ET and APT reconstructions.

Significance

This work has very significant applications for DOE missions in energy, nuclear security, and scientific discovery. This project is related to advanced hydrogen storage, and the analysis is directly applicable to nanoporous materials used in supercapacitors and batteries for electrical energy storage. The understanding gained from this project is anticipated to have a large impact due to the variety and importance of its applications.

Refereed Communications

I. Arslan, E.A. Marquis, M. Homer, M.A. Hekmaty, N.C. Bartelt, "Towards Better 3-D Reconstructions by Combining Electron Tomography and Atom-Probe Tomography," *Ultramicroscopy*, vol. 108, pp. 1579-1585, 2008.

I. Arslan, A.A. Talin, and G.T. Wang, "Three-Dimensional Visualization of Surface Defects in Core-Shell Nanowires," *Journal of Physical Chemistry C*, vol. 112, pp. 11093-11097, July 2008.

I. Arslan, J.C. Walmsley, E. Rytter, E. Bergene, and P.A. Midgley, "Toward Three-Dimensional Nanoengineering of Heterogeneous Catalysts," *Journal of the American Chemical Society*, vol. 130, pp. 5716-5719, 2008.

Nanoengineering for Solid State Lighting

102600
*Year 4 of 4
Principal Investigator: M. H. Crawford

Project Purpose

In this proposal, we seek to leverage the substantial nanoscience and nanotechnology investments at Sandia and transform them into nanoengineered solutions for energy-efficient solid-state lighting (SSL). While nanoscience will have broad impact on national security and energy areas, SSL is widely acknowledged to be "the low-hanging fruit" for early dramatic impact of nanotechnology. Our collaborative effort with Rennselaer Polytechnic Institute (RPI) focuses on developing and applying innovative concepts to achieving energy-efficient SSL by enhancing optical efficiency of light-emitting diode (LED) materials and includes: (1) nanoscale engineering of dielectric materials and integration with LED heterostructures for enhanced light extraction and (2) the study and manipulation of nanoscale InGaN materials properties to fundamentally improve internal quantum efficiency of light emitting materials, particularly at deep green wavelengths where high efficiency LEDs have never been demonstrated. This project will effectively leverage Microsystems and Engineering Sciences Applications (MESA) facilities and will involve top-rated students in the field of nanoengineering and its application to important national problems. The new nanoengineering approaches to SSL developed here are relevant to DOE's Basic Energy Sciences (BES) and Energy Efficiency and Renewable Energy (EERE) programs and are applicable to UV light emitters for chem-bio detection as well as high-efficiency photovoltaics.

Summary of Accomplishments

In the course of this project, we investigated a wide range of topics with the overarching goal of understanding and ameliorating the present limitations to InGaN LED efficiency. On the topic of InGaN materials, we focused on the impact of nanoscale crystalline defects on LED internal quantum efficiency (IQE). In our work on efficiency droop, we determined that nonradiative recombination at threading dislocations is not the primary high-current mechanism contributing to efficiency droop, while carrier leakage out of the InGaN active region is consistent with our findings. We further applied power-dependent photoluminescence (PL) to quantify both the IQE vs. carrier density relationship and the nonradiative coefficient A as a function of threading dislocation density. Our efficiency droop studies involved the exploration of a number of heterostructure designs and we observed that particular barrier doping designs reduced the anomalously high ideality factors of InGaN LEDs. We further addressed the existing controversy of the impact of v-defects on InGaN multiple quantum well (MQW) and LED efficiency. On the topic of light extraction, a major emphasis was the development of graded refractive index (GRIN) dielectric coating materials to eliminate Fresnel reflection from the GaN-air interface of the LED chip. As one example, we applied oblique-angle deposition techniques to realize GRIN ITO (indium tin oxide) nanorod coatings which were shown to enhance LED output efficiency by 24%. We found that additional lateral nanopatterning and micropatterning of GRIN dielectric layers helps to the extract waveguided modes and leads to even higher efficiencies. Beyond dielectric materials, we also investigated nanostructured metal coatings and the potential for surface-plasmon-induced improvements to LED efficiency.

Significance

By 2025, SSL could have a major impact by reducing US electricity consumption by 10%, saving ~$25B/year. The nitride semiconductor materials developed for SSL under this project can also be broadly applied to several

*This 36-month project spanned four fiscal years.

device technologies of interest to DOE and other agencies, and include InGaN photovoltaics as well as AlGaN ultraviolet LEDs and laser diodes for fluorescence-based chem-bio sensing, non-line-of-sight communications and trapped-ion based quantum computing.

Refereed Communications

D. Zhu, J. Xu, A.N. Noemaun, J.K. Kim, E.F. Schubert, M.H. Crawford, and D.D. Koleske, "The Origin of the High Diode-Ideality Factors in GaInN/GaN Multiple Quantum Well Light-Emitting Diodes," *Applied Physics Letters*, vol. 94, pp. 08113 1-3, February 2009.

J.K. Kim, A.N. Noemaun, F.W. Mont, D. Meyaard, E.F. Schubert, D.J. Poxson, H. Kim, C. Sone, and Y. Park, "Elimination of Total Internal Reflection in GaInN Light-Emitting Diodes by Graded-Refractive-Index Micropillars," *Applied Physics Letters*, vol. 93, p. 221111 1-3, November 2008.

"Bottom-Up" Meets "Top-Down:" Self-Assembly to Direct Manipulation of Nanostructures on Length Scales from Atoms to Microns

102660
[*]Year 4 of 4
Principal Investigator: B. S. Swartzentruber

Project Purpose

This project is centered on the development and application of state-of-the-art instrumentation for the fabrication and characterization of engineered nanopatterns and nanostructures on surfaces. We combine measurements using low-energy electron microscopy (LEEM) and scanning probe microscopy (SPM) to compare direct imaging of surface features on length scales from atoms to microns. We use these capabilities to investigate processes underlying the "bottom-up" generation of surface nanostructures. This bottom-up approach is complemented with the development of a novel nanomanipulator inside of a scanning electron microscope for "top-down" construction and characterization of unique nanostructures such as metallic and semiconducting nanorods and wires.

Summary of Accomplishments

The "bottom-up" portion of this project is concerned with the spontaneous formation of surface features that could possibly serve as templates for three-dimensional structures. Throughout this project, we studied a striking example of this phenomenon — the formation of stripe patterns on Si(001) induced by the presence of boron.

With the University of Wisconsin, we measured the diffusion of silicon atoms along the rows of the Si(111) 5x2-Au surface. Using scanning tunneling microscopy to image the motion of adatoms dynamically and analyze the detailed statistics of diffusion along the one-dimensional chains, we discovered that atom diffusion does not occur via a simple thermally activated hopping mechanism. Rather, silicon atom diffusion is mediated by meandering defects whose presence enables the silicon atom to hop over them to a new lattice site. The fundamental signature of defect-mediated diffusion is that sequential diffusion events are correlated. Other significant consequences of defect-mediated diffusion show up in measurements of the wait-time and jump-length distributions.

In the "top-down" portion of this project, we extended the capability of the single-probe nanomanipulator by adding an independent second probe. This enables not only more flexibility in the measurement of the electronic structure of a variety of nanorod systems, but also the capability to pick up and place nanostructures onto other measurement platforms. We have also used the nanomanipulator to build structures that would have been inaccessible by other means, for example, placing a 1-micrometer magnetic sphere on the end of an atomic force microscope cantilever to make a magnetic force microscope sensor.

Significance

Recently, a number of the mission-related technologies of Sandia have become invested in exploring the novel properties of nanostructures. These technologies include (but are not limited to): chemical sensors; water and

[*]This 36-month project spans four fiscal years.

gas purification; hydrogen storage; fuel cell applications; and the bio-inorganic interface. The nanometer-scale measurements enabled by our instrument will play a critical role in understanding and defining the function of nanostructures in these applications.

Refereed Communications

E. Bussmann, S. Bockenhauer, F.J. Himpsel, and B.S. Swartzentruber, "One-Dimensional Defect-Meditated Diffusion of Si Adatoms on the Si(111)-5x2-Au Surface," *Physical Review Letters*, vol. 101, p. 266101, December 2008.

A.A. Talin, F. Léonard, B.S. Swartzentruber, X. Wang, and S.D. Hersee, "Unusually Strong Space-Charge-Limited Current in Thin Wires," *Physical Review Letters*, vol. 101, p. 076802, August 2008.

F. Léonard, A.A. Talin, B.S. Swartzentruber, and S.T. Picraux, "Diameter-Dependent Electronic Transport Properties of Au-Catalyst/Ge-Nanowire Schottky Diodes," *Physical Review Letters*, vol. 102, p. 106805, March 2009.

Creation of Water-Treatment Membrane Technologies with Reduced Biofouling

102737
[*]*Year 4 of 4*
Principal Investigator: S. J. Altman

Project Purpose

The overall goal of this project is to use high-performance computing to direct polymer, material, and biological research to create the next generation of water-treatment membranes. Creation of low-cost, efficient water-treatment membranes helps ensure the availability of fresh water for human use, a growing need in both the US and the world. The three components of the project are, 1) creation of novel membranes, 2) computational optimization of membrane design, and 3) membrane testing. Two types of novel membranes are being developed. Micromixers are being imprinted on membrane surfaces to maximize turbulence and minimize stagnant regions on reverse osmosis (RO) membranes. Avoiding surface stagnation minimizes the deposition of microorganisms on the membrane surface, retards the biofouling process, and prolongs useful membrane lifetime. In addition, functionalized polyphenylenes and polysulfones are being used to make chlorine and biofouling resistant membranes. Computational fluid dynamic (CFD) modeling linked with the optimization DAKOTA toolkit are being used to (1) understand and predict the hydraulic behavior along the membrane and correlate the hydraulics to system performance metrics, (2) optimize the design and configuration of the micromixers, and (3) understand relevant processes that could impact fouling and system performance to guide the experimental design and characterization methods. A series of membranes have been tested on two cross-flow membrane testing systems that can monitor pressure, flow rate, temperature, salt rejection, and permeate flux in real time. Hyperspectral imaging with multivariate curve resolution is used to image microorganism and extracellular polymeric substance deposition to evaluate membranes and test modeling results. Sandia has a unique environment where experts in many fields can work together closely and efficiently. It is the integration of these disciplines that could put us at the leading edge of solving a nationally and internationally recognized problem and create the next generation of water-treatment membranes.

Summary of Accomplishments

We demonstrated the ability to print micromixers on the surface of reverse osmosis (RO) membranes using robocasting. We tested a series of membranes with micromixers on a cross-flow system and demonstrated that micromixers help prevent biofouling and that the design of the micromixers controlled where the bacteria adhered to the membrane surface. We also showed that micromixers do not significantly increase the pressure needed to maintain the same initial permeate flux and salt rejection. We synthesized a hydrophilic biocidal polymer coating (a series of poly(sulfone)s with attached quaternary ammonium groups). Exposure of the coated RO membranes to suspensions of *Escherichia coli* cells and subsequent testing for metabolic activity showed that all of the coatings exhibited significant biotoxicity. Testing of coated membranes in a cross-flow system showed increased biofilm growth on the coated membranes, presumably due to growth on top of a layer of dead cells that were in contact with the coating. We built a pilot system to test spiral-wound membranes. We developed two separate computational fluid dynamics (CFD) models, one using the code CFdesign® and the other using FLUENT®. Sensitivity studies run with the CFdesign model indicated that the greatest scouring on the membrane surface occurs when the chevron height is maximized and the chevron wavelength and spacing between chevrons are minimized. The same features that maximize scouring also increase the pressure drop. Operational factors need to be considered to maximize scouring while maintaining an acceptable pressure drop. The FLUENT code was used to simulate membrane processes including water and salt flow across the

[*]This 36-month project spanned four fiscal years.

membrane, concentration polarization, and particle trajectories. The FLUENT model was successfully coupled with DAKOTA, an in-house optimization code, demonstrating the coupling between a rigorous, parallel CFD analysis tool and a parallel optimization tool, which has not been carried out for this application.

Significance

This project supports Sandia's Water Initiative by creating safe and sustainable water through biofouling resistant water-treatment membranes. Improved water-treatment membrane technologies could enhance energy efficiency and productivity and help national security through mitigation of domestic and international sources of conflict. Thus, this works benefits the DHS, DOE, the Environmental Protection Agency (EPA), and the private sector. Technology transfer is possible in the oil and gas industry and for membrane manufacturers.

Refereed Communications

C.K. Ho, S.J. Altman, H.D.T. Jones, S.S. Khalsa, L.K. McGrath, and P.G. Clem, "Analysis of Micromixers to Reduce Biofouling on Reverse-Osmosis Membranes," *Environmental Progress*, vol. 27, p. 2, July 2008.

Discovery, Integration, and Interrogation of Biotic/Abiotic Materials and Systems

105722
Year 3 of 3
Principal Investigator: C. J. Brinker

Project Purpose

Our research exploits our recent discovery of the ability of living cells to create a unique bio/nano interface, contained within a robust silica host. Using amphiphilic phospholipids to direct inorganic self-assembly in the presence of living cells, we found that yeast and bacterial cells intervene, redirecting the assembly process to form a fluid, multilayered lipid interface at the cell surface that interfaces coherently with an ordered lipid/silica nanostructure. Remarkably this hybrid structure maintains fluidic accessibility and cell viability even after evacuation and electron imaging. Perhaps more importantly our cell-directed assembly (CDA) approach and its combination with aerosol-assisted self-assembly and patterning has enabled fabrication of precisely defined model systems in which to understand and control behavior at the individual cell level. This year, by engineering a physical system mimicking endosomal entrapment, we show unambiguously for the first time quorum sensing (QS) and genetic reprogramming to occur at the individual cell level. This should have profound implications on the interpretation of why QS occurs and how it evolves. Moreover it begins to uncover a general approach in which confinement induced self-signaling can be used to develop cellular characteristics like extremophile behaviors or synchronization. Additional highlights include the following: demonstration of a patternable, metabolically active, integration process that selects for living cells (over e.g., apoptotic cells) and is extendable to mammalian cell lines; integration of macrophage cells and demonstration of immune response triggered by addition of exogenous toxin; and preservation of Bacillus Calmette-Guérin (BCG) (weakened version of *Mycobacterium bovis*) for over eighteen months under hot dry conditions with 50% viability, suggesting a new direction for vaccine development for third world countries.

Summary of Accomplishments

The synthetic constructs we have developed have allowed us to explore several fundamental questions concerning the mechanisms by which cells actively control nanostructure formation and function and conversely the mechanisms by which nanostructured interfaces, matrices, and patterns can control cellular behavior. Highlights of our findings are summarized below:

- We showed that lipid localization at the cellular interface can be used to collocalize foreign transmembrane proteins and confer to the cellular system new behaviors. Importantly, we demonstrated that long-chained lipids added as protein-containing liposomes selectively partition to the immediate cell surface during CDA, thereby localizing foreign transmembrane proteins in their native/functional confirmations in close proximity to the cell surface.
- We developed several strategies enabling simple, efficient, in situ cell transformation. Patterned deposition of cells plus plasmids on a preformed lipid/silica film results in cellular integration, plasmid localization, and efficient transformation, providing a means for spatial patterning of cellular behavior.
- We have used CDA to incorporate model mammalian cells, such as adherent human embryonic kidney (HEK) cells, into our lipid-templated nanostructures and have found that mammalian cells localize phospholipids and create bio/nano interfaces similar to, yet distinct from, single-celled eukaryotes and prokaryotes. HEK cells immobilized within lipid/silica nanostructures had viability comparable to HEK in buffer.

- We developed a new optically and metabolically controlled lithography process, cell directed integration (CDI), to enable the patterned integration of arbitrary cell lines into solid state devices.
- We quantified the control parameters of the CDA process.
- We developed a nanostructured platform enabling interrogation of cellular behavior at the individual cell level.
- We observed that confinement of individual bacterial cells induces so-called quorum sensing pathways and genetic reprogramming important to understanding bacterial survival, virulence, and evolution and now recognized as potentially relevant to a spectrum of diseases, including cancer.

Significance

The novel biotic/abiotic materials we will develop are of interest to both basic and applied DOE and DHS missions. They are of interest for standalone cell-based sensors that could operate in extreme environments as well as platforms in which to study cell-cell communication, the onset of disease or infection, drug delivery, and cell differentiation. The possibility of engineering quorum sensing systems targeting new analytes could have general utility for chem/bio detection.

Refereed Communications

E.C. Carnes, J.C. Harper, C.E. Ashley, D.M. Lopez, S.M. Brozik, and C.J. Brinker, "Cell-Directed Localization and Orientation of a Functional Foreign Transmembrane Protein with a Silica Nanostructure," *Journal of the American Chemical Society*, vol. 131, pp. 14255-14257, October 2009.

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J. Liu, A. Stace-Naughton, X. Jiang, and C.J. Brinker, "Porous Nanoparticle Supported Lipid Bilayers (Protocells) as Delivery Vehicles," *Journal of the American Chemical Society*, vol. 131, pp. 1354-1355, January 2009.

L. Zhang, S. Singh, C. Tian, Y.R. Shen, Y. Wu, M.A. Shannon, and C.J. Brinker, "Nanoporous Silica-Water Interfaces Studied by Sum Frequency Vibrational Spectroscopy," *Journal of Chemical Physics*, vol. 130, pp. 154702 1-10, 2009.

E.C. Carnes, D.M. Lopez, H. Gresham, A. Cheung, G.S. Timmins, and C. J. Brinker, "Confinement-Induced Quorum Sensing of Individual *Staphylococcus aureus* Bacteria," to be published in *Nature Chemical Biology*.

Multimode Energy Scavenging from the Environment

106397
Year 3 of 3
Principal Investigator: C. A. Apblett

Project Purpose

The goal of this project is to develop an efficient energy scavenger for converting ambient low-frequency vibrations into electrical power. In order to achieve this, a novel inertial micropower generator architecture has been developed that utilizes the bistable motion of a mechanical mass to convert a broad range of low-frequency (< 30 Hz), and large-deflection (> 250 µm) ambient vibrations into high-frequency electrical output energy. The generator incorporates a bistable mechanical structure to initiate high-frequency mechanical oscillations in an electromagnetic scavenger. This frequency up-conversion technique enhances the electromechanical coupling and increases the generated power. This architecture is called the parametric frequency increased generator (PFIG).

Summary of Accomplishments

Three generations of the device have been fabricated. It was first demonstrated using a larger bench-top prototype that had a functional volume of 3.7 cm^3. The performance of this device has still not been matched by any other reported work. It yielded the best power density and efficiency for any scavenger operating from low-frequency (< 10 Hz) vibrations. A second-generation device was then fabricated. The device operates over a frequency range of 20 Hz. The internal volume of the generator is 2.1 cm^3 (3.7 cm^3 including casing), half of a standard AA battery. Lastly, a piezoelectric version of the PFIG is currently being developed. This device clearly demonstrates one of the key features of the PFIG architecture, namely that it is suitable for MEMS (microelectromechanical systems) integration, more so than resonant generators, by incorporating a brittle bulk piezoelectric ceramic. This is the first microscale piezoelectric generator capable of <10Hz operation. The device operates over a frequency range of 23 Hz. The internal volume of the generator is 1.2 cm^3.

Significance

Mechanical power harvesters are of importance to the DOE by providing a continuous low level supply of power for autonomous monitoring of critical assets. Small sensors that can detect motion of the assets without the need for a battery allow for continuous monitoring of state of health and of the position of any monitored assets. These systems can operate completely “off grid,” and have lifetimes measured in decades, allowing for unattended monitoring to be continuous and unobtrusive.

Passive and Active Electromagnetic Frequency Selective Surfaces for High-Power Beam Applications

106401
Year 3 of 3
Principal Investigator: H. Loui

Project Purpose

The purpose of this project is to create novel, reconfigurable, electromagnetic metasurfaces, materials-tensor instrumentation, and beam transmission measurement system for adaptive control over electromagnetic scattering relevant to the national security mission of the laboratory.

We intend to theoretically explain, numerically simulate, and experimentally demonstrate anomalous transmission of electromagnetic waves through compound subwavelength thick-metal gratings; and experimentally create an all-dielectric isotropic metasurface with negative index of refraction. We also intend to embed tunable materials into the periodic perforations of a thick metal plate, so that collectively the structure can affect electromagnetic (EM) beam propagation based on electrical configuration.

The leading-edge nature of this R&D effort is as follows: 1. understanding subwavelength scattering; 2. exploring metamaterial/surface physics; and 3. making chameleon-like radar deterrent surfaces.

Summary of Accomplishments

This project fostered creativity and stimulated exploration of forefront science and technology by conducting high-risk, potentially high-value R&D while forming strategic partnerships between Sandia, industry, and universities.

Contributions to science:

1. We theoretically explained and experimentally verified anomalous transmission of electromagnetic waves through compound thick-metal metallic gratings having subwavelength slits. We learned that the sharp stop bands appearing in pass-band transmission response are due to the extra degrees of geometric freedom afforded by compound-periodic surface.
2. We figured out how to control the resonance location and bandwidth of the band-pass anomalies mentioned in 1.
3. We created a double negative (DNG) composite metamaterial based on a cubic array of layered nonmagnetic spheres and numerical/experimental verified isotropic negative refractive index propagation using NaCl cubic lattices.

Contributions to engineering:

1. We created a high-order vector-basis Eigen-mode solver for determining the electromagnetic modes of inhomogeneous-filled waveguides for radar scattering analysis.
2. We invented a novel polarimetric calibration algorithm and patentable instrumentation for the broadband determination of ferrite permeability tensor critical to active radar applications.
3. We discovered an analytic formula for an entire class of spot-focusing lenses relevant to subwavelength imaging.
4. We created a magnetic tunable frequency selective surface and Gaussian-beam measurement system.
5. We investigated dispersion engineering and its applicability to radar components.

Significance

To the general S&T community, experimental validation of anomalous transmission opens up an entire field of study in compound periodic surfaces. These surfaces may be used for angle dependent frequency filtering of microwave signals. Experimental validation of all-dielectric, low-index contrast, double-negative, isotropic metamaterial enables low-loss frequency scaling of metamaterial applications to infrared and higher frequencies.

Tunable frequency selective surfaces (FSS) have potential application in DOE Defense Programs and national security missions. This technology is also relevant to radiofrequency (RF) systems, providing tailored radar response. Tunable ferrite structures support synthetic aperture radar, facilitating surveillance missions.

This project has built unique resources at Sandia for future research in subwavelength diffraction, metamaterials, radar-cross-section reduction, and military/commercial radome applications.

Improving Robot Navigation through Self-Supervised Online Learning

106408
Year 3 of 3
Principal Investigator: C. Q. Little

Project Purpose

This project with Carnegie Mellon University explores how self-supervised online learning techniques can be applied to robotics, particularly autonomous outdoor navigation, in order to allow robotic systems to improve their performance over time. While roboticists do everything they can to equip robots with capabilities relevant to a wide range of domains, in order for real-world applications of mobile robots to increase, they must be able to adapt to changing and unfamiliar aspects of their environments. In many domains that are prime candidates for mobile robotic applications, the risk of catastrophic failure, however small, is a primary reason why autonomous systems are still underutilized despite already demonstrating impressive abilities. The combination of the techniques developed throughout this project aim to improve the effectiveness and range of a robot's perception system, dramatically reduce the number of mission-ending errors by identifying potentially hazardous unfamiliar situations, reliably detect unexpected changes in previously traversed environments, and allow better utilization of the availability of limited human assistance.

Summary of Accomplishments

We developed and tested an online algorithm for dealing with scenarios where the robot must learn to trade off between multiple operating modes with no prior performance knowledge. The proposed approach relies on a bandit-based framework and uses confidence bounds to deal with the exploration / exploitation trade-offs. The algorithm was demonstrated on two scenarios relevant to the mobile robotics domain: trading-off online between autonomous and human tele-operation control and online optimization of the allocation of limited high-resolution overhead data to aid navigation. The use of online approaches showed significant improvement for both scenarios over any single-candidate system.

We also continued development of an online novelty detection system to allow a robot to identify situations that are outside of its experience base and therefore are potentially high-risk and require human oversight. Our approach relies on a supervised dimensionality approach that captures a lower dimensional space in which proximity implies similarity. Furthermore, our algorithm includes a query optimization scheme that bounds the computational and memory requirements of this algorithm, improving its suitability for real-time performance. We showed compelling real-time results on logged data that outperforms comparable approaches and are in the process of implementing this system for use onboard a mobile robot platform.

Significance

Autonomous robot navigation is a critical technology for several Sandia mission areas. These include nonproliferation and assessments, military technologies and applications, and homeland security. Under nonproliferation and assessments, autonomous robot technology can be used to aid robots performing site assessments. For homeland security, robots are used in a wide range of activities that include emergency response and physical security. The autonomous navigation technologies developed under this project will enhance robot performance for this wide range of applications, particularly when high degrees of reliability are necessary and single human operators must supervise many robots simultaneously.

Refereed Communications

B. Sofman, J.A. Bagnell, and A. Stentz, "Bandit-Based Online Candidate Selection for Adjustable Autonomy," *International Conference on Field and Service Robotics,* July 2009.

Network Design Optimization of Fuel Cell Systems and Distributed Energy Devices

110404
[*]Year 3 of 4
Principal Investigator: W. Colella

Project Purpose

This project involves the modeling of energy systems with the aim of designing them to achieve environmental, infrastructure security, and economic goals. Designs of alternative vehicles, power plants, and building thermal management systems, along with each technology's related energy supply chain, are being evaluated. Assessment criteria for these energy systems and supply chains include,

1. their impact on the environment including, a) greenhouse gas emissions, b) criteria air pollutants, c) solid waste production, d) human health, and e) energy efficiency;
2. their implications for national security including, a) the security of the fuel and energy supplied, b) the diversity of the fuel supply, and c) the dependence on foreign oil; and
3. their costs to consumers, governments, and incumbent energy suppliers.

Both mobile and stationary energy systems are being examined. Models of distributed energy networks are being constructed that, on the supply side, describe fuel cell system operation and, on the demand side, describe the energy demand profiles of buildings that these fuel cell systems may serve. Test data for key fuel cell system components is being incorporated.

This project combines Sandia's unique expertise in three main areas: 1) systems engineering, 2) the design of renewable and efficient energy technologies, and 3) the design of national infrastructure to increase homeland security.

Summary of Accomplishments

We developed two types of advanced energy models: 1) thermodynamic and chemical engineering energy device (TCEED) models, and 2) integrated engineering, economic, and environmental impact (IEEEI) models. TCEED models describe the detailed thermodynamic and chemical engineering processes within energy devices and systems. They include entirely new thermodynamic models of single, double, and triple- effect lithium bromide absorption chiller cooling cycles consuming low-temperature fuel cell waste heat (~ 80–150 °C) and chemical engineering process models of molten carbonate and solid oxide fuel cell systems. IEEEI models optimize the economic and environmental performance of fuel cells and low-carbon alternative energy generators operating in networks, by testing them against real-time building energy demand data. While first-generation models considered primarily heat and electricity, advanced versions now evaluate cooling power for the first time. On the demand side, to isolate cooling from electricity, real-time building chilled water consumption data is used to represent space cooling (but excludes refrigeration and freezing.) On the supply side, models describe cooling supplied by electric and steam turbine centrifugal chillers, and absorption chillers coupled to fuel cell waste heat. Advanced models also include a finer degradation of demand data and a greater variety of fuel cell system design, installation, operation, and control strategies. Model results indicate that greenhouse gas emissions are minimized with significant use of fuel cells coupled with absorption chillers, compared with other technologies.

[*]This 36-month project spans four fiscal years

Significance

This research supports key DOE environmental and energy efficiency missions. It supports goals of the Energy Efficiency and Renewable Energy (EERE) Office, the Office of Electricity Delivery & Energy Reliability (OEDER), the Office of Fossil Energy, and the Hydrogen Program for fuel cell technologies for distributed stationary power, making fossil energy systems more efficient, reducing carbon emissions, diversifying energy supplies, and modernizing energy infrastructure.

Refereed Communications

W.G. Colella, A. Rankin, and M. Parker, "Economic and Environmental Optimization Models for Refining Fuel Cell Use," International Association of Energy Economics (IAEE), , in *Proceedings of the 32nd International Association of Energy Economics (IAEE) International Conference -- Energy, Economy, Environment: The Global View,* June 2009.

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W.G. Colella, S.H. Schneider, D.M. Kammen, A. Jhunjhunwala, and N. Teo, "Part II of II: Deployment of MERESS Model -- Designing, Controlling, and Installing Stationary Combined Heat and Power (CHP) Fuel Cell Systems (FCS) to Reduce Costs and Greenhouse Gas (GHG) Emissions," to be published in the *ASME Journal of Fuel Cell Science and Technology*.

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W.G. Colella, "Designing Energy Supply Chains Based on Hydrogen," in *Climate Change Science and Policy, 2nd Edition,* S.H. Schneider, A. Rosencranz, and M.D. Mastrandrea, Eds. Island Press, 2009, pp

Advanced Materials for Water Treatment Membranes: Enhanced Rejection Performance and Surface Properties

110407
Year 3 of 3
Principal Investigator: S. J. Altman

Project Purpose

This project will leverage the biofouling testing capabilities of Sandia and the University of Texas (UT)-Austin capabilities in membranes, transport measurements, and water purification technologies.

Membranes are the technology of choice for water purification. Reverse osmosis processes produce high-purity water from saline water, but polyamide membranes, the state of the art, do not have good fouling resistance and their fundamental properties are poorly understood in terms of the mechanisms of salt rejection. The purpose of this work is to create new polymer membranes that have high flux for pure water, but are able to reject salt and have good fouling resistance. We plan to fabricate dense layers of functionalized poly(phenylene) and poly(aniline) on porous supports and test these membrane concepts for their performance in water purification bench-scale experiments.

Surface-modified reverse osmosis (RO) membranes are being created at UT-Austin by grafting hydrophilic poly(ethylene glycol)s to the surface of commercially available polyamide membranes. This treatment enhances the fouling resistance of the membranes while simultaneously maintaining their salt rejection capabilities. The anti-biofouling characteristics and salt rejection capability of these membranes will be tested at Sandia. Additional work in atomic force microscopy (AFM) will be conducted at the Center for Integrated Nanotechnologies (CINT), to measure the surface roughness of membranes.

The project supports technology and materials testing capability development in the area of water purification which is of strategic interest to Sandia and the nation.

Summary of Accomplishments

Surface modification, using the static top-surface contact method developed previously, has been performed on reverse osmosis (XLE) and nanofiltration (NF90) polyamide membranes. Two different molecular weight poly(ethylene glycol) diglycidyl ethers (PEGDEs) were grafted to the membrane surface using the top surface method of modification. Fouling resistance, measured as percent flux decline with time, was measured in four different feed streams: 150 ppm dodecyltrimethylammonium bromide (DTAB), 150 ppm sodium dodecyl sulfate (SDS), 150 ppm 9:1 decane:DTAB emulsion, or 150 ppm 9:1 decane:SDS emulsion. Additionally, flux recovery after cleaning was also investigated, to determine the extent of irreversible fouling. PEGDE-modified XLE and NF90 membranes demonstrated better fouling resistance and flux recovery than unmodified control RO membranes when tested in surfactant-only fouling feed (DTAB or SDS). They also showed slightly better fouling resistance in oily water emulsions (decane:DTAB or decane:SDS).

In addition to performance testing of PEGDE-modified membranes, surface characterization of these membranes has also been performed to probe the cause of the observed performance changes. Fourier transform infrared spectroscopy (FTIR) and x-ray photoelectron spectroscopy (XPS) were used to verify the presence of PEGDE on the membrane surface. Graft density was measured using a magnetic suspension balance capable of measuring mass changes on the order of micrograms. An electrokinetic analyzer was used to measure the surface charge of the PEGDE-modified and unmodified membranes. Surface charge is thought to be one potential cause of observed fouling behavior. Polyamide membranes are negatively charged at normal operating pH (7–8), and PEGDE-modified membrane surfaces were only slightly less negatively charged. PEG is a neutral molecule and a PEG film has virtually no surface charge, which indicates incomplete or patchy surface coverage of PEGDE on the NF and RO membranes.

Significance

This university collaboration will benefit the national security mission of the DOE by creating technology that is targeted toward maintaining a sustainable and secure water supply for human use. New science will facilitate lowering the energy requirements for water purification.

Refereed Communications

E.M. van Wagner, A.C. Sagle, M.M. Sharma, and B.D. Freeman, “Effect of Crossflow Testing Conditions, Including Feed pH and Continuous Feed Filtration, on Commercial Reverse Osmosis Membrane Performance,” to be published in the *Journal of Membrane Science*.

A.C. Sagle, E.M. van Wagner, H. Ju, B.D. McCloskey, B.D. Freeman, and M.M. Sharma, “PEG-Coated Reverse Osmosis Membranes: Desalination Properties and Fouling Resistance,” *Journal of Membrane Science*, vol. 340, pp. 92-108, September 2009.

Interfacial Property Control of Elastomeric Nanocomposites

113483
Year 3 of 3
Principal Investigator: T. J. Boyle

Project Purpose

Polymeric nanocomposite materials promise to revolutionize the optical, electronic, catalytic, and mechanical properties of elastomeric materials by allowing for controlled manipulation of the final materials' properties. However, it has been demonstrated that simply mixing advanced, nanoscale materials into standard polymeric materials results in deviations from the enhanced properties expected from standard composite theory. The overarching reason for this difficulty is the failure to control and predict the influence of the nanomaterials-elastomer interface. This is due to the surface area to volume ratio in nanocomposites being so large, that its effect dominates the rules of mixtures behavior for the individual components themselves. For instance, a change from a 100- to 10-nm diameter nanoparticle results in a 900% increase in the surface-to-volume ratio.

To overcome these challenges, this project will develop unique Sandia capabilities that will allow for the systematic variation of the nanoparticle-polymeric interfaces and predict the interfacial effect on composite properties. We will use advanced synthetic routes to intentionally vary the shape of the nanoceramics (NC) and to tune the strength of their interaction with an elastomeric matrix. Throughout this project, it will be necessary to characterize the surface chemistry, nanostructure, and the mechanical behavior of the designed interfaces in both liquid and solid matrices. These measurements will be performed in conjunction with molecular-scale modeling to yield a fundamental understanding of the nanocomposite interface and create a predictive capability that will provide a connection between synthesis and resultant properties. Sandia's ability to tailor the properties of the elastomeric/NC composites will have a substantial impact on existing programs at Sandia (e.g., Center for Integrated Nanotechnologies [CINT]). Further, numerous American industrial applications, especially the automotive industry, require this information and will be partners in directing and testing these concepts and materials.

Summary of Accomplishments

- Developed new routes to high-aspect-ratio nanowires of ceramic materials that are very reproducible.
- Demonstrated through computational calculations that "jack" morphologies are of the most interest.
- Determined new methods for coating nanomaterials of interest.
- Functionalized with silanes to interact with squalene.
- Functionality leads to negative charge on surface!
- Modeling indicates both chain and terminus affect surface charge.
- Test beds from electrospinning indicate nanoparticle distribution can be controlled by ligand functionality.
- Sent large batches to Goodyear, Inc. for testing in real-life systems: (i) uncoated and (ii) functionalized.
- Silane functionalized rods found by cryo-ultramicrotome transmission electron microscopy (TEM) to "nest."
- Preparation for large-scale MnO_x and $M'MnO_x$ "nanojacks" is underway.

Significance

Tailored nanocomposite materials are expected to be stronger, lighter, more resistant to aging, or provide any other desired property in a predetermined manner, contributing greatly to a number of DOE critical missions (e.g., nuclear security and energy security).

Refereed Communications

J.M.D. Lane, A.E. Ismail, M. Chandross, C.D. Lorenz, and G.S. Grest, “Forces Between Functionalized Silica Nanoparticles in Solution,” *Physical Review E*, vol. 79, p. 050501, May 2009.

M.K. Petersen, J.M.D. Lane, and G.S. Grest, “Shear Viscosity of Extended Nanoparticles,” to be published in *Physical Review E*.

T.N. Lambert, C.A. Chavez, B. Hernandez-Sanchez, P. Lu, A. Ambrosini, T. Friedman, T.J. Boyle and D.R. Wheeler, “Synthesis and Characterization of Titania-Graphene Nanocomposites,” to be published in the *Journal of Physical Chemistry C*.

Improving Electronic Structure Calculations to Predict Nano-optoelectronics and Nanocatalyst Functions

113484
Year 3 of 3
Principal Investigator: K. Leung

Project Purpose

Current density functional theory (DFT) implementations, while extremely successful for many solid-state applications, often predict incorrect binding energies, catalytic behavior, and spin-states for common transition metal centers and integrated porphyrin systems. We propose to emphasize the concept of spatial locality to improve the treatment of heavy atoms, and apply it towards fundamental investigations of porphyrin-based nanocatalysts and molecular electronics. Our theoretical expertise includes new DFT functionals (Sandia); DFT+U (Massachusetts Institute of Technology [MIT]; University of California, Santa Barbara [UCSB]; Sandia); and quasi-self-interaction free DFT (UCSB). Our predictions will be validated with comprehensive experiments on cobalt porphyrin structures, which are potential catalysts for solar energy-based reduction of the greenhouse gas carbon dioxide in aqueous solutions. We will also study novel porphyrin nanosheets, potentially useful for molecular electronics-based memory chip applications.

Other than these nanoengineering catalysis and optoelectronics applications, our electronic structure methods will also potentially strongly impact the modeling of lanthanide and actinide materials pertinent to Sandia's national security needs (nuclear materials), the Qualification Alternatives to the Sandia Pulsed Reactor [QASPR] project, and ongoing modeling efforts related to unique Sandia capabilities such as radiolysis-aided metal nanoalloy synthesis and biological sensors (DHS programs). Students and postdocs from MIT and UCSB will visit and interact with experimentalists and industrial experts at the Center for Integrated Nanotechnologies (CINT), giving the next generation of US scientists a post-university experience and education in the science-based integrated nanoengineering effort unique to national laboratory/industry settings.

Summary of Accomplishments

The use of transition metal ion (especially cobalt) based porphyrins, corrins, and other macrocycles to catalyze CO_2 reduction has been pursued by John Shelnutt and coworkers at Sandia. They have applied polymerized cobalt macrocycles layers coated on gas diffusion electrodes. The overall reaction likely takes place in four steps:

$CoP + CO_2 \rightarrow CoP\text{-}CO_2$
$CoP\text{-}CO_2 + H^+ \rightarrow CoP\text{-}COOH$
$CoP\text{-}COOH \rightarrow CoP\text{-}CO + OH^-$
$CoP\text{-}CO \rightarrow CoP + CO$

The two electrons can be added to any of the 4 products/intermediates. Thus, the above reaction actually represents 10 different mechanisms depending on when electrons are injected.

In this work, we apply density functional theory and *ab initio* molecular dynamics techniques to study the reaction intermediates of these reactions in water. We addressed several general issues regarding CoP-catalyzed CO_2 reduction. (1) The difference between aprotic and protic solvents is that various charged intermediates are strongly stabilized by water, which also acts as a proton source critical to form the key $CoP\text{-}COOH^-$ intermediate. (2) We elucidated the optimal charge- and spin-states of the cobalt ion in the intermediates, determined by the electrochemical potentials used in experiments, using redox potential calculations. These calculations confirmed, for example, that CoP-$COOH^-$ may be the key intermediate. (3) We found that almost all steps of the multistep reaction go downhill in free energy. (4) We discovered that high pH conditions facilitate this reaction because $CoPCOOH^-$ is only very weakly acidic (pK_a>8), contrary to CoPCOOH, which behaves like a carboxylic acid (pK_a~4.5).

Significance

This work is aligned with DOE goals for energy security, nuclear security, and scientific discovery and innovation. The project will provide important new understanding that could result in solutions for greenhouse gas reduction and CO_2 sequestration. This work can also improve theoretical tools for lanthanide/actinide modeling, reduce optoelectronic device size and power consumption, and increase reliability.

Developing a Thermal Microscopy Platform for In-Situ Thermal/Thermoelectric Structure-Property Studies of Individual Nanotubes and Nanowires

113485
Year 3 of 3
Principal Investigator: J. Huang

Project Purpose

The main goal of this project was to advance the state of the art in-situ structure and property characterization for low-dimensional nanostructures, including nanowires and carbon nanotubes (CNTs). Creation of a characterization platform capable of performing thermal and thermoelectric transport analysis as well as transmission electron microscopy (TEM) structural analysis on the same structure is an as yet nonexistent capability. No fundamental understanding exists of the relationships between nanowire structure and thermal properties, hindering both cooling and power-conversion developments. Presently, the thermal/thermoelectric properties of nanowire arrays are measured via bulk techniques providing an aggregate average of millions of nanowires. However, such arrays consist of nanowire structures with varying diameters, defects, grain boundaries, etc. No direct thermal property-nanostructural correlations exist for individual nanowire structures. The lack of structure and property correlation in nanomaterials creates problems in understanding their intrinsic properties.

Summary of Accomplishments

We developed a microelectromechanical systems (MEMS) thermal microscopy platform that is compatible with both a cryostat for thermal property measurement and transmission electron microscopy (TEM) for microstructure investigation of the same nanostructure. The thermal properties and atomic structures of individual Si and GaN nanowires were investigated, and this investigation demonstrated that the thermal microscopy platform works. Theoretical modeling tools were developed to study atomistic phonon scattering in model systems, such as CNTs. We are extending our study to other materials systems, such as Bi, BiTe, and CNTs.

Significance

We believe these studies will provide unprecedented details regarding size, defects and surface effects on the electron and phonon transport processes in nanowires, nanotubes, and other nanomaterials (e.g., graphene), and will open a new path to study nanoscale transport phenomena in general. The results will provide the foundational science needed to tailor nanostructure fabrication for integrated device applications.

Refereed Communications

J.Y. Huang, F. Ding, B.I. Yakobson, P. Lu, Q. Liang, and J. Li, "In-Situ Observation of Graphene Sublimation and Multilayer Edge Reconstructions," *Proceedings of the National Academy of Science*, vol. 106, pp. 10103-10108, June 2009.

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Fundamentals of Synthetic Conversion of CO_2 to Simple Hydrocarbon Fuels

113486
Year 3 of 3
Principal Investigator: R. A. Kemp

Project Purpose

The production of useful energy is inherently linked to national security and quality of life, yet depends on depletable resources and poses the risk of catastrophically altering the environment. There is no greater problem than sustainable production of usable energy. We have begun to attack this problem by developing technologies for recycling CO_2 into hydrocarbon-based transportation fuels, with the intent of helping to ensure domestic and battlefield energy supplies while mitigating global climate change. This approach is "bio-inspired" as nature employs the same inputs, CO_2/energy/water, to produce oxygenated hydrocarbons or biomass. Our work addresses two identified strategic goals by partnering with key academic/industrial institutions, and simultaneously meet the goals stated in Sandia's nanoengineering initiative. First, although CO_2 recycling is "bio-inspired," detailed process analyses comparing possible gains achievable using nanotechnology to convert CO_2 and water to fuel synthetically, i.e., in the form of nanostructured biomimetic catalysts, to Nature's biomass route have not been completed. Understanding "advantages-disadvantages" of these alternate routes is essential to success in directing research towards establishing credibility and identifying key hurdles and promising research directions. It is critical to understand early whether any as yet unforeseen "showstoppers" exist in synthetic chemical route(s).

We are partnering with the University of Wisconsin to perform this analysis. We also address the science of applying nanotechnology to direct chemical or electrochemical production of a key intermediate, namely methanol, from CO_2 and water (or H_2). Calculations suggest that copper nanocatalysts alone, or possibly on the surface of electrodes (produced collaboratively with the University of Vermont and the University of Texas), can directly affect this reaction.

Summary of Accomplishments

Based on previous density functional theory (DFT) calculations on the Cu(111) surface, we developed a microkinetic model for methanol synthesis from mixtures of $CO/CO_2/H_2$. Several reaction pathways were included with over 60+ elementary steps evaluated. The model was then fitted to published kinetic data using a commercial $Cu/ZnO/Al_2O_3$ catalyst. Our model indicates that about 2/3 of the MeOH produced is synthesized from CO_2 via the intermediates HCOO, HCOOH, $(HO)CH_2O$, CH_2O, and CH_3O. Due to the ease of cleaving the C-O bond, the intermediate $(HO)CH_2O$ has been shown to be of special importance. Also, the Cu(111) surface may not be the most reactive facet on the operating catalyst. Process analysis and economic studies for two CO_2/H_2 reaction systems have been performed. The first process has two isothermal reaction systems: a) a water-gas shift (WGS) reactor, and b) a methanol synthesis reaction, and one separation system for the methanol recovery. We developed a second alternative with an amine-based CO_2 separation system to remove CO_2 from the WGS stream output. Our calculations show that in the current environment, splitting of CO_2 becomes economically attractive if it costs less than \$284.58/MTON CO_2. However, this value is expected to increase, as the price of methanol is expected to increase. Both processes have overall efficiencies significantly higher than their biological counterpart. The efficiency for the production of methanol from CO_2 and H_2 is 50%, but we have shown in simulations that changes to this process can increase this yield up to ~87%. A new route to electrically conducting polymers has been developed with the University of Texas group, using metal "seed points" to grow metal nanoparticles as catalysts. While not yet demonstrated for methanol, the catalyst system does show promise for an oxygen reduction reaction.

Significance

Overall, work performed in this project has concluded that the proposed concept of recycling waste CO_2 back into a usable fuel (for example in this case, methanol) via reduction with hydrogen is clearly feasible in the near future. In other words, we have focused on the re-conversion step of taking CO_2 back into a fuel, and the process analysis performed here indicates no technical or economic "showstoppers" are present in this step. Additionally, the economic sensitivities of each variable in the process were evaluated. These results are particularly applicable to the "Sunshine to Petrol" Grand Challenge LDRD project currently ongoing at Sandia.

Density functional theory (DFT) results obtained during this project have indicated the roles of many presumed intermediates in the reaction of CO_2 with H_2. Over 60 possible intermediate structures have been calculated on Cu(111) surfaces, and a particular one — $OCH_2(OH)$ — has been shown to be important because the C-O bond is easily broken. These scientific results will play an important role in guiding and helping to design future catalysts to improve the CO_2/H_2 conversion to methanol. An important technical contribution was the modification and optimization of the CAMERE (carbon dioxide hydrogenation to form methanol via a reverse-water-gas-shift reaction) process to yield a calculated increase of methanol production from 53% to 87%. This optimization was primarily based on changes to reactor conditions and recycle streams. Attempts to grow electrically conducting polymers containing metal nanoparticles were also successful. These polymers could be grown on electrode surfaces to yield seed points for nanoparticle growth. Further development of this polymer growth procedure will be of interest to a wide range of energy-related researchers. Catalysts of this type have recently been shown to be active for the oxygen reduction reaction, thus indicating interest in a variety of processes.

Refereed Communications

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Electrostatic Microvalves Utilizing Conductive Nanoparticles for Improved Speed, Lower Power, and Higher Force Actuation

113487
Year 3 of 3
Principal Investigator: C. A. Apblett

Project Purpose

This project seeks to use nanoparticles suspended in a polymer matrix to form a microfluidic valve that has the force and actuation speed of a pneumatic valve with the ease of integration of an electrostatic valve. We have incorporated carbon nanotubes above the percolation threshold to provide electrical continuity in the polymer membrane of the valve as it deflects through the entire range of motion. The critical findings from this year's efforts have been the tradeoff between thickness of the membrane and the amount of force that the valve can sustain prior to being forced open. Computer predictions of this nanoparticle valve have guided the design and fabrication of prototypes with the established microfluidic process, and focused on efforts to reduce process complexity by removing a patterning step within the nanotube layer by using actuation bias only above or below this layer. Incorporation of the nanoparticles through various means has been achieved, and there is current work in characterizing the electrical properties of the membrane as a function of displacement. The current actuation voltages are too high to be useful on chip, so efforts are now focused on reducing this actuation voltage. Once the valve material set has been optimized by selection of appropriate particle size, morphology, loading, and composition, it will be integrated into a microfluidic array that will be used to grow a large array of identical protein nanocrystals. Successful completion of this project will allow Sandia a novel microfluidic technology that has a much higher level of integration of valve control with higher force than has been previously achieved. This technological advantage can be leveraged into opportunities in homeland security for biological hazard analysis and in the National Institutes of Health (NIH) for use in infectious agent research.

Summary of Accomplishments

We have designed and built electrostatically actuated microvalves compatible with integration into a polydimethylsiloxane (PDMS)-based microfluidic system. The key innovation for electrostatic actuation was the incorporation of carbon nanotubes into the PDMS valve membrane, allowing for electrostatic charging of the PDMS layer and subsequent discharging, while still allowing for significant distention of the valveseat for low-voltage control of the system. Nanoparticles were applied to semicured PDMS using a stamp transfer method, and then cured fully to make the valve seats. DC actuation in air of these valves yielded operational voltages as low as 15 V, by using a supporting structure above the valve seat that allowed sufficient restoring forces to be applied while not enhancing actuation forces to raise the valve actuation potential. Both actuate-to-open and actuate-to-close valves have been demonstrated, and integrated into a microfluidic platform, and demonstrated fluidic control using electrostatic valves.

Significance

Microfluidics are a critical component of several microsystems integrations, and a technique to more tightly integrate microfluidics and microelectronics will provide opportunities in homeland security for biological hazard analysis and in NIH for use in infectious agent research. Use in defense, energy, and environmental applications can be envisioned for a small gas control system or integrated chemical/biological gas analyzer.

Nanoengineering by Optically Directed Self-Assembly

113488
Year 3 of 3
Principal Investigator: A. M. Grillet

Project Purpose

Optical microdevices have many advantages over traditional electronic devices including lower energy losses and reduced interference from radiation. However, lack of robust manufacturing technology to produce photonic crystals currently limits development and application of these technologies. Traditional methods such as spontaneous self-assembly cannot generate the complex structures required to produce a full bandgap photonic crystal.

The goal of this work is to develop and demonstrate novel methods of directed self-assembly of nanomaterials using optical fields. To achieve this aim, our work will employ laser tweezers, a technology that enables noninvasive optical manipulation of particles, from glass microspheres (diameter[D] ~3 microns) to gold nanoparticles (D ~ 20 nm). Laser tweezers will be used to create ordered materials with either complex crystal structures or using aspherical building blocks that are free of random defects, thereby enabling realization of novel nanomaterial characteristics such as full photonic bandgaps. Additionally, laser tweezers allow defects to be systematically engineered into the photonic crystals, which would be impossible with spontaneous self-assembly. The product of this research effort will be a demonstrated capability to perform nanomanufacturing of particle structures with controlled optical properties.

This project brings together a multidisciplinary team from Sandia, Yale University, and the University of Delaware. With active collaboration with industrial partners, this partnership will provide a unique educational opportunity for engineering graduate students and postdoctoral researchers, while enabling new nanoengineering manufacturing technologies especially focused in economically competitive next-generation technologies.

Summary of Accomplishments

This project has developed significant new capabilities to measure femtonewton-scale forces acting between colloidal particles. We have expanded existing techniques to understand interactions of aspherical particles, multiparticle effects and interactions in electric fields. Understanding interactions is critical to controlling stability and assembly of particles. For example, multibody effects have been found to reduce stabilizing electrostatic repulsions between particles resulting in particle aggregation (i.e., unstable particle suspensions). Using holographic optical trapping methods we have built metastable crystal structures such as the A4 diamond structure which is predicted to have a large photonic bandgap. We have additionally developed novel optically switchable coatings to functionalize particles and applied them to build complex three dimensional structures. Using electric field assembly, we have demonstrated the ability to create ordered arrays of spherical and aspherical particles. Applying this technique, we have created ordered arrays of two industrially relevant nanoparticles: ZSM-5 a catalyst used in oil refining and titanium dioxide which is used in many industrial processes including paints and sunscreen. Coupling electric field with convective assembly, nanostructured titania films are assembled with controlled orientation. Optical and thermal properties of these films are under further investigation.

Significance

This novel nanomanufacturing capability for photonic bandgap crystals may enable an optical computing revolution. Photonic computing offers many advantages over electronic computing such as reducing energy-loss mechanisms, increasing bandwidth, and reducing interference in radiation-sensitive applications. This project addresses the current technology limitation of optical computing — the lack of robust techniques for manufacturing photonic bandgap crystals.

Refereed Communications

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Optimized Nanoporous Materials

113489
Year 3 of 3
Principal Investigator: D. Robinson

Project Purpose

In many applications including batteries, supercapacitors, fuel cells, and water purification, functionality depends on an interaction with a surface, such as an electrostatic attraction or chemical reaction. To maximize functionality, we want materials that maximize surface area by arranging so that every point in the material is within a few nanometers of a surface. Unfortunately, this means that electrical charge or chemical reactants must travel long distances through very narrow channels to reach all of that area. This results in tradeoffs between functionality and transport. In the case of a supercapacitor — the target application on which we focus — this means charge capacity and discharge rate. Our goal is to learn how to overcome this tradeoff. We plan to achieve this by creating larger channels into the interior of a supercapacitor that allow rapid transport with minimal sacrifice of storage material.

Solving this problem requires development of new methods to synthesize materials with regular arrays of pores on several defined length scales, coupled with a thorough understanding of nanoscale mass and charge transport that is being developed by others at Sandia in separately funded modeling efforts. We are applying new templating and self-assembly methods to synthesize conducting materials with optimized pore geometries. We characterize their structure and performance via electron microscopy and electrochemical kinetic measurements.

These materials could improve performance of both low-voltage and high-energy pulsed-power supplies in weapons, and also support our energy security role by helping accommodate intermittent generation and loads in hybrid vehicles and wind or solar power plants. This work is fundamental in nature and requires significant breakthroughs to succeed, but promises significant advances in the design and synthesis of nanoporous materials for energy and defense applications, making the work appropriate for the LDRD program.

Summary of Accomplishments

It became apparent in this project that there is a significant lack of basic understanding of charge transport in nanoporous conductors and many easy opportunities to learn about and exploit the unique phenomena that occur in this context.

We studied the relationship between resistance inside and outside a nanoscale pore. To boost charging rates, opposing electrodes should be as close together as possible, but there is a point beyond which there are diminishing returns, and increasing practical limitations to fabrication and operation. This presents optimal length scales for design of energy storage devices.

In nanoscale pores, the amount of salt that adsorbs to the electrode can become comparable to the amount of salt in the pore. When the salt concentration goes down, the electrode becomes more resistive, and charges more slowly. We quantified this effect through modeling and demonstrated it in experiments. Added wall adsorbates — and sometimes the adsorbed ions themselves — can change the chemical potential of free ions in the pores, changing the conductivity. Control of these effects is necessary for fabrication of optimal energy storage devices.

With the University of Illinois, we developed new ways to fabricate hierarchically porous electrodes that may overcome some of these limitations on charging rate. We also applied a combination of advanced deposition techniques to make finely interpenetrating but still highly conducting capacitor electrodes.

With North Carolina State University, we proved that porous conductors are also of potential use in drug delivery applications because they can store significant concentrations of charged drugs, and the release rate can be controlled by changing voltage.

We determined that there are many opportunities for future advancement of understanding and application of nanoporous conductors, and they are worthy of future research and development investments.

Significance

This project supports our energy and nuclear weapons (NW) missions by providing new tools and methods enabling optimized nanoporous materials for use in electric power generation (fuel cells), hybrid vehicles, and intermittent renewable sources (supercapacitors). It further supports the American Competitiveness Initiative (ACI) and objectives of Sandia's National Institute for NanoEngineering (NINE) and Strategic Partnerships investment area (IA) through a new collaboration between Sandia and the University of Illinois.

CO_2 Reduction Using Biomimetic Photocatalytic Nanodevices

113490
Year 3 of 3
Principal Investigator: J. E. Miller

Project Purpose

Nobel Prize winner Richard Smalley has called energy research the single most important problem facing humanity today and has promoted nanotechnology as a means to harness solar energy. Applying nanotechnology to create solar fuels (i.e., fuels created from sunlight, carbon dioxide, and water) is especially attractive as it impacts not only energy production and storage, but also climate change. Furthermore, solar irradiation is the only sustainable energy source of a magnitude sufficient to meet projections for global energy demand. Biofuels meet the definition of a solar fuel but the efficiency of photosynthesis is estimated to be less than 10% of that needed for biofuels to serve as a replacement for fossil fuels. Alternately, bio-inspired nanostructured photocatalytic devices that more directly and efficiently produce fuel can be envisioned. To be competitive, these devices need to be robust, multifunctional, and capable of promoting and coupling the multielectron, multiphoton water oxidation and CO_2 reduction processes in one complete system. The purpose of the project was to design, fabricate, and characterize just such nanodevices using key components that are inspired by nature —specifically synthetic analogs of the light-harvesting chlorosomal nanorods of photosynthetic bacteria. Cobalt porphyrins that are catalytically active for CO_2 reduction are incorporated into self-assembled photocatalytic porphyrin nanostructures that were first discovered at Sandia. These hybrid nanomaterials can then be joined to semiconductors capable of oxidizing water to O_2, or to electrodes for use in electrochemical systems. The completed nanodevices or nanostructured electrodes can then use the energy in sunlight to perform or assist in the creation of a solar fuel, in this case CO.

Summary of Accomplishments

We applied ionic self-assembly to create new porphyrin nano- and/or meso-structures with unique morphologies and properties. This approach has proven to be fairly general and useful for combining different functionalities into a single nanostructure. For example a light-harvesting tin porphyrin and catalytic cobalt porphyrin can be assembled into a single structure. We also applied other techniques, for example metal-ion-induced polymerization, to create porphyrin structures such as uniform cobalt porphyrin nanospheres. Morphologies produced in this effort range from fairly simple geometries such as sheets, rods, tubes, plates, and spheres, to complex geometries that appear cabbage- or clover-like, or like wheels and spokes. We successfully grew porphyrin nanostructures on electrochemical reactor supports (gas diffusion layer) and applied these nanostructures for the first time to reduce carbon dioxide to carbon monoxide with high selectivity. Carbon monoxide is a key synfuel intermediate. In collaboration with others, we gained insight into the reaction mechanism that allows for this high selectivity. Finally we demonstrated visible light enhancement (up to 30%) of CO_2 reduction with these devices.

Significance

Development of nanotechnology to produce carbon-based solar fuels will help provide a pathway to a more secure, sustainable and environmentally benign energy future. The work directly supports the DOE energy security goals and the goals of Sandia's Energy, Resources and Nonproliferation strategic management unit. The research enhances core laboratory strengths including nanotechnology, materials, and energy, and helps establish Sandia's National Institute for NanoEngineering. Finally, the work is helping to solidify Sandia's role as a leader in "solar fuels."

Refereed Communications

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Stress-Induced Chemical Detection Using Flexible Coordination Polymers

113491
Year 3 of 3
Principal Investigator: M. D. Allendorf

Project Purpose

Real-time, compact, and highly sensitive chemical detectors remain a critical need for embedded surveillance, detection of explosives, water-quality monitoring, high-throughput medical analysis, and monitoring personal exposure to environmental toxicants. The latter application is particularly demanding. Existing exposure assessment methods provide little information about changes over time and have technology problems concerning sensitivity, specificity, and portability. In each of these applications, high sensitivity to multiple analytes, coupled with a low-cost, compact design, are desirable. Static microcantilevers (SMC), which detect adsorption-induced stresses, outperform resonant-beam designs and have sensitivities superior to quartz crystal microbalances and conventional piezoelectric gravimetric sensors. However, to achieve sub-ppb sensitivities, equivalent to picomolar concentrations in water and femtomolar concentrations in air, recognition chemistries are needed to induce differential stress in the cantilever while simultaneously providing specificity for a broad range of analytes. Interdisciplinary approaches and tools are needed to create completely new sensing materials, enabling real-time monitoring of sub-ppb analyte levels.

The objectives of this project are to discover new recognition chemistries based on a novel class of nanoporous materials known as coordination polymers (CPs), and integrate them with SMCs to create a new generation of versatile sensors with unprecedented sensitivity and selectivity. CPs have chemically tailorable pores and unit cell dimensions that vary by as much as 10% upon guest sorption. Because of their crystalline nature, CPs can be modeled by high-level methods (e.g., molecular dynamics), allowing sorption chemistry to be linked with induced mechanical stress. Thus, a fully rational design process is possible to guide the synthesis of CPs with desired adsorption capabilities. This project includes collaboration with the Georgia Institute of Technology School of Engineering, creating nanoengineering expertise for this new class of sensing materials.

Summary of Accomplishments

Using a chip with microcantilevers (MCL) coated with a nanoporous coordination polymer (CP) we demonstrated the concept of stress-based chemical detection, which is the major hypothesis tested in this project. We showed that the CP-coated device responds to water vapor, alcohols, and CO_2 in a manner consistent with the reported isotherms. Furthermore, we demonstrated that controlling the hydration state of the CP layer can be used to impart selectivity to CO_2. The results were published in a reviewed journal and a patent application was filed. Building on this discovery, we developed methods to grow several other CP on microcantilevers, and collaborated with Prof. R. Fischer (Ruhr Universitat, Bochum, Germany) to create a new capability for producing CP films on substrates. A second CP was integrated with a microcantilever and shown to respond to H_2O and alcohol vapors, but in a different way than the first, suggesting that MCL arrays can be designed for selective detection. We also developed new force fields to enable atomistic simulations of a range of CPs. These models were used to predict the uptake of explosives, nerve agents, volatile organics, and polyaromatic hydrocarbons by CPs. The results demonstrate that the response of these nanoporous materials is strongly dependent upon their chemical structure and that an array of sensors coated with different CP can be used for selective chemical detection. This work performs model gas uptake by CPs of interest in collaboration with Prof. T. Timofeva at New Mexico Highlands University. Three journal articles were submitted to reviewed journals as a result of this work. A total of 15 conference presentations were given during the project and two reviewed proceedings papers were published.

Significance

Our results are the first-ever integration of a nanoporous CP with an actual electronic device, as well as the first use of a CP as part of a sensor and as such are of considerable scientific interest. In follow-on projects we expect it to be possible to develop CP coatings tailored for personal environmental monitors, trace-contaminant detection, and explosives detection. Our efforts to develop force fields to describe the uptake of small molecules by these materials created new tools that can be used to guide synthetic efforts to create new CPs with tailored properties. During the project we collaborated with several universities and as a result engaged both students and postdocs in the research. Other benefits include improved understanding of, 1) transport phenomena in porous media; 2) gas sorption; 3) and separation methods.

Aligned Mesoporous Architectures and Devices

118841
Year 2 of 3
Principal Investigator: C. J. Brinker

Project Purpose

During the last decade, mesoporous materials with tunable periodic pores have been synthesized using surfactant liquid crystalline templates thus opening a new avenue for a wide spectrum of applications. However, potential applications for these materials are somewhat limited by their unfavorable pore orientation. Although considerable effort has been devoted to align the pore channels, fabrication of mesoporous materials with perpendicular pore channels remains a major challenge.

Our work in the previous year demonstrated that pore channels of mesoporous silica can be aligned by exploiting capillary forces. Alignment was achieved by contacting a nanocomposite thin film that contains inorganic clusters or oligomeric building blocks and lyotropic surfactant liquid crystalline phase with an anodized porous alumina membrane. Wetting of the nanocomposite on the porous membrane creates a fluid meniscus, generating a capillary force that fills the alumina pore channels with the nanocomposite. During the capillary rise, the mesostructure within the nanocomposite is aligned by the shearing force and subsequently forms aligned mesoporous channels after further polymerization and surfactant removal. This work leads to the formation of long fibers or fiber bundles with aligned pore channels.

We propose to explore the use of the aligned architectures for ionic transport channels. Ionic channels are of great interest for fuel cells and neuron signal transmission. Success of this work may provide new fabrication techniques and insight leading to better materials for many energy-related or biological applications.

Summary of Accomplishments

This work, with PECASE (Presidential Early Career Award for Scientists and Engineers) recipient Yunfeng Lu at the University of California, Los Angeles, resulted in reaching the following milestones:

1. We further optimized the synthesis conditions and demonstrated alignment of the mesostructures. This was achieved by optimizing the pH, temperature and aging time, which allowed us to minimize the polymerization reaction kinetics and maximize the mobility of the building blocks.
2. We conducted both fluidic mechanical calculations and experimental studies to understand the aligning mechanism. Viscoelastic properties and contact angle of the nanocomposite were measured and used to calculate the capillary force and shearing force. A mechanism was proposed based on these studies.
3. We investigated the alignment of mesostructures within different-sized alumina pore channels. Alumina membranes with different pore diameters were used as the template to study the assembly of the mesostructure within this confined environment.
4. We synthesized aligned metal and semiconductor nanowire arrays using electrochemical deposition using the aligned mesostructure as template.

Significance

This work will support the DOE mission for scientific discovery and innovation, by developing a novel material platform with potential application in water purification, separations, chem/bio sensors, templated synthesis, microelectronics, optics, controlled drug release, and highly selective catalysis.

Refereed Communications

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Rheological Properties of Nanocomposites

118842
Year 2 of 3
Principal Investigator: B. A. Simmons

Project Purpose

The overarching goal of this project with Presidential Early Career Awards for Scientists and Engineers (PECASE) recipient, Bill King, at the University of Illinois, is to develop an understanding of nanometer-scale polymer flows as a function of composition, shear, strain, and temperature. Of particular interest are large strain flows in nanocomposite materials, as are relevant for manufacturing and reliability. Nanometer-scale polymer flows exist at interfaces and surfaces, near inclusions, and in a number of manufacturing applications. Hot embossing offers the opportunity for large area manufacturing with nanometer-scale features. In embossing for micro-/nanoscale patterning, a relief mold is pressed into a soft polymer medium. Typically the stamp is heated such that the polymer melts beneath the stamp. Feature sizes are possible as small as 10 nm over several square centimeters. Our previous work has shown that the most important mechanism of polymer flow during nanoimprint lithography is the squeeze flow of the polymer that is extruded between the hard imprinting template and a supporting hard substrate.

We propose to continue our direct mechanical measurements on polymer squeeze flow of nanoparticle-polymer blends. The measurements are capable of simultaneously extracting both stress and strain of a polymer down to extruded thicknesses of < 5 nm. The measurements can be performed at temperature between room temperature and 200 °C, which allows interrogation of both glassy and viscoelastic polymer mechanical response. The polymer films of interest include nanoparticle quantum dots, which are of size 2–20 nm. The measurements will be the first of their type in that the nanoparticle inclusions are of size comparable to the polymer molecule. The high resolution of the measurement technique will allow mechanical properties to be extracted on the molecular scale, which in turn may guide simulations and design of manufacturing processes.

Summary of Accomplishments

The accomplishments of this FY were to determine the impact of nanoparticle morphology and size on different polymer nanocomposites. It was determined that the size of the nanoparticles, correlated with the intrinsic properties (e.g., molecular weight and hydrophilicty/hydrophobicity) of the polymers, over the ranges of 10–150 nm, have a significant impact on the rheological properties of the nanocomposites as compared to particle-free polymers. The use of traditional polyolefins with tailored nanoparticles and specific surface chemistries appear to be the strongest candidates in terms of developing a model system for future work. The development of a model system for further study will enable the discovery into the fundamental understanding of these systems that are necessary to develop robust nanocomposites for industrial applications. The insight gained by this work indicates that the surface energy and surface composition of the nanoparticles plays a significant role into the ultimate properties of the nanocomposites. These results are in the process of being developed into manuscripts for submission in the scientific literature.

Significance

This project will develop a fundamental, science-based approach to understanding polymer flows at the nanoscale. This project therefore supports DOE's mission in scientific discovery and innovation, especially for nanoscience, and contributes to Sandia's Basic Energy Sciences (BES) programs and the Center for Integrated Nanotechnologies (CINT). The development of nanocomposites that can be patterned down to the nanometer scale will also have applications in advanced photovoltaic materials, and therefore links to the DOE energy security mission (e.g., solar and renewable energy programs).

A New Chamber Design for Aerosol Evolution Studies in the Ambient Environment

118843
Year 2 of 3
Principal Investigator: B. D. Zak

Project Purpose

Atmospheric aerosols impact climate, both directly through scattering and absorption of radiation and indirectly through cloud processes. Because of the complex composition and spatial and temporal distribution of the atmospheric aerosol, understanding such impacts is challenging. To better understand the effects of aerosols, we study the processes that transform aerosols, such as new particle formation, condensation/dissolution, coagulation, and cloud processing. Numerous studies have utilized laboratory smog chambers to help predict the behavior of the atmospheric aerosol. Using the results of such laboratory experiments to predict the behavior of the ambient aerosol, however, is difficult given the complexity of the atmosphere and the inability to replicate such conditions. Recently, we designed, tested and deployed a new-type chamber in order to study the evolution of an initially monodisperse aerosol in ambient conditions over intervals of one or more days. The work is in collaboration with Texas A&M University (TAMU).

The ambient aerosol chamber for evolution studies (AACES) is a cubical chamber of rigid Acrylite OP-4 acrylic outer shell, which transmits UV radiation both in the UV-B (280–215 nm) and UV-A (315-400 nm) ranges. FEP Teflon lines the inside of the chamber on all sides and the top, while expanded-PTFE (ePTFE) Teflon is used on the bottom of the chamber. The fibrous structure of the ePTFE acts as a barrier to particulates, while allowing gas molecules to move virtually unimpeded from one side of the membrane to the other, creating an initial environment inside the chamber that is free of particles and continuously mimics the ambient air. Two to three chambers will be deployed in various field locations. Each chamber will be used to study the effects of aerosol transformation given different initial ambient conditions as well as both inorganic and organic particle types.

Summary of Accomplishments

During the course of FY 2009, data was collected in a remote forested location north of Woodland Park, Colorado. Analysis of the aerosol transformations occurring in this terpene forest showed significant production of secondary organic aerosol with growth rates as high as 15 nm per hour of additional organic material being added. Following the completion of data analysis, AACES was brought back to TAMU and modified to provide a more rigid framework allowing for ease in transportation and greater sealing efficiency. To do this, an aluminum framework was designed and fitted to the existing structure. Rural measurements were then taken using a mobile experimental facility setup at Lick Creek Park south of College Station, TX. This area is known for relatively high concentration of isoprene leading to significant aerosol growth over 48 hour measurement periods. Following this field campaign, two chambers were deployed on the top of the Moody Towers at the University of Houston campus. AACES was used to better understand processes such as:

- The transformation and growth of ammonium sulfate in an urban environment under heavy anthropogenic loading of trace gases
- The process of soot aging in the atmosphere via sulfuric acid deposition to the soot surface.
- The production of HONO as a result of surface reactions involving soot and NO_x

Each process was monitored using a range of instrumentation including: a differential mobility analyzer / tandem differential mobility analyzer system, aerosol particle mass spectrometry, ion drift - chemical ionization mass spectrometer to monitor HONO production, and a cavity ringdown and nephelometer system used to measure total aerosol extinction and scattering. Measurements collected over an 11 week period will allow insight into heterogeneous processes involving aerosols as well as their overall impacts on climate.

Significance

This project relates to DOE's 4th strategic goal: "Improve energy security by developing technologies that foster a diverse supply of reliable, affordable, and environmentally sound energy..." To ensure environmental soundness, the behavior of energy-related aerosols in the environment needs to be understood. This project contributes to this goal by providing an improved and innovative means for studying selectable energy-related aerosol behavior in an ambient gaseous and radiative environment.

Spatial Optimization for Regional Stormwater Infrastructure: Balancing Water Quality, Supply Augmentation and Ecosystem Function

119634
Year 2 of 3
Principal Investigator: V. C. Tidwell

Project Purpose

River meander migration is one of the most perplexing and intriguing problems in all of open channel hydraulics. Significant progress in understanding this phenomenon has been accomplished only in the past few decades. However, there remains to be achieved any consensus regarding how to model this most basic behavior of natural rivers. Dr. Jennifer Duan of the Civil Engineering Department at the University of Arizona is one of the leading scientists in developing models of this phenomenon. She has developed a numerical representation that uses a mass balance sediment solution to determine the rate of meander migration rather than only the velocity profile of the river. The proposed work will extend this model by exploring the importance of different parameters in the velocity solution, analytical and numerical solutions to the velocity profile, and analyze the effect of different sediment transport solutions. The work will be two-fold, first development of a theoretical model involving those issues discussed above, then model verification through its application to the Middle Rio Grande (MRG).

Through the partnership established between Sandia, the University of Arizona Departments of Hydrology and Water Resources and Civil Engineering, and the Army Corps of Engineers Hydrologic Engineering Center, we will explore geomorphic and hydraulic effects on river meander in the MRG. Several studies have attempted to predict the future course of the river and areas where potential water quality mitigation and infiltration can occur, along with the identification of sites threatened by future flood events. The meander migration model developed during this project will be used to predict the river's future course under different scenarios in an effort to manage the river for those objectives set out by state and federal agencies.

Summary of Accomplishments

Processes occurring in unlined stormwater channels and their relationship to land use, water quality and surface-groundwater interactions are complex. The interaction of hydraulics and sediment in curved open channels is not well understood; the research is focused on this aspect of channel design. Curved open channels are best represented as helices in the polar coordinate system. Much work has been done to solve the system of partial differential equations representing flow in channel bends. A zero-order solution was developed using one parameter to represent the strength of the secondary (normal to downstream) flow. By setting the integral of half of the total stream flow equal to the integral of the flow from the inside bank to an unknown location normal to the downstream direction, the center streamline is determined. This location is then used to determine the velocity in each channel half. The ratio of longitudinal and transverse sediment transport was found to be proportional to 7.0 × height/radius. Using these two solutions, the rate of meander migration is established.

A meandering stream is well represented by a cosine generated curve, $\text{theta} = \text{theta}_{(\text{initial})}\cos(ks)$where theta is the angle between the channel centerline and the down-valley direction. During meander propagation, the stream no longer maintains this shape and may take an arbitrary curve. Trigonometric functions are used to determine the new radius of curvature and angle at each node. To plot the results of these solutions a transformation from polar to Cartesian coordinates must be made.

During this year, a FORTRAN code was developed to represent the above solution and the post-processing to plot the results for inspection. Verification of the model was done by comparing model results with those found from laboratory experiments in the literature.

Significance

There is a strong linkage between energy, water, and the environment. Here, we investigate the interdependencies between waste water infrastructure, water supply, water quality, and the environment. Energy demand is directly influenced through the resultant need to treat and pump water and waste water. This work supports the objectives of Sandia's Water Initiative, the Energy-Water Nexus Program, and the National Infrastructure Simulation and Analysis Center (NISAC).

Using Reconfigurable Functional Units in Conventional Microprocessors

119638
Year 2 of 3
Principal Investigator: A. F. Rodrigues

Project Purpose

Scientific applications use highly specialized data structures that require complex, latency sensitive graphs of integer instructions for memory address calculations. In our prior work, we have demonstrated significant differences between the Sandia's applications and the industry standard SPEC-FP (standard performance evaluation corporation-floating point) suite. The integer dataflow in Sandia's applications average 40% more instructions and 50% more operands than the SPEC benchmarks. Furthermore, 92% of the data produced by these graphs is used to generate a memory address. Therefore, integer dataflow performance is critical to overall system performance.

Previously, this problem could be handled with specialized address generation units. However, Sandia's large and complex applications do not have identical access patterns. We demonstrated that each application has between 16 and 32 unique important graphs. It is not feasible to implement unique address generation units for each graph type, and each new application may use a different set of graphs. Thus, a reconfigurable functional unit (RFU) is an attractive accelerator because its functionality can change to accelerate a variety of different graphs. In this work with the University of Wisconsin-Madison, we use an RFU tightly integrated with a microprocessor to accelerate integer dataflow, improve the number of outstanding memory operations and therefore improve overall system performance.

We have developed compile-time algorithms that detect and select common graphs for acceleration. In addition, we have developed an RFU execution model that efficiently encodes a large number of inputs and outputs (needed for the complex Sandia graphs) for execution in an RFU. The execution model also includes architectural techniques to improve RFU performance by improving both issue time, output pipelining, and minimizing register file bandwidth. Research is underway to maximize the number of cases where our techniques may be applied. Future research will investigate the potential of run-time techniques for detecting common dataflow graphs for acceleration.

Summary of Accomplishments

An operating system (OS) for multitasking reconfigurable systems manages access to both CPU and reconfigurable hardware (RH) resources. As in traditional multitasking systems, the OS periodically performs a thread context-switch to time-share the CPU. Similarly, the RH allocator periodically reallocates RH resources based on the needs of active applications. There are multiple ways that a thread scheduler's behavior can impact the behavior of the RH allocator. Thus far, we have addressed two of these: the issue of hardware preemption in response to software context-switches, and the problem that recent RH kernel requests near a context switch does not correctly predict near-future RH kernel needs. To evaluate the system performance of these techniques, we also developed metrics for heterogeneous systems. We have also developed alternative preemption techniques that yield the benefits of preemptable hardware, but without the overhead associated with full save and restore of configuration and data.

The OS thread scheduler performs thread context switches at periodic intervals to time-share access to the CPU. Similarly, the RH allocator periodically determines the allocation of hardware based on recent requests for access to RH resources. However, a thread context switch affects the hardware needs of applications that will execute in the near future. We have developed two RH allocator techniques that consider application thread context switches when allocating RH so that the allocation is based both on the hardware use of the recent past and on the predicted needs of applications that will execute in the near future.

Significance

Sandia's missions in nuclear security and scientific discovery and innovation require high performance science and engineering codes. A major obstacle to performance is the rate of memory addresses which can be generated. This work will address this bottleneck, and allow major improvements in the performance of Sandia's applications.

Heat Conduction and Particle Motion in Stationary Nanofluids

119639
Year 2 of 3
Principal Investigator: J. A. Zimmerman

Project Purpose

Fluidic cooling systems have been shown to remove more heat than conventional air systems while using less power than thermoelectric coolers. However, the demand for more heat removal necessitates advancements beyond existing technology. Nanofluids, nanoscale particles suspended in fluids, have been studied over the last decade for applications ranging from fluidic cooling to nanolubrication. Much of the research found thermal conductivity enhancements greater than predictions by effective medium theory, at low volume concentrations. However, large variations in data and dependencies have been observed. The goal of this project with Stanford University is to show how these variations can occur due to particle thermal diffusion away from the heated portion of the fluid and particle aggregation over time by measuring the full field temperature and thermal conductivity distribution of nanofluids in a temperature gradient over time.

This is the first experiment to measure the impact on the thermal conductivity distribution of thermodiffusion and aggregation of particles in a nanofluid. It is also the first experiment to temporally measure the effect of aggregation on a stable stationary nanofluid showing an increase in the thermal conductivity over time during the course of natural aggregation. Through a more complete understanding of the complicated physical mechanisms governing nanofluids and the dependence of thermal properties on these mechanisms, the applicability to cooling solutions can be better understood.

Summary of Accomplishments

Light scattering measurements of aggregates in the nanofluid have been completed and show fractal dimensions decreasing with temperature for the stabilized alumina nanofluid. For the unstabilized alumina nanofluid the fractal dimension is found to be higher.

Three simulations of the nanofluid in a parallel plate apparatus have been completed. The first numerically solves the Onsager relation governing the dependence of the heat flux and particle flux on the temperature and concentration gradients. The second models the Brownian motion of non-interacting particles through a Monte Carlo method. Each particle position is tracked and randomly displaced based on Brownian motion theory. The steady state concentration profiles of these two models are compared and the Soret coefficient is used as a fitting parameter. The two models are compared at various times and both the magnitude and shape of the concentration versus position curves match well. Finally, aggregation has been added to the Monte Carlo simulation by tracking if particles touch and randomly selecting from these particle pairs which of these to aggregate, based on well known models of Brownian-based aggregation. The average particle size and number of particles in each aggregate are tracked. The fractal dimension measured via light scattering is used to determine the aggregate's radius of gyration and the thermal conductivity of the fluid. Calculations of thermal conductivity using fractal theory for aggregation based effective medium theory have been compared to the values measured through the previous thermal measurements and are found to agree. The increase in thermal conductivity is found to be due to aggregation and the current aggregation-based models are able to correctly predict the thermal conductivity without the use of empirical constants.

Significance

In alignment with DOE's mission of scientific discovery, these measurements improve the understanding of nanofluid behavior due to particle diffusion and aggregation and show the importance of taking these effects into account. They give insight into how nanofluids may act in practical applications including microscale heat exchangers. These experiments also give insight to the evolution of certain types of nanofluids over time, showing how some degrade in their performance while others improve.

Refereed Communications

P.E. Gharagozloo, J. K. Eaton, and K.E. Goodson, “Diffusion, Aggregation, and the Thermal Conductivity of Nanofluids,” *Applied Physics Letters*, vol. 93, p. 103110, September 2008.

J. Buongiorno and P.E. Gharagozloo, et al., “A Benchmark Study on the Thermal Conductivity of Nanofluids,” to be published in the *Journal of Applied Physics*.

Nanotransport and Control of Molecules Through Molecular Gates

119640
Year 2 of 3
Principal Investigator: K. D. Patel

Project Purpose

Development of sophisticated tools capable of manipulating molecules at their own length scale enables new methods for chemical synthesis and detection. Although nanoscale devices have been developed to perform individual tasks, little work has been done on developing a truly scalable platform: a system that combines multiple components for sequential processing, as well as simultaneously processing and identifying the millions of potential species that may be present in a biological sample. The development of a scalable micro-/nanofluidic device is limited in part by the ability to combine different materials (polymers, metals, semiconductors) onto a single chip, and the challenges with locally controlling the chemical, electrical, and mechanical properties within a micro- or nanochannel.

Our collaborators at the University of Illinois at Urbana-Champaign (UIUC) have developed a unique construct known as a molecular gate: a multilayered polymer-based device that combines microscale fluid channels with nanofluidic interconnects. The molecular gate differs from other nanofluidic systems in that microfluidic and nanofluidic elements are assembled in a 3-dimensional construct where the nanofluidic connections are made with a nanoporous membrane, as opposed to single etched nanochannels. This allows for selective control of chemical and mechanical properties of each layer, and enables solution properties such as pH and ionic strength to be independently maintained in each layer. By utilizing dense arrays, nanofluidic transport phenomena can be exploited while maintaining high throughput. Molecular gates have been demonstrated to selectively transport molecules between channels based on size or charge. Processes have also been developed to metallize and modify the surface chemistry of the nanopores, changing the electrokinetic transport characteristics. This research is focused on individually addressable nanopores for developing a scalable system to efficiently utilize nanoscale transport.

Summary of Accomplishments

A key accomplishment during FY 2009 was the successful fabrication of nanochannels with multiple addressable electrodes inside the channels. The previous approach to fabricating these nanochannels involved stacking alternating layers of metal and polymer (poly[methyl methacrylate]) layers and etching a nanopore using a focused ion beam (FIB). This FIB process was believed to change the surface chemistry of the polymer nanopore, and electrical leakage was frequently observed between layers. In order to successfully integrate metal electrodes into nanochannels, a new device design was created. Sequential patterns of gold and copper were deposited on glass substrates and coated with a photodefinable polymer. The copper layer was then dissolved in a copper etching solution, leaving a nanoscale channel spanning over gold electrodes. Since normal chemical etching is limited by diffusion of reactants, creating a long-aspect-ratio channel will take several days. In order to accelerate the etch process, a potential is applied to the sacrificial electrode to assist in dissolution. This allows channels with over 1000:1 aspect ratios to be fabricated in several minutes.

Initial tests on the anodic dissolution of copper showed that residue formed in the channel could inhibit complete etching. Bubble formation also occurred, which could increase the overall etch rate but also risked permanently clogging the nanochannel. By optimizing the applied potential, etchant solution composition, and device geometry, open nanochannels could be created with multiple gold electrodes spanning the channel surface.

Significance

Development of molecular gates as a scalable architecture for controlling molecules and nanotransport ties to DOE's mission to advance scientific understanding of nanoscale phenomena. Tools to help understand nanoscale transport will ultimately lead to the development of new diagnostic devices and methods to explore alternative, environmentally sound energy sources.

Solar Hydrogen Generation with Porous Semiconductor Electrodes

119644
Year 2 of 3
Principal Investigator: B. R. Antoun

Project Purpose

The production of hydrogen fuel using solar-illuminated semiconductor photocatalysts in an electrolytic solution is an attractive renewable energy technology. An especially desirable reaction is the overall splitting of water into stoichiometric amounts of hydrogen and oxygen. In this process the semiconductor photocatalyst behaves as both the cathode and anode in an electrochemical system driven solely by solar irradiation. The activity of many photocatalysts has been investigated with, at most, moderate efficiency, and more research to explore new potentially active materials is warranted to increase the energy conversion efficiency.

Pulsed laser deposition (PLD) of films is an experimentally convenient approach to photocatalyst synthesis. The physical mechanisms of pulsed laser-material interactions facilitate the deposition of a wide variety of semiconductor materials in a controllable fashion. Thin films prepared by PLD have proven to possess desirable characteristics for many applications, including highly sensitive electronic and optical devices. Deposition conditions strongly affect film properties including crystallinity, porosity, thickness, and morphological features. Chemical composition also dictates the stability and activity of photocatalysts, and in this regard, PLD offers unique opportunities for systematic variation and optimization.

Efficient photocatalysts must absorb solar energy in visible and infrared wavelengths as well as possess microstructure and surface characteristics suitable for electrochemical catalysis reactions. There are strict requirements for electronic band properties to maximize absorption as well as to match reaction potentials. The experimental study and optimization of these materials is an important step toward economically viable and environmentally clean solar-energy-driven production of hydrogen fuel. This work is in collaboration with the University of California (UC)-Berkeley.

Summary of Accomplishments

Several interesting photoelectrode material systems have been fabricated and characterized. Specifically, cation- and anion-doped niobium oxide films, nanostructured tungsten trioxide photoanodes, and nanostructured mixed oxide photoanodes incorporating combinations of titanium dioxide, niobium pentoxide, tungsten trioxide, and bismuth trioxide have been developed.

A unique pulsed laser deposition system that allows for deposition of photoelectrodes with complex stoichiometries and layered structure was designed and constructed. This involves a motorized, electronically programmable system for variation of the deposition source material and therefore film composition. Using this technique, it is possible to systematically vary dopant and co-catalyst loading concentration, as well as vary layer compositions in multiple-bandgap heterostructure photoelectrodes.

A photoelectrochemical characterization system was assembled to study the performance of deposited electrodes. Potentiostatic control, artificial solar light simulation, and gas chromatography are integrated in a setup capable of fully characterizing the photoelectrochemical properties and hydrogen production efficiency of a given material system.

Presentations on pulsed laser deposition of metal oxide photoelectrodes for solar-driven hydrogen production were given at two technical conferences and publications were accepted in their respective printed proceedings: Solar Hydrogen and Nanotechnology IV, part of SPIE Optics + Photonics, 2009; and the 6th International Symposium on Multiphase Flow, Heat Mass Transfer and Energy Conversion, 2009.

Significance

This research benefits DOE's science strategic goal by encouraging and developing future world-class scientists that can contribute to advancing scientific knowledge in the future. This research that is conducted in this project has great relevance and potential benefit to the DOE's energy strategic goal. This project will assist development of a technology capable of providing a reliable, affordable and environmentally sound energy source.

Signature Molecular Descriptor: Advanced Applications

119645
Year 2 of 2
Principal Investigator: E. E. May

Project Purpose

The signature molecular descriptor is a very powerful and robust way to encode the local environment of a particular atom in a molecule. Our collaborator, Presidential Early Career Awards for Scientists and Engineers (PECASE) recipient Prof. Visco at Tennessee Technological University, has demonstrated this feature in several refereed journal articles, conference presentations, and invited speaking engagements. Much of this previous work has been done associated with removing algorithmic bottlenecks in the use of the molecular descriptor, Signature for inverse design problems.

This project has two purposes. First, the primary purpose is to evaluate Signature for its utility in high-throughput screening (HTS) studies. A vast amount of information exists in public databases (such as PubChem) concerning the activity of molecules against certain protein targets. With Signature, in conjunction with support vector machine (SVM) classifications and powerful clustering/feature selection techniques, information can be mined from the databases to make predictions on the activity of compounds not yet tested against a particular protein target. The second purpose is to continually evaluate Signature for use in inverse-design problems. As additional studies are performed using Signature in this capacity, more information is gained on the strengths and weaknesses of the approach.

Summary of Accomplishments

The bulk of this year was spent determining whether the previous year's efforts on using Signature in HTS for a single PubChem bioassay can be applied to any bioassay within PubChem. It was determined that the technique used for the single bioassay was not robust for use in general. The major problem was that the smaller bioassays could use feature selection via clustering, but larger bioassays required a recursive feature elimination technique. Subsequent investigation led to efforts to utilize a cross-validation technique which removes the bias from the feature selection method. This evaluation is currently ongoing and will be finalized during the extended work period.

Additionally, a computer-aided molecular design (CAMD) study was performed in order to identify green solvents to supplement a list provided by GlaxoSmithKline. Our work not only identified some known green solvents not part of the original set, but new compounds which are predicted to have optimal properties associated with waste, environmental impact, health and safety.

Significance

The HTS technique developed in this work has the potential to explore not only the PubChem database for new inhibitors, but for other large databases as well. Additionally, the results of the CAMD study can be used to help guide the selection of green solvents.

Signature, in conjunction with advanced screening techniques, provides a means to identify novel compounds which may be of interest in protecting our nation's national security. The results of this project will be of interest to DOE Basic Energy Research and other agencies such as the National Institutes of Health (NIH) Biomedical Information Science and Technology Initiative (BISTI) program.

Physiological Models and Inference Based on Optical Imaging

119647
Year 2 of 3
Principal Investigator: C. F. Diegert

Project Purpose

A multilevel, multiresolution mathematical model describing the relationship between cortical brain electrical activity in epilepsy and optical reflectance spectroscopy measurements of the cortical surface has been defined and partly implemented in software. Because of the surface nature of the measurements, the model is 2.5-D not 3-D. The levels in the model are as follows:

1. electrical: a 2-D version of cable equation theory describing electrical activity in terms of space-variant resistance and capacitance.
2. vascular: the vascular system responds to average (spatial and temporal) metabolic demand due to the electrical activity of (1) via alteration of resistances and capacitances. A key contribution is the ability to model flow into a brain region both directly from larger arterial structures (which are deep in the brain and therefore not directly modeled in this 2.5-D model) and from adjacent brain regions.
3. mixing: the concentrations of oxygenated and deoxygenated hemoglobin are the primary controllers of the spectroscopy results and so careful accounting for blood volume and fractional concentrations is crucial.
4. spectroscopy: there are extensive standard results on the spectroscopy of hemoglobin. The multiresolution characteristic is due to the fact that different levels need not have the same spatial sampling (digital context) or the same spatial bandwidth (analog context).

The basic ideas in the model are described in terms of temporal nonlinear ordinary differential equations (ode) for spatially-sampled variables. In the limit of zero spatial sampling distance, the model becomes a system of nonlinear partial differential equations (pde). The two software systems under development are based on the ode versus pde description. Both software systems are of interest: the ode system because the spectroscopy data is only available in a spatially sampled form and the pde system because there are fast solution methods for the pdes. The work is in collaboration with Cornell University.

Summary of Accomplishments

The main contribution was the implementation of a novel scaling algorithm for fusing information from different trials of the same experiment. Based on this work, we have a much clearer understanding of the difficulty of the overall problem and especially the challenges created by the spatial variation of the cortical tissue. While spatial variation can easily be incorporated into our models for forward calculations, performing system identification to determine a complete set of spatial variation from data, i.e., the inverse problem, is very challenging. Therefore, we have begun work toward methods based on circular averaging of the video around the site of the stimulus.

From lab experience at Cornell Weill Medical College, we have a much improved understanding of the physiology of the neurovascular interaction. Based on this improved understanding, we have correspondingly modified one level, the so-called vascular level, of our mathematical model. In particular, we now think of each volume of brain tissue not as a well-mixed compartment containing a certain amount of oxy- and deoxy-hemoglobin but rather as a well-mixed balloon so that it is possible to introduce the relationship between wall stress and internal pressure. Then, the interaction between the vascular level and the neurovascular coupling level is via control of the relationship between wall stress and internal pressure.

Significance

This project is relevant to the science missions of DOE and DOD. Advances from this project would enable better fusion of data from various modalities and much more precise physiological models of the brain that will be useful for national security applications such as treatment and prevention of post-traumatic stress disorder (PTSD) and traumatic brain injury (TBI), advances in lie detection and intent detection, and classifying and improving human performance in critical tasks (e.g., decision-making under high stress).

Passive High-Flux Thermal Management of Electrochemical Systems with In Situ Microchannel Phase Change

120207
Year 2 of 3
Principal Investigator: M. P. Kanouff

Project Purpose

Energy-storing electrochemical batteries are the most critical components of hybrid and electric vehicles. Lithium-ion batteries are proposed to improve the fuel economy of these vehicles because of their higher specific energy, but face thermal management challenges. Thermal management to maintain a specific operating temperature window of individual cells and packs is essential to maintain the batteries' performance. This research, in collaboration with the Georgia Institute of Technology, addresses the singular limiting feature of all battery cooling systems proposed thus far — the cooling systems are external to the batteries, which implies that substantial temperature gradients exist between the heat generation location (the cells) and the skin of the battery. A cooling system integrated with the internal heat generation sites and utilizing efficient, passive, thermal transport between heat generation sites and external heat sinks will be developed. Thermal energy dissipated during electrochemical reactions is transferred across chemically inert microchannels embedded into the cells to a phase-change fluid. This energy evaporates the fluid, and the vapor rises through the microchannel core to the top of the batteries. Air-cooled heat sinks condense the fluid, which returns to the microchannels inside the battery via a return line due to capillary and gravitational forces. This system represents revolutionary advances over the state of the art by passively removing heat almost isothermally with negligible thermal resistances. Electrochemical heat generation mechanisms will be studied, and will serve as source terms and boundary conditions for a microchannel phase change heat transfer investigation. The resulting models will be used to design, fabricate and test a representative battery cooling system. The minimization of peak temperatures and gradients within batteries allow increased power and energy densities unencumbered by thermal limitations. These storage devices will see application in the spatial and temporal concentration of renewable energy sources and in the harvesting of low-grade energy.

Summary of Accomplishments

A comprehensive review of the literature on thermal issues in lithium-ion batteries has been submitted for publication in the *Journal of the Electrochemical Society*. In addition, a wind tunnel, which allows for precise control of the battery temperature by providing high surface convection to or from an air stream and maintains constant battery temperature during operation, was fabricated. The air stream is cooled or heated by a small-volume coolant recirculation loop using a potentiometer-controlled electrical resistance heater and by the laboratory chiller. Testing has been completed on a commercially-available battery over a temperature range of 12 to 50 °C and current range of 0.125 to 3C for both charge and discharge. During the majority of tests, the battery surface temperature was controlled to within +0.75 °C, and the battery surface temperature across various locations was within +0.5 °C. These data will be used in the previously developed coupled electrochemical-thermal model to yield improved accuracy in the simulation of scaled-up batteries. The thermal model has also been modified to accept hybrid electric vehicle (HEV) simulation input data, and several simulations have been conducted. A preliminary design for the internal cooling device for the battery has been completed, and potential manufacturers for the large footprint (~200–1000 mm^2) and small channel (~200 µm) sheet have been identified. In addition, a flow visualization test piece using 180 µm acrylic tubes is being fabricated to observe the internal flow mechanisms under simulated heating conditions and validate the header geometries. These experiments will therefore identify the underlying physical mechanisms, and validate and refine the preliminary internal cooling device design prior to fabrication of the actual cooling device.

Significance

Unlike other systems, the wind tunnel has allowed for precise temperature control even during high heat generation events (e.g., high discharge rates). The data collected using this test facility will be used to improve the accuracy of the coupled electrochemical-thermal model, which will in turn be used to design and fabricate a representative battery cooling system. The minimization of peak temperatures and gradients within batteries will allow increased power and energy densities unencumbered by thermal limitations. These storage devices will also see application in the spatial and temporal concentration of renewable energy sources and in the harvesting of low-grade energy.

This work will contribute to the DOE energy strategic goal by advancing technology for electrical energy storage. This technology will help realize a low-emission energy source that is suitable for transportation applications, and will also enable solar energy collection systems to provide energy throughout a 24 hour cycle.

Cosmic-Ray Hydrometrology for Land Surface Studies

120208
Year 2 of 4
Principal Investigator: D. Desilets

Project Purpose

Energetic cosmic rays continually bombard Earth, with implications important to humanity. For example, cosmic rays interact with microelectronic components, generating soft errors in advanced computing systems and posing challenges to the design of reliable aerospace components. Cosmic rays also interact with materials in the upper meter of Earth's crust, producing rare radionuclides that are retained in the lattices of rock minerals. The buildup of these radionuclides (e.g. ^{10}Be and ^{36}Cl) can be used to determine numerical ages of previously undatable geologic hazards such as prehistoric earthquakes, volcanic eruptions and landslides. Cosmic rays also produce rare radionuclides in the atmosphere, providing a valuable tracer for atmospheric transport and mixing processes. Investigators at Los Alamos National Laboratory (LANL) have shown that highly penetrating cosmic rays can be used as an imaging tool to locate fissile materials hidden in shipping containers. More recently, the utilization of cosmic rays has been extended to the field of hydrology, where it has been discovered that measurements of slow cosmic ray neutrons can potentially be used to remotely and passively monitor soil water content and snow water equivalence at a footprint not attainable by other instruments.

This proposed work is centered on the novel application of cosmic rays to remote sensing of soil water content and snow water equivalence — two of the most important variables in the hydrologic cycle. This new technology can be put to a variety of uses, including monitoring slope stability, forecasting spring snowmelt and flash floods, and monitoring soil moisture in croplands. In addition to exploring applications in hydrology, the proposed work will investigate fundamental aspects of cosmic ray physics and neutron transport, and therefore provide ancillary benefits to all areas of applied cosmic ray research.

Summary of Accomplishments

Two field sites have been established in northern New Mexico. One site is on the Valles Caldera National Preserve, where neutron detectors are operating in a trailer adjacent to a snow pillow and buried neutron detectors. Neutron data have been collected over the 2008-09 winter season and are currently being analyzed. Algorithms for converting neutron count rates to snow water equivalent depth are being evaluated.

A second field site has been established in a municipal watershed supplying the city of Santa Fe. Neutron detectors have been installed in adjacent sub-basins having different vegetation properties but that are similar in topography, aspect, elevation and climate. Data will be evaluated for differences in temporal patterns in neutron intensity that are potentially associated with differences in snow pack and soil water content between the two basins. These data will in turn be used to evaluate the effects of forest thinning on watershed hydrology.

A technical note has been submitted to Water Resources Research and a contribution to the Encyclopedia of Remote Sensing has also been made. Presentations have been made at the American Geophysical Union and National Ground Water Association annual meetings, LANL seminar series, and at two National Aeronautics and Space Administration (NASA) remote sensing workshops.

Significance

This work is relevant to DOE's goals in energy security and scientific discovery and innovation. Energy abstraction, processing, and transmission are dependent on the availability of water. Likewise, the ability to produce biofuels is extremely dependent on water resource availability. The ability to meet growing demands for energy could be compromised by rapidly increasing demands placed on our nation's water supply by all demand sectors. This project will develop and demonstrate tools that can be used to generate essential soil water and snow pack data. This technology can be used in monitoring permafrost — an important link in the global carbon system.

Multiscale Schemes for the Predictive Description and Virtual Engineering of Materials

120209
Year 2 of 3
Principal Investigator: O. A. von Lilienfeld-Toal

Project Purpose

The predictive power of computational materials simulation shall be enhanced dramatically by delivering a tool which enables engineers and experimentalists not only to routinely characterize, but also to identify, customize, and subsequently also synthesize, from scratch new materials which exhibit valuable and desired properties. Such in silico rational compound design (RCD) efforts are not only hampered by the difficulty of reliably predicting macroscopic properties for any given material but also by the sheer size of chemical space, i.e., the mind-bogglingly large number of all the stable and potentially interesting chemical compositions which define a material. Methods from seemingly different areas and levels of theory, such as physics, chemistry, materials sciences, applied mathematics, and even molecular biology will be combined in order to account in a rigorous way for fluctuations in chemical composition and link them to their macroscopic properties, which can be exploited for a purposefully guided exploration of chemical space. The feasibility and versatility of the underlying theory shall be evidenced by applying the devised RCD algorithms towards two prototypical materials discovery problems, namely the RCD of a photocatalyst for the efficient generation of energetically rich material such as methanol, methane, molecular hydrogen, or ammonia, as well as RCD of heat transfer fluids with optimized physical properties for enhanced efficiencies of solar power facilities. While the potential benefit of such a tool, for science, engineering, and eventually society, can hardly be overestimated, the technological and technical barriers on the way to its assembly appear immense for the involved research fields are only now on the edge of making such a project conceivable.

Summary of Accomplishments

FY 2009 Accomplishments:

- The molecular grand-canonical ensemble (MGCE) density functional theory (DFT) scheme was furthered. A Monte Carlo protocol was devised for the unified sampling of chemical space and phase space (with Mark Tuckerman, New York University, and Michel Cuendet, Swiss Institute for Bioinformatics).
- Interatomic many-body dispersion forces have been analyzed for a variety of gas and bulk systems. These effects were shown to reach up to 30% of relevant energy contributions (with Alexandre Tkatchenko, Fritz-Haber Institute, Berlin).
- Defect formation energies in GaAs have been studied.
- Study of methane surface adsorption on metal nanocluster (with Robin Hayes, currently at New York University).
- Alchemical paths and finite difference derivatives, from the MGCE, were implemented into VASP and tested for chemical reactions.
- Development of an empirical scheme for linearizing chemical compound space.
- Development of accurate analytical ab initio energy gradients in chemical compound space.
- Randomized aromatic hydrocarbons with variable number of atoms or beads were successfully generated.

Quantitative structure-property relationships were devised that yield good predictions of reorganization energies, relevant for charge mobilities according to Marcus theory (with Denis Andrienko, Max-Planck Institute, Mainz, and Jean-Loup Faulon, University of Evry, Paris).

- Engineering molecular conductivity (with I-Chun Lin, currently at New York University, and Koichi Yamashita, Tokyo University).
- Calculation of free energies of aqueous solvation.
- Discovery that proton tunneling protects DNA from spontaneous damage (with Alejandro Perez and Mark Tuckerman, New York University).

Significance

Enhancing the predictive power of computational materials simulation is instrumental to the DOE missions in scientific discovery and energy security. The virtual tuning of material's properties through the engineering of the atomistic composition and structure represents a potential impact which can hardly be overestimated. Entire technologies, e.g. involving biohazards, water purification, explosives, molecular electronics, or harvesting light for renewable energy, will benefit from a successful outcome of this project.

Refereed Communications

K. Leung, S.B. Rempe, and O. von Lilienfeld, "Ab Initio Molecular Dynamics Calculations of Ion Hydration Free Energies," *Journal of Chemical Physics*, vol. 130, p. 204507, 2009.

R.H. French, et al., "Long Range Interactions in Nanoscale Sciences," to be published in *Reviews of Modern Physics*.

O. von Lilienfeld, "Accurate Ab Initio Energy Gradients in Chemical Compound Space," to be published in the *Journal of Chemical Physics*.

S. Jayaraman, O. von Lilienfeld, A.P. Thompson, and E.J. Maginn, "Molecular Simulation of the Thermal and Transport Properties of Three Molten Alkali Nitrate Salts," to be published in *Industrial and Engineering Chemical Research*.

Cross-Layer Design for Secure Communications in MANETs

120254
Year 2 of 3
Principal Investigator: Y. R. Choe

Project Purpose

With the exponential growth of personal devices, we have witnessed a plethora of uses for interconnection on-the-go. The interconnection can be made between mobile-to-stationary devices or mobile-to-mobile devices. The latter can be seen as a new paradigm of how people can communicate with each other. Without the need for established infrastructures, an ad-hoc network can be formed for the purpose of communicating in the immediate session. However, people are not stationary, and as such, we cannot expect the network topology to remain static. As such, mobile ad-hoc network (MANET) becomes the network paradigm that encompasses the mobility and spontaneity current devices allow us to have. While security is a major concern, it should not be the only one. A network that is not resilient and robust can be a secured yet useless network; thus, security needs to be built in concert with resilience and robustness in mind. To this end, we are proposing the investigation of recent developments in online social networks (OSN) to accomplish security, resilience, and robustness of MANETs in collaboration with The University of California (UC)-Davis. OSN emphasizes the idea of community, allows nodes to inherently build notions of trust — through the establishment of community and explicit evaluation of peers — and communicate based upon this notion of trust. Resilience and robustness is accomplished via the maintenance of multiple friends (either directly or indirectly connected). OSN is flexible enough that one could implement different layers using its concept. As such, a cross-layer approach could be used to identify and route to a particular peer (routing work has been done, in works such as Davis Social Link). If successful, OSN can provide a way for MANET nodes to quickly locate each other, establish a trusted path, and maintain control of its identity that is not possible in current network paradigm.

Summary of Accomplishments

Over the past year, we looked into a concrete example that could apply the use of social networks and MANETs. We realized that although there has been burgeoning research in social networks (especially online social networks), not much has been investigated regarding the fundamentals that could bridge the gap between social networking and traditional networking (MANET is included in this context). We felt that such lack of fundamental understanding would impinge on any development of cross-layer social/traditional network solutions. Therefore, the direction we took was the following:

1. We devised a concrete example under which the traditional approach alone would be insufficient, and justified the use of social networks.
2. Under the concrete example, we brainstormed several research topics that are fundamental to the success of a cross-layer solution of said example.
3. Developed necessary primers for the reasonable operation of the new cross-layer paradigm.

The result of the three approaches produced the following:

1. We looked into the development of a decentralized emergency announcement system that utilizes both social networks and traditional networks, as to make the decision process more intelligent (e.g., decide who to forward the announcement to in order to optimize the task objective).

2. Under the problem domain specified in (1), we identified some problem areas where specific interesting research could arise:
   a. Distributed storage and retrieval of information with little privacy intrusion
   b. Localized authentication that could be based on:
      i. Locality
      ii. Social context
      iii. Traditional means (e.g., password-based, group authentication)
   c. Distributed forwarding decision based on situation context and social relevance

3. Recognition of “virtual profile” as an important primer in realizing a social-based emergency announcement system.

Significance

This work is relevant to communication systems that are critical to DOE missions and to DOD and DHS. This project proposes a mechanism for robust and secure communication for mobile ad-hoc networks, which is needed to support advanced concepts for robust and reliable wireless systems. It is also applicable to communications systems that need to operate in the presence of hostile network attacks and for ensuring that first responders to national emergencies can communicate under adverse conditions.

Mobile Agent Systems for Distributed Embedded System Reasoning and Complex Warfare Simulation

120460
Year 2 of 2
Principal Investigator: J. Wu

Project Purpose

The proposed research studies fundamental issues in developing reconfigurable intelligent software architecture capable of dealing with unforeseen events that synergistically works with other agents in dynamic and unstructured environments. The proposed framework for mobile agent systems is applicable to a wide range of applications, such as mobile intelligent systems working in hazardous waste removal, search and rescue operations, and swarm based wireless sensor networks for fire or target tracking networks. The software architecture will also be used as a platform for complex warfare simulations.

The use of mobile agents in intelligent embedded systems enables the creation of a lean infrastructure for rapid deployment. The agent-based approach to intelligent embedded system control allows viral-like distribution of application specific algorithms instead of traditional power hungry communication methods such as network-wide dissemination. The computing environment will provide an interface for task-level commands to dictate highly complicated low-level maneuvers.

The work is in collaboration with the University of California (UC)-Davis.

Summary of Accomplishments

This project developed and demonstrated a mobile agent-based dynamic run-time task allocation architecture that provides flexible mission-based control of a system of heterogeneous mobile robots. The architecture follows a noncentralized control scheme where mobile task agents, each assigned to a specific mobile robot, can autonomously appropriate a task from a global database of available tasks. Once a task has been assigned and collaboration has been initiated with a control agent, a behavior agent is used to gather the required behaviors for the task, based on pertinent robot information. Dynamic behavior modification demonstrated that the system could provide real-time adaptation to environmental changes. The validity of the architecture was proven through a feasibility case study involving the border patrolling of a designated area using a K-Team Khepera III mobile robot. A new simple, yet effective, wall-following behavior algorithm was also demonstrated.

Significance

This work will improve the intelligence and versatility of agent collectives and is directly applicable to a wide variety of DOE and Sandia application areas, including homeland security response operations, sensors and data acquisition, etc.

Advanced I/O for Large-Scale Scientific Applications

120479
Year 2 of 2
Principal Investigator: R. A. Oldfield

Project Purpose

The next-generation of supercomputing systems will have unprecedented demands for storage access. Applications will require access to petabyte datasets that may be distributed to a variety of locations (perhaps across administrative domains) and may require a number of transformations before they are in a proper format for the scientific computation. The goal of this project, in collaboration with the Georgia Institute of Technology (GA Tech), is to evaluate the integration of lightweight storage architectures and data-transformation technologies to manipulate data at strategically located processors in the network between the data source and the data sink. The ultimate purpose is to: (1) enrich data sources with application-specific functionality that manages data being streamed out on behalf of clients, and (2) take advantage of nodes "in between" the source and sinks to perform processing and data-movement actions that benefit sinks and reduce bottlenecks from resource contention. Our technical approach is to leverage work in lightweight file systems at Sandia and the input/output (I/O) graph technology developed in collaboration with Sandia, GA Tech, and the University of New Mexico (UNM) to investigate the viability of such an approach for selected high performance computing applications in the areas of astrophysics and fusion.

Summary of Accomplishments

We developed the ADIOS (ADaptable IO System) application programming interface (API) that provides an I/O abstraction that is nearly as simple as standard POSIX (portable operating system interface for Unix), but with support for selecting the I/O method to employ at runtime via an external XML configuration file. We demonstrated that allowing adaptable I/O configurations achieves as much as 75% of peak I/O performance. We developed a data format called BP (binary packed) that enhances I/O performance by offering data annotation and automatic characterization with minimal coordination among the collective processing performing I/O.

Significance

This work has the potential to advance the computing capabilities for DOE applications by reducing I/O overheads and providing mechanisms to effectively manage and process data with minimal impact on the core scientific application. Such an advance will improve performance and scalability of the application and reduce the amount of work required by the scientist to manage data. This work ties strongly with the DOE science strategic goal to advance science through advanced computation.

Fundamental Studies of Electrokinetic Phenomena in Polymer Microsystems

124007
Year 2 of 3
Principal Investigator: B. A. Simmons

Project Purpose

Despite the ubiquity of hydrophobic colloids and the importance of hydrophobic micro/nanodevice substrates, generally accepted descriptions of electro-osmotic phenomena that provide predictive capability at hydrophobic surfaces are lacking. Models and descriptions of these systems are often contradictory, and those models that do agree with each other have not to date offered detailed predictions. The long-term goal of this project with Presidential Early Career Awards for Scientists and Engineers (PECASE) recipient Brian Kirby at Cornell University is to characterize the dynamic effects of nanobubble formation and decay on electrokinetic system response in polymer-water systems and use this knowledge to enable rational design of micro/nanofluidic devices with hydrophobic interfaces. The overall objective of the proposed research is to characterize both the microscopic (nm) and macroscopic (μm) effects of nanobubbles produced at hydrophobic interfaces upon solvent or temperature cycling, with specific attention to nanobubble stability as a function of shear and transverse electric field. We will combine (a) electrokinetic measurements at hydrophobic interfaces; (b) techniques for controlled formation of surface nanobubbles; and (c) atomic-force microscopy of surface interfaces so as to identify (i) the thermodynamic parameters that define the charge processes at hydrophobic surfaces, (ii) the role of gas bubbles on electrokinetic transport, and (iii) the effect of shear and electric field on nanobubble stability. Our central hypotheses are as follows: (1) the interplay of nanobubbles in electrokinetic phenomena is tied to the size of the bubbles as compared to double-layer shielding, and (2) electrokinetically induced shear will decrease the characteristic time for nanobubble decay, by overcoming diffusion-limited transport of dissolved gas.

Summary of Accomplishments

We conducted experiments in both TOPAS® (plastic copolymers of cyclic olefins and ethylene) and silica microfluidic channels in order to measure their electrokinetic properties as a function of the time history of the microfluid-solid interface. Detailed procedures for phase-sensitive streaming potential experiments and automated current monitoring experiments are described in previous published works. We measured the zeta potential as a function of time, (1) in pressure-driven flow inferred from streaming potential measurements; (2) in electro-osmotic flow inferred from current monitoring experiments; (3) in pressure-driven flow after an initial exposure to an electric Del(E); and (4) after exchanging ethanol as the solvent in the system for water.

We examined the effect of an initially applied electric Del(E) in disrupting electrokinetic transients in pressure driven flow. TOPAS microchannels were filled with aqueous solution, and an electric field of magnitude 500 V/cm was then applied across the microchannel for 12 minutes. The electric field was then switched off, flow actuated via pressure, and the streaming potential measured. The zeta potential remained relatively constant from the time the electric field was switched off over a period of 10 hours. Variation in the data is not explained by an exponential decay, as an exponential fit to the data resulted in a nonsensical time constant and a low R-squared value.

Significance

The proposed work ties directly to Sandia's mission to ensure the security and sustainability of our water resources. By developing unique capability to characterize electrokinetic effects in microsystems, the proposed work will inform engineering design of cyclic olefin polymer microstructures used to analyze environmental and drinking water. The fundamental insights gained by this effort will support the DOE mission of furthering fundamental science.

Novel Methods for Detecting and Defending Against Advanced Malware

124009
Year 2 of 2
Principal Investigator: J. Margulies

Project Purpose

We propose a multipronged approach to understanding and improving our abilities in the field of vulnerability identification: develop training systems that teach security analysts to find vulnerabilities; use experimental methods to understand how analysts approach the training systems; feed our understanding of analyst approaches back into training systems, allowing the systems to benefit from co-evolution; and use our results and improved understanding to ascertain the fundamental science behind vulnerability identification. We expect our approach to yield a number of benefits: better-trained security analysts with unparalleled experience identifying vulnerabilities; deep understanding of the science of identifying vulnerabilities; and a truer understanding of how capable we, as a nation, actually are of identifying vulnerabilities, and how many vulnerabilities may be flying under our collective radar.

Summary of Accomplishments

The purposes of this LDRD project were threefold: 1) to better understand complex vulnerabilities; 2) to develop strategies to mitigate such vulnerabilities; and 3) to develop a training program to teach software security evaluators to identify complex vulnerabilities. Addressing the third objective, discussions with the two beta test teams resulted in a number of ideas for future experiments based on the training model. Among the more practical findings of this study was a metric for the complexity of a given vulnerability. The research team also defined a new term, *flexibility*, to help reason about the difficulty of inserting a complex vulnerability into a given system. As a result of our findings, members of our team have begun spearheading a variety of new security solutions based on making systems less predictable.

Significance

The results of this R&D effort will build on our current strengths in uncovering vulnerabilities and will enhance Sandia's information assurance capabilities and Sandia's ability to protect critical information systems.

The tools and techniques developed during this project will benefit information systems analysis at Sandia. The project team will develop new evaluation tools and skills to be used in detecting and eliminating vulnerabilities.

Solid-Oxide Electrochemical Reactor Science

126613
Year 2 of 3
Principal Investigator: A. Ambrosini

Project Purpose

The general topic area of this collaboration between Sandia and the Colorado School of Mines (CSM) is solid-oxide electrochemical reactors targeted at solid oxide electrolyzer cells (SOEC), which are the reverse of solid-oxide fuel cells (SOFC). Solid-state electrolyzers are a focus area that complements Sandia's efforts in thermochemical production of alternative fuels. An SOEC technology would co-electrolyze carbon dioxide (CO_2) (produced by and captured from coal-burning power plants or other CO_2 waste streams) with steam to form synthesis gas (H_2 and CO). Synthesis gas forms the building blocks for a number of petrochemical substitutes which can then be applied to transportation vehicles or distributed energy platforms.

There are potentially great benefits associated with developing both fuel-cell and electrolyzer technologies. They offer high conversion efficiency for fuels to electricity and produce very little pollutant emissions. Electrolyzers offer the possibility to convert CO_2 back to CO, and then to logistics fuels. Thus there are societal, political, and environmental benefits to be realized by bringing the technology to the developmental level where cost-effective commercial products are viable in the marketplace.

These systems operate at high temperature, around 800 °C, which provides both challenges and benefits. Research is certainly needed to improve materials, optimize cell architectures, and produce cost-effective systems. The effort proposed here concentrates on research concerning catalytic chemistry, charge-transfer chemistry, and optimal cell-architecture. Functional-layer design, including optimal particle-size distribution, is particularly important. Other important considerations include degradation mechanisms, for example, carbon deposits or Ni electrode reoxidation. The technical scope will include computational modeling, materials development, and experimental evaluation.

Summary of Accomplishments

The literature review completed early in FY 2009 revealed two areas of opportunity: 1) generation of key electrochemical-performance data needed to improve understanding of SOEC reaction kinetics; and 2) development of advanced electrochemical devices specifically designed for use as high-temperature electrolyzers.

Reaction Kinetics: To clarify the electrochemical processes underpinning SOEC operation, Mizusaki et al. [1] conducted experimentation on "patterned anodes." Such experimental data is unique for inferring the details of the elementary electrochemical reactions and transport of the fuel-side electrode when using steam and hydrogen reactants. No such data exists for co-electrolysis of both H_2O and CO_2. Construction of a dedicated SOEC test stand has been completed and measurements of the electrochemical performance of fabricated solid-oxide electrochemical cells are underway. These results will be compared to models of the charge-transfer chemistry developed at CSM based on a modified Butler-Volmer formulation.

Materials Development: Most SOEC developers employ cells originally designed for operation as fuel cells, by simply operating these fuel cells under reverse bias. SOEC performance can be improved through development

[1] J. Mizusaki, et al., "Kinetic-Studies of the Reaction at the Nickel Pattern Electrode on YSZ in H_2-H_2O Atmospheres," *Solid State Ionics*, vol. 70/71, pp. 52-58, 1994.

of electrochemical devices specifically designed for use in electrolysis mode. We are conducting an effort to develop nickel-free fuel-side electrode materials for SOECs based on the perovskite mixed electronic-ionic conductor, $(La_{0.75}Sr_{0.25})_{(0.95)}Mn_{(0.5)}Cr_{(0.5)}O_3$ (LSCM). The lack of nickel in the electrode enables SOEC operation with a hydrogen-free fuel supply. Fabrication of these novel electrodes is ongoing; the first goal is demonstration of a dense YSZ (yttria-stabilized zirconia) electrolyte on a porous LSCM fuel-side electrode. Efforts are focused on improving the density of the electrolyte by creating a functionally graded electrode structure. Once the LSCM-based cell fabrication process is established, we will test these cells in co-electrolysis mode. Computational modeling will help to guide the cell fabrication process, providing insight on the desired cell architecture to optimize the novel cell.

Significance

Sandia has been establishing a leadership position in recycling CO_2 into liquid hydrocarbon fuels. High-temperature electrolysis from carbon-neutral electricity is a promising complementary field that builds on the foundation of ongoing research on solid-oxide fuel cells at CSM and advanced research in doped-perovskite materials and has the potential to substantially improve electrode performance at Sandia. The collaboration will bring new capabilities to Sandia, build a strategic partnership with CSM in the science of high-temperature electrochemical reactors, and build on Sandia's considerable strengths in nanofabrication and experimental diagnostics. Successful completion of this project will benefit DOE by creating growth in the areas of environmental carbon management and the synthesis of domestic liquid transportation fuels. Such fuels will better enable energy independence, thereby strengthening national security.

Biodefense and Emerging Infectious Disease Collaborations with UTMB

129297
Year 2 of 2
Principal Investigator: A. Hatch

Project Purpose

The project was a collaborative work in the area of biodefense and emerging infectious diseases that Sandia is conducting with our strategic institutional partner, University of Texas Medical Branch (UTMB) at Galveston. The project is composed of three primary Research and Development tasks. These included, 1) the development of a dynamical fluorescent labeling system to investigate the dynamics of the dimerization of the toll-like receptor TLR4/MD-2 receptor, 2) the analysis of stochasticity in immune system signaling pathways, and 3) development of rapid and accurate diagnostic method for detection of ultralow levels of rickettsial pathogens.

The technical benefits of this continuation project were, 1) to understand the initial stages of host-pathogen recognition and receptor dynamics in the important TLR4 cellular signaling pathway, a crucial constituent of the innate immune response to bacterial pathogens, 2) to characterize the poorly understood influence of stochastic cell-to-cell noise and variability in the host signaling response triggered by invading pathogens, and 3) to develop a novel rapid, portable, and sensitive diagnostic tool for diagnosis and monitoring of human infection by Category A, B, and C biodefense bioagents.

In addition to the technical benefits, the project strengthened our strategic partnership with UTMB, which taken together allows Sandia and UTMB to provide unique understanding and solutions for the nation to defend against biological weapons of mass destruction and emerging infectious diseases.

Summary of Accomplishments

For pathogen diagnostics, the technical challenges addressed included the need for sample preparation, and the need for order-of-magnitude improvements in assay sensitivity for antibody-based approaches. Technical innovation centered on using a high capture area porous polymer monolith containing photografted antibodies, on-chip sample handling and preparation (using size-exclusion monolith elements), and diagnostic instrumentation (amenable to field or point-of-care deployment). Significant results were achieved in these areas including 1) selective capture of bacteria with large-pore monoliths, 2) demonstration of a powerful photopatternable monolith framework for arrays of immobilized capture elements and 3) at least 10-fold improvements in speed and sensitivity of capture immunoassays compared to the traditional planar format. Taken together, these accomplishments are significant progress toward meeting the needs for a rapid, specific, sensitive, low-cost, portable and easy to use diagnostic device format.

For processing samples for vaccine development, an automated, fully enclosed system that can be used in BSL3 facilities was designed. The device concentrates and processes intact viruses to enable subsequent viral structure determination using cryogenic scanning electron microscopy (cryoSEM). Viable elution conditions were determined, a critical parameter in the design of antiviral drugs and vaccines. The system was proven suitable for addressing complex conditions for viral structure determination and vaccine development applications.

Toward understanding impacts of stochastic cell signaling, advanced Bayesian inference methods and sensitivity analysis methods, in combination with time-resolved single-cell translocation data has enabled the determination of NF-κB model parameters that give good quantitative agreement between the model predictions and observed behavior. Furthermore, the model was enhanced by accounting for the existence of a reservoir of inactive NF-κB molecules, ultimately showing that this reservoir is indeed a major contributor to the dynamical system behavior. We provided quantitative insights into translocation dynamics enabling the study of cell-cell variability in model parameters.

Significance

This collaboration between leading infectious disease experts at UTMB and Sandia's bioanalytical, computational and advanced imaging experts provided innovative solutions toward improving the nation's ability to defend its population and deployed military forces against biological weapons of mass destruction and emerging infectious diseases. Defending against biological weapons of mass destruction was recently highlighted by the "World at Risk" report issued by Senators Graham and Talent. These interdisciplinary efforts allow us to address in new ways, the pressing needs to protect the US from bioterrorism threats and infectious disease outbreaks. Outstanding postdoctoral researchers have been trained by joint institutional teams to help equip the next generation of scientists with broad multidisciplinary skills needed to address the growing problem area of biothreats and emerging infectious diseases.

Computational Models of Intergroup Competition and Warfare

130810
Year 1 of 3
Principal Investigator: R. G. Abbott

Project Purpose

Warfare is an extreme form of intergroup competition in which individuals make extreme sacrifices for the benefit of their nation or other group to which they belong. Among other animals, limited, nonlethal competition is the norm [1]. It is not fully understood what factors lead to warfare, or to more moderate examples of intergroup competition like territorial fighting in social insects. Agent-based models and genetic algorithms will be used to discover how natural selection shapes the behavior of individuals to give rise to group level traits for success in intergroup competition. These powerful computational techniques give novel insights and allow us to test hypotheses about what drives intergroup competition and warfare.

This project will focus on the development of computational models of intergroup competition. In particular, the conditions under which natural selection for individual sacrifice for the benefit of the group will be studied, and how changes in the intensity of intergroup competition over time apply pressure for the attunement of effort devoted to individual vs. group goals, both over the course of generations, and within the lifetime of an individual.

There is a tradition of examining these properties using mathematical and computational models. However these models have failed to take advantage of genetic algorithms to simulate the evolution of intergroup aggression by natural selection. The emergent properties of groups of organisms lend themselves to study with computational models because group properties are the result of the repeated interactions of discrete, individual members of those groups and this is a largely untapped resource for answering these questions. This project is a collaboration with the University of New Mexico.

Summary of Accomplishments

During the past year, agent-based models of ant foraging, based on the foraging behavior of three species of desert harvester ant, genus *Pogonomyrmex* have been developed. Field observation of ant foraging behavior, with a focus on the ants' use of information to direct and optimize colony foraging success has been conducted. These observations, along with other data from the literature, have been used to parameterize the models. Field observations were used as a reference for discovering and developing the individual ant behaviors that are important in capturing a colony's emergent foraging behavior. In order to optimize other, unmeasured parameters, and in order to investigate the effect of colony size on differential foraging success when feeding on more or less heterogeneously distributed food sources, this model was incorporated as the fitness function in a genetic algorithm, which allows for simulating the evolution of behavior under various conditions. This enabled the study of evolution of recruitment behavior across a wide range of colony sizes, with colonies foraging on foods distributed in a wide range of homogeneity to heterogeneity. We have found that the conditional laying of pheromone trails, based on a foraging ants' perception of how much food is nearby when it begins its return to the nest, allows most efficient foraging on a wide range of food distributions, and in all but the very smallest colonies. This conditional trail-laying behavior may be an important contribution to models of recruitment in a variety of ant species, and may be a valuable technique in the engineering application of ant colony algorithms. Results of this work will be presented as a talk at the Swarmfest 2009 agent-based modeling conference.

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[1] J. Maynard Smith and G.R. Price, "The Logic of Animal Conflict," *Nature*, vol. 246, pp. 15-18, 1973.

Significance

This research will yield insight for domains involving the modeling and simulation of human combatants including DOE threat models and DOD conflict simulations. For example, the Office of Naval Research Human Social Cultural Behavior Modeling program seeks to provide the ability to understand and effectively operate in human/social/culture terrains inherent to nonconventional warfare missions.” The use of invertebrates (ants) as models to elucidate the influences shaping the evolution of human conflict behavior facilitates controlled experimentation that could not be conducted on humans and that enhances tools and capabilities for modeling and simulation.

Data Mining for Improved Computer System Architecture

130811
Year 1 of 1
Principal Investigator: K. S. Hemmert

Project Purpose

Designing microprocessors has become a delicate balancing act between numerous decisions, each potentially having a large impact on the others. Data mining and machine learning techniques can be applied to computer system design to aid in optimizing these decisions, improving system runtime performance. For example, data mining and machine learning can be used to improve predictors, such as branch predictors or prefetchers, which speculate in order to improve performance.

Data mining and machine learning for computer system architecture optimization will be studied in the context of FAST (FPGA-accelerated simulation technologies) full-system simulators, developed and used for research at the University of Texas, Austin. These simulators are capable of running unmodified applications and operating systems. FAST simulators are vital for data mining analysis because they are hardware accelerated, enabling them to run about three orders of magnitude faster than other current cycle-accurate simulators. As a result, data mining and machine learning algorithms are provided with the large amount of data required to identify patterns and train improved predictors.

Branch prediction is essential to performance in modern processors. A data mining analysis can be used to determine which architectural features most highly correlate with branch outcomes. Initial investigation suggests that intermediate, potentially stale, data values from program execution can improve branch prediction accuracy. Additionally, preliminary research indicates that certain data mining algorithms, such as pruned decision trees, have high potential for replacing or augmenting traditional branch predictors.

This investigation into applying data mining and machine learning to computer system design, with specific case studies in branch prediction and data prefetching, will result in a methodology and toolset that can be applied to many areas of computer systems. FAST simulators can be used to train and evaluate new predictors, with the goal of improving computer system performance on real world applications.

Summary of Accomplishments

It was found that decision trees and boosting algorithms can outperform state-of-the-art branch predictors like the perceptron and GTL. Trees use a relational representation to form a possibly disjunctive boundary which enables it to correctly navigate through a noisy space. Additionally, information gain serves as a successful ranking tool to identify potentially helpful input features to decision trees and boosting algorithms. Finally, it was observed that decision trees and boosting algorithms are capable of creating small and simple trees that can dramatically improve branch prediction accuracy.

Significance

Our missions in defense, energy, and science increasingly rely on simulation to reduce experimentation. Nationwide, simulation is stepping up to the challenge where extensive experimentation is impossible. Successful research in this area could provide key advances that will improve the performance of microprocessors which are at the heart of modern supercomputers used for large scale simulations.

Data-Driven Optimization of Dynamic Reconfigurable Systems of Systems

130812
Year 1 of 3
Principal Investigator: J. P. Eddy

Project Purpose

In this research, we define a system-of-systems (SoS) as a dynamic, interdisciplinary network of individual communicating, collaborating entities with varying levels of autonomy and decision-making capability. Entities may be humans, autonomous machines, or human operated equipment. The concept of a system-of-systems is different from that of a traditional large-scale system that is complex but static. To understand the nature and mechanisms of complex systems, researchers have addressed the core components of static, single system design optimization using traditional systems engineering and mathematical programming for more than two decades. With the emerging notion of dynamic design and operations of a system-of-systems, we are faced with an important generalization of the architecture and mechanism.

Our vision of this research is to develop new methods for a quantitative reconfiguration of a system-of-systems that can respond to unforeseen operating scenarios by integrating distinctive domains of knowledge in systems engineering, data management and mining, multidisciplinary optimization, and parallel computing. We identify key research themes: a) the dynamic aspect of systems architecture is modeled, b) the decision-maker remains in the loop for the coordination process, and c) the SoS optimization framework is easily scalable to model realistic operating conditions and models.

This research will transform the conventional paradigm for designing and operating multiple system infrastructures into a new paradigm of autonomous, reconfigurable system-of-systems. The outcome of the research will potentially benefit areas such as homeland security, emergency response, and future combat systems, where the dynamic paradigm plays a key role. Human and capital losses from natural disasters, unforeseen attacks or system failure may be significantly smaller than those observed in the cases of hurricanes, tsunami disasters, or food contamination outbreaks. The collaboration between Sandia and the University of Illinois at Urbana-Champaign will leverage expertise in the core research areas addressed above.

Summary of Accomplishments

During FY 2009, algorithms and expertise in the areas of data mining and optimization have been developed. Each of these areas are critical to this project. Sandia tools for performing system-of-systems (SoS) analysis and optimization were used. A proof-of-concept example and expertise in data-mining were created and proved of benefit to our SoS analysis. These capabilities may prove valuable to some of our DOD customers.

Significance

Sandia is engaged in SoS research as a tool for furthering its strategic goals. Examples include the US Army programs for defense, logistics modeling of disaster relief efforts for national security, and power grid analysis and water systems modeling for energy and security. This research is intended not only to improve our ability to model these kinds of systems but also to provide tools to aid in real-time operation of such systems for optimal decision-making and resource allocation.

Development and Characterization of 3D, Nanoconfined Multicellular Constructs for Advanced Biohybrid Devices

130813
Year 1 of 3
Principal Investigator: B. J. Kaehr

Project Purpose

Inspiration for the design of new materials and devices is increasingly found in biological systems where sensitive detection, energy conversion, and molecular/nano machinery have been continually improved upon by evolution. To impart the useful properties of biological systems into devices requires new ideas and technologies. Although there has been much focus on material functionalization using biomolecules, incorporation of self-sustaining and self-replicating components (e.g., cells, tissues and organisms) into solid-state platforms has received scant attention. Outside of native and well-controlled environments, cells are fragile and cell behavior is difficult to manipulate into complex systems such as tissues. In order to bridge the organic structures and functionalities of cells to the inorganic, solid-state materials of modern devices, functional biotic/abiotic interfaces are required. This research will take advantage of recently developed strategies that allow the cell-directed assembly (CDA) of nanomaterials to form functional bio/nano interfaces. This approach is an important step toward building solid-state devices that are enabled by cellular functions. Devices for sensing and computation will be further facilitated if higher order cellular functions, such as differentiation and intercellular communication can be maintained and exploited in biohybrid materials. Recent breakthroughs in 3D microfabrication that enable the topographical and chemical microenvironments of developing cell populations to be precisely defined will be employed to direct bio/nano interfaces to multicellular constructs. Patterning of multicellular constructs that can direct assembly of nanostructured films combined with the emerging tools of cellular (re)programming (i.e., synthetic biology) will permit the design of communication networks between engineered cell populations — enabling the development of cell-based circuitry. Incorporation of cellular functions into integrated microplatforms may allow the development of new technologies including cell-powered robots and "personalized" bionic implants.

Summary of Accomplishments

- Thin films (20–60 nm) comprising a variety of crosslinked proteins (e.g., serum albumin, catalase, avidin, glucose oxidase) have been prepared and shown to direct assembly of meso-structured silica films. This work demonstrates the compatibility of the cross-linked protein matrices with the lipid-silica self-assembly process and represents a fundamental step towards year 2 and 3 goals. Moreover, protein function (e.g., catalytic and binding properties) is maintained under these conditions and can be deactivated using standard UV lithography—allowing functional patterning with nanoscale resolution.
- A new strategy that employs cell growth to direct functional inorganic/cell interfaces has been developed. Bacterial cell walls (such as *Escherichia coli* rod shaped cells) can be targeted with catalytic precursors (charged metal nanoparticles) to form a biocompatible coat which can be developed into an electrically percolating network via metal-ion reduction chemistry. By allowing the cell to undergo one growth and division cycle results in sequestration of catalysts to cell poles forming new (central) template that can be targeted with additional catalysts. This work demonstrates a new route for Janus (asymmetric) metallic particle synthesis and should provide a foundation to realize biohybrid systems based on more complex biological architectures and developmental pathways (crucial toward achieving year 2 and 3 goals).

Significance

The development of a robust platform bridging biological systems to devices and systems will yield an entirely new class of biohybrid technologies and is thus of interest to basic and applied science DOE missions. These materials, to be developed and analyzed in a collaborative effort with the Center for Integrated Nanotechnologies (CINT), can be explored across a broad range of applications such as extreme environmental sensing, biocomputation, bioenergy conversion and artificial tissue fabrication.

Development of a Structural Health Monitoring System for the Assessment of Critical Transportation Infrastructure

130814
Year 1 of 3
Principal Investigator: D. P. Roach

Project Purpose

Recent structural failures such as the I-35W Mississippi River bridge in Minnesota have underscored the urgent need for improved methods and procedures for evaluating our aging transportation infrastructure. This research seeks to develop a structural health monitoring (SHM) system to provide more quantitative information about the condition of metallic structures for making appropriate management decisions and ensuring public safety. The system will employ advanced structural analysis and nondestructive testing (NDT) methods for sensing/measurement and decision-making purposes. Metal bridges will be the focus since many of these structures are over 50 years old and are classified as fracture-critical. A fracture-critical structure is one where failure of a single component may result in complete collapse such as the one experienced by the I-35W bridge. Failure may originate from sources such as loss of section due to corrosion and cracking due to fatigue loading. Because standard inspection practice is primarily visual, these types of defects can often go undetected due to an oversight or lack of access to a critical area. Another issue is that inspections are typically done every 1 to 2 years leaving the opportunity for failure to occur between inspections. An SHM system has several advantages for overcoming these limitations, a few of which are: a larger area of the structure is monitored; monitoring is continuous and/or long-term; multiple types of sensors are employed; and sensing/measurements are automatic or semiautomatic. The research needed to apply SHM to metallic structures will be performed and field demonstrations will be carried out to show the potential of SHM for assessing the condition of our critical transportation infrastructure. This project will combine the expertise in the transportation infrastructure arena at New Mexico State University (NMSU) with the expertise at Sandia in the emerging field of SHM.

Summary of Accomplishments

Project milestones 1 through 4 have been addressed. Milestone 1 was to perform initial inspection and analyses of railroad bridges using the American Railway Engineering and Maintenance-of-Way (AREMA) guidelines, which was addressed by performing the load ratings for 13 steel through-girder railroad bridges and 3 through-truss bridges. Milestone 2 involved identifying critical locations for damage and deterioration, particularly fatigue damage. It was found that the most heavily stressed members were the floor beams and stringers, which also experience the greatest number of load cycles. It was also found in the literature review that the connections between floor system elements typically resist significant moment and that this can lead to fatigue problems. Milestone 3 was the selection of instrumentation to be used in the study, which will be strain gauges due to equipment availability and applicability to the preliminary SHM system design. Milestone 4 was to design an SHM system, which is currently in the very early stages; however, it has been decided that the SHM system will consist of strain gauges and a data acquisition system that will use rainflow counting to determine the remaining life of a metallic structure. A literature review was also carried out with a focus on fatigue in steel bridges and on SHM systems for bridges. It was found that the fatigue life of steel bridges is typically estimated using Miner's rule and/or fracture mechanics principles using either a deterministic or probabilistic approach. It was found that the most common method of SHM for bridges is monitoring changes in the dynamic behavior of a structure to locate and quantify damage. It was found, however, that no system was validated for field use even though some algorithms were capable of detecting damage in a laboratory setting.

Significance

SHM shows great promise for critical infrastructure assurance and homeland security. Although advanced methods and techniques are available to SHM professionals, deployment of SHM systems for in-depth evaluation has been slow due to the lack of specific procedures for properly designing, installing, and operating the SHM system for making decisions. This project will enable more widespread use of SHM to improve the assessment of our critical infrastructure.

Distributed Video Coding for Arrays of Remote Sensing Nodes

130815
Year 1 of 2
Principal Investigator: B. J. Merchant

Project Purpose

The focus of this research collaboration with New Mexico State University will be to apply bitstream-based processing techniques to the problems of distributed video compression. The basic goal of distributed compression (more formally called distributed source coding) is to take advantage of correlations between sensor measurements in order to reduce the amount of communications bandwidth required to transmit these measurements to some collection site. There has been a great deal of research related to distributed source coding in recent years, but virtually all of this work has assumed the availability of sensor correlation information at both the sensor nodes and the collection site. In reality, such information must be extracted by the sensors in the network and efficiently distributed as needed. Typically, this would require a sensor node exploiting the distributed coding paradigm to have essentially the same capabilities as the decoder at the collection site — i.e., it would have to be capable of fully decoding the transmissions that it picks up from all of neighboring nodes in the array and analyzing them to determine what, if any, correlations exist. In the case of video, this decoding process converts the very sparse compressed representation of the data into a very large number of image pixels which must then be processed by the sensor node. Both the process of decoding the compressed bitstream and that of analyzing the reconstructed video sequence consume large amounts of computational bandwidth and node power, making sensor nodes more expensive and reducing their effective lifetimes in the field.

In previous work, it has been shown that spatial overlap between the video frames of neighboring sensors can be determined with relatively high accuracy by directly processing the bits produced by a motion-JPEG (joint photographic experts group) video encoder.

Summary of Accomplishments

In the past year, we were able to investigate new bitstream domain processing techniques as well as produce the groundwork for a distributed video coder using conditional entropy. It was shown that areas of correlation can be identified with relatively high accuracy using the bitstream information alone. This scheme used the motion-JPEG video encoder to produce bitstreams. The results have produced two conference papers, one of which received the best graduate paper award at the International Test and Evaluation Association (ITEA) Live Virtual Constructive Conference.

During this time, we have explored methods for image segmentation and edge detection using bitstream information. These methods have proven helpful in refining methods for identifying correlations. As of right now, a working distributed video coder that is capable of exploiting these correlations and dependently encoding information is nearing completion.

Significance

Many Sandia mission areas utilize distributed sensor systems (monitoring for security, environment, production processes, etc). The DOE/NNSA ground-based nuclear explosion monitoring research program is seeking unobtrusive sensors for deployment near testing areas. In some cases communications will be severely limited due to the location of these systems. This work will advance the technology available for application to these monitoring systems.

Refereed Communications

I. Mecimore and C.D. Creusere, "Unsupervised Bitstream Based Segmentation of Images," *Digital Signal Processing Workshop and 5th IEEE Signal Processing Education Workshop*, vol. 1, pp. 643-647, January 2009.

Evaluation of Baseline Numerical Schemes for Compressible Turbulence Simulations

130817
Year 1 of 2
Principal Investigator: R. B. Bond

Project Purpose

Numerical and modeling errors in turbulence simulations are difficult to isolate and quantify. An approach that has previously shown promise in this area is the method of nearby problems (MNP), developed by Presidential Early Career Award for Scientists and Engineers (PECASE) recipient, Dr. Christopher Roy of Virginia Polytechnic University. MNP is a novel approach that can be used to assess numerical errors in complex calculations. In MNP, exact solutions are generated by spline fitting highly resolved numerical solutions. These solutions are "nearby" the numerical solutions from which they were derived, and thus are representative of the relevant physical and mathematical properties, yet they are exact and can thus be represented to machine precision. These exact solutions are solutions not to the original equation set, but rather, to a "nearby" equation set, with the same differential operator and a source term generated by applying the original differential operator to the exact solution. The source terms generated are small and distributed, preserving the "nearby" nature of the new equation set. Multidimensional MNP can be applied to problems in code and solution verification in many different areas of computational science and engineering. This project will focus on applying multidimensional MNP to 3D (2 spatial and 1 temporal) and 4D (3 spatial and 1 temporal) solutions to the Euler and Navier-Stokes equations. This will allow baseline numerical schemes for these equation sets to be evaluated. We will extend this work for unsteady turbulent simulations, to allow dissipative and dispersive errors to be quantified. Quantification and study of these numerical errors will lead to the development of new subgrid turbulence models which can account for the presence of numerical error, as estimated by MNP. This contribution will be particularly useful for modeling of compressible turbulent flows, since computer codes used for simulating compressible flows are often limited to second-order accuracy.

Summary of Accomplishments

Over the past year, we have accomplished a number of key objectives of this work. These accomplishments are summarized below.

- The 2D MNP approach for generating exact solutions and for estimating discretization error was applied to 2D heat conduction and the 2D incompressible Navier-Stokes equations and published in the *Journal of Computational Physics.*
- The spline fitting approach has been extended from 2D to 3D, but not yet tested. The weighting functions used to ensure Ck continuity at spline fitting boundaries have been extended to arbitrary dimensions by combining the 1D weighting functions in multiple dimensions. Results were presented at the 19th AIAA Computational Fluid Dynamics Conference.
- Insight into the source of the high-frequency oscillations seen previously in the 2D results has been gained by going to higher-order local fits. Results were presented at the 19th AIAA Computational Fluid Dynamics Conference.
- Two new 2D problems have been analyzed which have exact solutions: unsteady Burgers equation and 2D ringleb flow (Euler equations for expansion past an arc). Results were presented at the 19th AIAA Computational Fluid Dynamics Conference. An additional 2D problem of a subsonic airfoil is currently under investigation.

Significance

This work is relevant to our nuclear security mission; it will provide a platform for evaluating numerical schemes for compressible turbulent flows. The work will also advance the state-of-the-art in discretization error estimation, which indirectly impacts the predictive capability of modeling and simulation for the Stockpile Stewardship Program.

Refereed Communications

C.J. Roy and A.J. Sinclair, "On the Generation of Exact Solutions for Evaluating Numerical Schemes and Estimating Discretization Error," *Journal of Computational Physics*, vol. 228, pp. 1790-1802, March 2009.

Interfacial Electron and Phonon Scattering Processes in High-Powered Nanoscale Applications

130818
Year 1 of 3
Principal Investigator: P. E. Hopkins

Project Purpose

A significant limiting factor in next generation nanoelectronic systems is the large heat fluxes generated from operation. Inadequate power dissipation capabilities in these systems result in self-heating and increased operating temperatures that degrade device gain and efficiency and shorten device life. The materials used in the design and construction of the nanoelectronic devices and the dissipation of the heat from these devices contributes to overheating. Nowhere is this problem more pronounced than in high-powered systems, such as sensor, and signal processing systems and energy conversion systems, such as thermoelectric coolers and power generators. Therefore, thermal management in current and future nanoelectronic systems is a growing concern. As these nanoelectronic systems continue to decrease in characteristic sizes, the thermal management issues arise at the interfaces or junctions of different materials where energy carrier scattering is prominent. The key to thermal engineering of next-generation nanosystems is to understand the intrinsic properties of materials that affect interfacial thermal transport.

The objective of this project is to study heat transfer processes around structurally imperfect regions at interfaces involving both traditional and novel nanostructures used in high-powered nanoelectronic and energy conversion applications. Deposition, fabrication, and post-processing procedures of nanocomposites and devices can give rise to interatomic mixing around interfaces of materials leading to stresses and imperfections that could affect heat transfer. As nanoapplications continue to decrease in characteristic sizes, the degree and depth of the interatomic mixing can be on the same order or greater than the sizes and length scales of the individual materials comprising the device. An understanding of the physics of energy carrier scattering processes and their response to interfacial disorder will elucidate the potentials of applying these novel materials to next-generation high powered nanodevices and energy conversion applications.

Summary of Accomplishments

We set up three optical experiments to measure thermal properties of thin films systems: a phase-sensitive thermoreflectance technique and two transient thermoreflectance (TTR) techniques. We are currently examining thermal transport in phononic crystals, semiconductor photovoltaics (with the University of California [UC] Berkeley), thin film semiconductors used for nanowire contacts (with the Massachusetts Institute of Technology [MIT]), nanoporous metals for use in irradiated applications (with Los Alamos National Laboratory [LANL]), and diamond contact thermal spreaders (with the University of New Mexico [UNM]). We have also been studying thermal transport across traditional interfaces that are heavily disordered; we have studied electron phonon coupling, thermal boundary conductance, and substrate thermal conductivity changes resulting from changes in the interfacial structure.

In addition to these experimental initiatives, we have also progressed in modeling and simulation, studying upper and lower limits to electron and phonon scattering with various Boltzmann-based theories and nonequilibrium Green's function (NEGF) simulations. Using Boltzmann based theories, we have developed a ballistic-diffusive approximation to electron transport in thin film limit and isolated the effects of interface scattering on ballistic and diffusive transport. We have also looked extensively at the effects of interface structure and morphology on phonon transport at interface, developing new lower limits for thermal conductance across interfaces as a function of structure. In addition, we have outlined a new phonon modeling technique for one dimensional thermal transport, the NEGF technique, and have used this method to analytically predict a new phonon transport mechanism that results from interface scattering which parallels Fabry-Perot interference in optics. These phonon wave interference mechanisms can be controlled to give rise to asymmetric heat conduction, i.e., thermal rectification.

This work from this project has thus far resulted in 15 journal publications (8 accepted and 7 under review) and 7 conference presentations.

Significance

A key to future success in national security and defense lies in improving the fundamental scientific understanding of the complex dynamic behavior in energy conversion systems used in military applications. This project will advance the understanding of thermal transport at interfaces in current and future nanoelectronic and energy conversion applications. The physical insight gained by this study will be used to design future nanoelectronic devices.

Refereed Communications

P.E. Hopkins, J.L. Smoyer, J.C. Duda, R.N. Salaway, and P.M. Norris, "Effects of Inter- and Intraband Transitions on Electron-Phonon Coupling and Electron Heat Capacity After Short-Pulsed Laser Heating," *Nanoscale and Microscale Thermophysical Engineering*, vol. 12, pp. 320-333, 2008.

P.E. Hopkins, "Effects of Electron-boundary Scattering on Changes in Thermoreflectance in Thin Metal Films Undergoing Intraband Transitions," *Journal of Applied Physics*, vol. 105, p. 093517, May 2009.

P.E. Hopkins and E.S. Piekos, "Lower Limit to Phonon Thermal Conductivity of Disordered, Layered Solids," *Applied Physics Letters*, vol. 94, p. 181901, May 2009.

J.C. Duda, J.L. Smoyer, P.M. Norris, and P.E. Hopkins, "Extension of the Diffuse Mismatch Model for Thermal Boundary Conductance Between Isotropic and Anisotropic Materials," *Applied Physics Letters*, vol. 95, p. 031912, July 2009.

P.E. Hopkins, "Multiple Phonon Processes Contributing to Inelastic Scattering During Thermal Boundary Conductance at Solid Interfaces," *Journal of Applied Physics*, vol. 106, p. 013528, July 2009.

P.E. Hopkins and D.A. Stewart, "Contribution of D-Band Electrons to Ballistic Transport and Scattering During Electron-Phonon Nonequilibrium in Thin Au Films Using an Ab Initio Density of States," *Journal of Applied Physics*, vol. 106, p. 053512, September 2009.

P.E. Hopkins, "Contributions of Inter- and Intraband Excitations to Electron Heat Capacity, Electron-Phonon Coupling, and Temporal Temperature Decay in Noble Metals," to be published in the *Journal of Heat Transfer*.

P.E. Hopkins, P.M. Norris, M.S. Tsegaye, and A.W. Ghosh, "Extracting Phonon Thermal Conductance Across Nanoscale Junctions: Nonequilibrium Green's Function Approach Compared to Semiclassical Methods," to be published in the *Journal of Applied Physics*.

Laser Doppler Vibrometer Measurements of Carbon Nanotubes' Vibration Spectra: A High Frequency Resolution Technique with Sensor Applications

130819
Year 1 of 1
Principal Investigator: S. W. Howell

Project Purpose

The purpose of this project is to evaluate the utility of nanowires for ultrasmall mass detection and high-bandwidth piconewton force detection. A real-time, nondestructive technique to measure the vibrational spectra of nanowires will help enable these applications. Furthermore, reliable estimates for the elastic modulus and spring constants of nanowires and the quality factors of their oscillations are of interest to characterize these nanowires. During the previous FY, our collaborators at Purdue University developed this laser Doppler vibrometry (LDV) technique to measure the resonant frequencies and quality factors of multiwalled carbon nanotubes (MWNTs) under ambient conditions. In FY 2009, the mechanical properties and vibrational spectra of crystalline silver-gallium (Ag_2Ga) nanowires will be measured and compared with those of MWNTs and silicon microcantilevers.

Laser Doppler vibrometry (LDV) is used to measure the thermal and driven vibrations of nanowires under ambient and low-vacuum conditions. The high frequency resolution of LDV enables a precise determination of the resonant frequencies and quality factors of the different eigenmodes of a vibrating nanowire. LDV is promising for automated detection since the predominant noise in the measured vibration spectra is a low power white noise background, which is clearly distinguishable from the optically reflected signal from the oscillating nanowire.

An important byproduct of this research is the ability to determine the elastic properties of an oscillating nanowire in an unobtrusive way. Successful completion of this proposal will enhance Sandia's ongoing nanosensing programs by enabling fundamental research in carbon nanotube-based sensing and device development.

Summary of Accomplishments

To evaluate the suitability of Ag_2Ga nanowires as resonators for mass sensors and force transducers, we used laser Doppler vibrometry (LDV) to measure the thermal and driven vibrations of Ag_2Ga nanowires in atmospheric and low-vacuum conditions. These experiments were done in collaboration with Purdue and the University of Louisville.

Atmospheric measurements of the thermal vibration spectra of Ag_2Ga nanowires allowed determination of the eigenfrequencies, quality factors, elastic modulus, and modal spring constants of the Ag_2Ga nanowires. In low-vacuum conditions (<1 Torr), the quality factors increased by a factor of ~50 due to the elimination of mass loading and viscous damping by the surrounding gas. Furthermore, the high-frequency resolution of the LDV measurement allowed nanowires with radially asymmetric cross sections to be identified.

For mass sensing applications where the minimum detectable mass, δm, is transduced from the resulting resonant frequency shift, δm for the Ag_2Ga nanowires studied was estimated to be in the tens of femtograms range at atmospheric pressure and the attogram range under vacuum conditions. The low spring constants and high-frequency bandwidth (up to 2 MHz) would allow piconewton force detection for nanowire displacements on the order of 1 nm.

Overviews of this research were presented at the 2008 Fall Materials Research Society (MRS) meeting and the 2009 March American Physical Society (APS) meeting.

Significance

This research evaluates the relative figures of merit for force and mass sensing using nanocantilevers, such as Ag_2Ga nanowires. The small mass, low stiffness, and relatively high Q-factors at atmospheric conditions favor the use of Ag_2Ga nanowires as nanocantilevers in accelerometers, chem-bio sensors, acoustic sensors, and in femtogram/attogram mass sensing applications with relevance to our nuclear security, energy, and science missions.

Refereed Communications

M.L. Bolen, S.E. Harrison, L.B. Biedermann, and M.A. Capano, "Graphene Formation Mechanisms on 4*H*-SiC(0001)," *Physical Review B*, vol. 80, p. 115433, September 2009.

L.B. Biedermann, R.C. Tung, A. Raman, and R.G. Reifenberger, "Flexural Vibration Spectra of Carbon Nanotubes Measured Using Laser Doppler Vibrometry," *Nanotechnology*, vol. 20, p. 035702, January 2009.

L B. Biedermann, M.L. Bolen, M.A. Capano, D. Zemlyanov, and R.G. Reifenberger, "Insights Into Few-Layer Epitaxial Graphene Growth on 4*H*-SiC(000) Substrates from STM Studies," *Physical Review B*, vol. 79, p. 125411, March 2009.

Nanocomposite Materials for Efficient Solar Hydrogen Production

130820
Year 1 of 3
Principal Investigator: J. E. Miller

Project Purpose

Solar energy is the most abundant sustainable energy option and as a result is of great interest. Materials that utilize concentrated solar energy to produce hydrogen will potentially enable a long-term viable alternative to fossil fuels. The focus of this research will be fabricating and understanding nanostructured composite materials that are active for a thermochemical process that converts solar energy into chemical energy in the form of hydrogen in a more-efficient, straightforward, and possibly more cost-effective manner than solar driven electrolysis. The nanocomposite materials should provide an improvement over the current generation of materials because the active phase will have a higher surface area to volume ratio within the oxygen-conducting bulk phase that should allow for greater materials utilization during each thermochemical cycle. The composites will be fabricated into monolithic structures with defined and controlled macroscale surface to volume ratios that can be evaluated and compared at the National Solar Thermal Test Facility (NSTTF) at Sandia in a solar water-splitting reactor. Several known and novel formulations will be evaluated. Key metrics important to achieving high efficiency that will be considered include overall active phase utilization (reaction extent) and reaction kinetics as a function of particle size within the composite and of the critical macroscale dimension. The processing of the materials will take place in the Materials Science and Engineering Department at the University of Arizona. This work will help create a partnership between Sandia National Laboratories and the Arizona Research Institute for Solar Energy (AzRISE) whose mission is to help create innovative collaborations in order to accelerate research, development and practical implementation of solar energy solutions to our energy needs.

Summary of Accomplishments

The research for FY 2009 focused on fabricating composite materials that are active for solar thermochemical processes into monolith parts suitable for on-sun evaluation. The specific project activities addressed the critical need for alternative processing methods that would allow rapid and reproducible fabrication of uniform substrates comprising different constituent materials and different compositions suitable for testing at the National Solar Thermal Testing Facility (NSTTF). Obtaining meaningful data at a reasonable throughput with the small scale solar water-splitting semi-batch reactor requires simple uniform structures with well defined and known macroscale surface-to-volume ratios. Additionally, the processing method should also be scalable to at least kilogram quantities to produce parts for the larger CR5 solar reactor. The feasibility of manufacturing bulk monolithic honeycomb structures via an advanced polymer co-extrusion process was evaluated with a series of Fe_2O_3-YSZ sintered composites. Honeycomb and similar structures appear to be ideal substrates because of their high strength and high surface area. However traditional ceramic processing of honeycombs via bulk extrusion cannot accommodate the curved ring design of the advanced CR5 thermochemical reactor. Co-extruded polymer based honeycombs can be easily fused together in an arc shape with minimal size and shape deformation of the final part as each channel of the comb is supported by a polymer/carbon black core during manipulation of the green ceramic into shape. Firing the green part burns the polymer away, revealing the hollow channels. Parts with several open channels have been successfully fabricated.

Significance

The design and implementation of new thermochemical materials that have ideal compositions and structures are needed to enable new, viable, and sustainable alternatives to fossil resources. This work impacts DOE strategic goals in the areas of defense, energy, science, and environment, and it will help to strengthen our nation's national security and provide a pathway to long term energy independence.

Nanotexturing of Surfaces to Reduce Melting Point

130821
Year 1 of 3
Principal Investigator: E. J. Garcia

Project Purpose

The reduced melting point of nanotextured silicon surfaces is far below theoretical prediction and has practical application for bonding in microsystems packaging.

In collaboration with the University of Texas, El Paso (UTEP), we will focus on: (Year 1) advancing the science and technology of reduced melting point (RMP) in nanotextured silicon-on-insulator (SOI) wafers, (Year 2) using RMP for bonding applications and (Year 3) implementing the RMP bonding technique for microsystems.

Year 1 research focuses on comparing theoretical predictions to results from melting experiments in which the geometry and size of the surface silicon on SOI wafers is varied. Preliminary experiments have shown that the melting point of silicon nanocrystals measuring 100 nm in diameter and 40 nm in thickness but with very fine features (< 5 nm) is reduced from its bulk value of 1412 °C to 1055 °C. This reduction deviates strongly from simple theoretical modeling that predicts that for a melting temperature of 1055 °C the particle diameter would have to be ~0.8 nm. In this project, theoretical models will be adapted and used to predict the size-dependent melting of nanostructured silicon crystals using the appropriate characteristic dimension such as the size of fine features. An experiment will be designed to nanopattern the surface silicon on SOI wafers and heat the samples to determine their size-dependent melting point. The silicon nanocrystals will be characterized for morphology, size and crystallography, before and after heat treatment. Experimental results will be analyzed relative to theoretical predictions. Year 2 research will study the effect of doping the surface silicon to further reduce the melting point. Localized heating via electrical current through doped regions will be attempted. Bond strength and character will be studied as a function of temperature, pressure and other critical parameters. Year 3 will implement the RMP bonding technique on actual microsystems chips.

Summary of Accomplishments

Sharp diamond-like shaped structures were patterned successfully for the initial experiments using nanoimprint lithography on silicon-on-insulator wafers. Heating experiments were conducted at a number of temperatures (1000 °C, 1200 °C, 1250 °C, etc.) approaching the bulk melting point of silicon (1412 °C) to investigate changes in the patterned structures. These devices were characterized with a scanning electron microscope and it was discovered that some undesirable oxidation occurred on the surface of the structures resulting in unexpected behavior of the structures. These experiments are being rerun using a different furnace and using a different forming gas to reduce the unwanted oxidation. A method has been developed to perform in-situ measurements to determine structural changes to the test devices as a function of temperature. A new dry etch process was also conducted at UTEP this summer to observe the effects of an alternate etch process on the diamond-shaped structures. Test data generated this summer is being compared with an existing theoretical model.

Significance

This research benefits our efforts towards developing microsystem-based components for application to security functions. The work is furthering the advancement of advanced microsystem packaging methodologies, in particular how we can achieve hermetic bonding of packages in reduced temperature processing environments. Such environments will lessen the deleterious effects of high temperature processing on microdevices during the packaging stage.

Neural Correlates of Attention

130823
Year 1 of 2
Principal Investigator: T. J. Shepodd

Project Purpose

Sandia has a great interest in the decision-making process. Within the brain, the complex process can be simplified into a three-step process: perception, association of perception with motivation/reward, and preparation to behave towards the stimuli. Recent advances with in situ brain monitoring show that posterior parietal cortex is necessary for such sensorimotor integration, representing target locations, intended actions and even reward-related signals. These studies elucidate the causal relationships of various functional areas within the intraparietal sulcus during voluntary decision-making behavior. In preparation for studies on the human brain, primate brain function will be evaluated while $GABA_A$ agonists will inactivate either the parietal reach region (PRR, an area encompassing macaque area 5 and MIP) or the lateral intraparietal area (LIP) while the other region is monitored with electrophysiological recording and functional magnetic resonance imaging (fMRI). Later in this project, in humans, an analogous technique of repetitive transcranial magnetic stimulation (rTMS) will be employed to create temporary, virtual lesions in the homologous parietal regions while reach and saccade decision tasks assess any behavioral deficits, and simultaneous functional magnetic resonance imaging (fMRI) reveals the underlying neuronal changes responsible for any behavioral changes. The purpose of these studies is to determine which way and what kind of information flows between parietal areas LIP and PRR as well as other prefrontal and subcortical structures in the sensorimotor decision-making circuitry. This work, in collaboration with the California Institute of Technology (Caltech), is key to understanding the spatial/temporal nature of the decision-making process in the human brain.

Summary of Accomplishments

A macaque was subjected to the planned task paradigm at Caltech, except that the paradigm was modified to use an adaptive staircase method for determining the asynchronous timing of the target presentation during choice tasks. Baseline behavioral data was acquired for 15 sessions, to firmly demonstrate the monkey's pre-inactivation biases. The injectrode design was modified to improve its performance and its integration into the NAN drive (electrode micromanipulator system). Saline testing of the injectrode device has begun, as a preliminary step before the inactivation using THIP (4,5,6,7-tetrahydroisoxazolo[5,4-c] pyridin-3-ol). The FY 2009 results should leave us ready for the fMRI work in 2010.

Significance

A significant part of what DOE and DHS do for the nation involves risk-informed decision-making. This project addresses the human cognition element of those critical national and homeland security decisions. It will examine cognition under uncertainty in decision-making. Issues include: attentional demands; ambiguity; physiological state; individual ontogeny; role of intuition and memory.

Optical Properties of Dielectric/Metal Composites

130825
Year 1 of 1
Principal Investigator: M. V. Pack

Project Purpose

Composite metal-dielectric films have been of interest to researchers in various areas for a number of years. These films, which are sometimes described by fractal self-similarity or effective medium theories, have shown promise in the areas of both sensing and superlensing. In sensing, semicontinuous metal films (SMFs) can produce strong, local electromagnetic field enhancements due to the excitation of localized plasmon oscillations in the metal nanostructure. These enhancements can be applied for highly sensitive sensing applications such as surface-enhanced Raman scattering (SERS), surface-enhanced infrared absorption (SEIRA), and enhanced fluorescence.

Metal-dielectric composite films are also under study for use in near-field superlens (NFSL) designs, where planar slab focusing and enhancement of near-field electromagnetic modes can yield exciting results including subwavelength imaging and the translation of evanescent fields. Current planar superlenses based on bulk metal films exhibit negative refraction and planar slab focusing at only one particular wavelength, usually in the ultraviolet range. Using effective medium theories and careful material selection, however, metal-dielectric composite superlenses can be designed to operate within a broad range of wavelengths, including the visible and near-infrared regions.

The ultimate goal of our work, which is in collaboration with Purdue University, is the combination of the enhancement and superlensing aspects of composite films into a single system that will allow remote, enhanced sensing of analytes.

Summary of Accomplishments

Our single-layer results show that the metal-dielectric SERS substrates we have created and studied actually show some very useful features in SERS sensing. Chief among these features is the adaptation of the metal nanoparticle structure of the substrates during biomolecule solution deposition. This adaptation acts to create a final structure that is very well-suited for electromagnetic field enhancement and SERS.

The multilayer results can be broken into two overlapping categories: samples with distinct layers in cross-sectional views and those with indistinct layers. We have found that multilayer SERS-active samples show improved performance over single-layer SERS films, due to image charge coupling and long-range effects in a bulk silver sublayer included below the typical SERS layer and spaced a few nanometers away from the semicontinuous SERS-active layer.

Our multilayer structures with indistinct layers are particularly interesting, with applications as exotic as superlensing and further improvements to biosensing. We have shown that these samples show promise as tunable near-field superlenses for the visible and near-IR wavelength ranges.

We have shown marked progress in the computation and simulation of 2D semicontinuous metal films and have demonstrated preliminary results on 3D random metal-dielectric composites. In our 2D film simulations, we have shown that it is possible to develop full-wave (finite-difference time domain) techniques based on real scanning electron microscope (SEM) images of a sample's metal nanostructure, and to approximate a sample's far-field and near-field responses using a number of averaged responses calculated from a pool of SEM images.

We have begun working on extending this technique to 3D composite structures in order to obtain more reliable predictions of a sample's response.

Significance

Plasmonic enhancement of optical fields provides novel solutions to problems in chemical sensing and subdiffraction imaging; both are important for national security. SERS can be an extremely powerful technique for the sensitive and selective detection of low-concentration analytes as commonly encountered in the detection of toxic industrial chemicals, chemical warfare agents, and biochemicals.

Refereed Communications

P. Nyga, V. P. Drachev, M. D. Thoreson, and V. M. Shalaev, "Mid-IR Plasmonics and Photomodification with Ag Films," *Applied Physics B*, vol. 93, pp. 59–68, October 2008.

PIV Investigation of the Richtmyer-Meshkov Instability after Reshock

130826
Year 1 of 3
Principal Investigator: B. B. Cipiti

Project Purpose

Inertial confinement fusion (ICF) is hampered by a hydrodynamic instability where any imperfection on the interface between the ablator and deuterium-tritium (DT) fuel is impulsively accelerated, resulting in mixing between the fuel and the ablator. The mixing can reduce the yield of the fuel and distort the converging shock wave so thermonuclear conditions are not reached. In ICF experiments, such as the Z Machine at Sandia and the National Ignition Facility (NIF) at Lawrence Livermore National Laboratory (LLNL), a thorough understanding of this instability is crucial to successful advancement of controlled nuclear fusion. This phenomenon is also important in stellar evolution behind a supernova and in the mixing of fuel and oxidizer in hypersonic vehicles. This instability, known as the Richtmyer-Meshkov instability, has been studied in shock tubes by observing the growth of the interface between a pair of gases.

This work will advance this research by using a membraneless interface accelerated by a strong shock and reshock at the University of Wisconsin-Madison Shock Tube Laboratory. Reshock represents an important physical condition because the shock wave will pass from the heavy gas into the light gas, analogous to a shock wave passing from the heavy ablator to the light DT fuel. After this heavy to light transversal, the perturbation reverses phase and continues to grow in amplitude with enhanced turbulent mixing. The work will utilize the Mie scattering of solid particles entrained in one of the gases to clearly distinguish the interface and to obtain density measurements from the spatial concentration of the particles. With this setup, a portion of the field will be focused in on and successive images will be used for particle image velocimetry (PIV) analysis. The velocity field from PIV will resolve the location of vortex cores and produce turbulence statistics.

Summary of Accomplishments

Work over this past year studied the Richtmyer-Meshkov instability of a shocked membraneless interface of a helium/argon mixture over pure argon into late times after reshock and rarefactions. The interface was initially accelerated by shock waves of strengths /M /= 1.3 and /M /= 1.9. Particle image velocimetry (PIV) was used in the University of Wisconsin Shock Tube Laboratory for the first time, producing velocity fields within the argon gas (seeded with Al_2O_3 particles). These velocity fields will allow for a more detailed comparison of the experiments to hydrodynamics codes. Another diagnostic was introduced using a pair of high speed cameras and continuous lasers to track the positions of the bubble and spike as they are accelerated by the shocks and rarefactions. This method acquired images at 100 kHz, producing hundreds of data points per experiments, where past methods yielded only one or two. This bubble/spike data gives a measure of mixing width over time and was found to closely match the mixing width predicted by two analytic bubble/spike growth models and a hydrodynamics simulation.

Experiments are also being performed on an interface of helium over sulfur hexafluoride. An analytic model was developed along with experiments to determine the frequency-wavelength response of the membraneless interface between the two gases. This allowed for better control of the interface in creating a standing wave initial condition.

The growth of the interface after acceleration by /M/ = 1.2 shock waves is being studied using PIV. Previous experiments have shown some differences between experiments and simulations at this high Atwood number (/A /= 0.95), so the velocity fields produced from the PIV data, particularly the distribution of vorticity deposited on the interface, will allow for a better comparison to the simulation results.

Significance

This experimental study will provide essential physical insight and relevant data for the Richtmyer-Meshkov instability, which is crucial to successful advancement of controlled nuclear fusion, a major DOE mission.

Relating Polymer Dynamics to Molecular Packing

130827
Year 1 of 3
Principal Investigator: D. B. Adolf

Project Purpose

A number of technologically important processes, from the design of bullet-proof vests to the fabrication of plastic films and bottles to the implosion dynamics of plastic-bonded high explosives (PBX), depend in a critical way on the dynamic response of polymeric materials when subjected to a strong impulse. Polymers constitute an especially difficult class of materials to describe due to the varied and complex rheological behaviors seen in their semicrystalline, crosslinked, or liquid states. Indeed, depending on the temperature and the time scale of observation, a single polymer can exhibit glassy, rubbery, or liquid-like dynamic response. Moreover, lethargic relaxation rates make the response not only dependent on the current state of the material (e.g., temperature, density, strain rate) but also on its past history.

Our goals are to understand the interplay between molecular packing, nano- and microrheology, and macroscopic response of bulk materials leading to a predictive capability for the dynamic response of polymers undergoing deformation. The work is in collaboration with New Mexico Institute of Mining and Technology (NM Tech).

Polymer relaxation rates depend on the average potential energy in equilibrated systems, and this relationship has led to constitutive equations capable of predicting polymer response. This work will address two important, outstanding questions: 1) is this relationship valid in unequilibrated systems (or more generally, how does unequilibrium molecular packing affect relaxation) and 2) how does the distribution of potential energy change as the glass transition is approached. The first question provides the foundation for constitutive equations based on potential energy that can be applied to practical, nonequilibrium behaviors such as creep and yield. The second question may offer insight into the divergence of these rates at the glass transition.

Summary of Accomplishments

The primary scientific accomplishment was the development and implementation of a simulation methodology for calculation of the dynamic heat capacity by directly modulating the temperature over a range of frequencies. Experimentally, the dynamic heat capacity is a probe of potential energy rearrangement; however it is difficult to interpret. Simulation studies of simple models permit clarification of features seen experimentally. The Sandia molecular dynamics code, LAMMPS (large-scale atomic/molecular massively parallel simulator), was modified to permit sinusoidal variation of temperature. Scripting procedures were developed for efficient implementation of the technique because it is necessary to run in a multiprocessor environment (each dynamic heat capacity calculation requires hundreds of simulations). Three systems have been analyzed. Two polymeric: freely-jointed chains, freely-rotating chains; and a spin system: the East-model. Variation of characteristic times and of the relaxation "shape"-parameter were tracked. The degree to which time-temperature superposition holds was assessed. Results were presented at the March meeting of the American Physical Society both in a talk (entitled "Cole-Davidson Glassy Dynamics in Simple Chain Models") and a poster (entitled "Specific Heat Spectroscopy of Simple Chain Models"). A paper has been written on the basic method and submitted to the *Journal of Chemical Physics* (entitled "Driven Simulations of the Dynamic Heat Capacity"). Finally, initial analysis of energy clustering has been performed.

Significance

This project benefits the DOE science and DOD and DHS national security missions by addressing the time/frequency rheological response of plastic-bonded high explosives. Although a small percentage of the whole, the polymer binder has a marked effect on properties. Understanding the relationship between the molecular structure of an elastomer and its complex modulus (viscoelastic behavior) would, for example, permit the chemical aging of PBX to be linked to the mechanical properties of the material.

Refereed Communications

J.R. Brown, P. Jenks, D. Turner, J.D. McCoy, and D.B. Adolf, "Driven Simulations of the Dynamic Heat Capacity," to be published in the *Journal of Chemical Physics*.

High-Fidelity Nuclear Energy System Optimization

131333
Year 1 of 3
Principal Investigator: S. B. Rodriguez

Project Purpose

Nuclear technology sustainability and nuclear waste management are the key challenges for nuclear energy technology on its path towards broad acceptance and deployment. Minimization or elimination of high level waste (HLW) inventories (transuranics [TRUs] and long-lived fission products [FP]) warrants expansion of nuclear energy as a sustainable energy source ensuring energy independence and security. This research effort is focused on the high-fidelity nuclear energy system optimization towards an environmentally benign sustainable and secure energy source. The analysis takes advantage of Generation IV reactor technologies and advanced fuel cycle options. This proposal defines a nuclear energy system as a configuration of nuclear reactors and corresponding fuel cycle components. The nuclear energy system performance is optimized under constraints of nuclear waste minimization and sustainability requirements targeting an environmentally benign energy source limit.

Recognizing the difficulties of spent nuclear fuel reprocessing and virtual technical impossibility to reprocess transmutation fuel compositions containing higher actinides after their first irradiation cycle, it is desirable to assess technical characteristics of a nuclear system that would achieve the highest incineration rate of spent nuclear fuel compositions as a result of one-cycle irradiation. This project will identify system needs and performance requirements leading to the actinide-free high-level waste and perform technology optimization studies towards an environmentally benign system.

The analysis focuses on Generation IV VHTRs (very high temperature reactors) operating in an OTTO (once-through-then-out) mode with 3D reloading schemes in combination with fast spectrum systems (VHTR-FR scenarios), specifically accounting for performance optimization and nuclear waste management including nuclear waste minimization. The analysis will be performed for technologically feasible configurations with full accounting for the core physics in the 3D whole-core exact-geometry fuel cycle analysis using hybrid Monte Carlo methods. The modeling approach will be validated in experiment-to-code benchmark studies. The work is in collaboration with Texas A&M University.

Summary of Accomplishments

Year 1 Accomplishments (FY 2009)

- On Task 1.1. The conceptual fuel cycle system has been defined. Consistent with the defined fuel cycle, advanced nuclear energy system parameterization has been completed including basis high-fidelity pressurized water reactor (PWR) and VHTR models (whole-core exact geometry), and external-source-driven system models for final stage cleanup/sterilization assuming the process taking place either immediately after VHTR or with some post-processing targeting energy recovery from used fuel and fuel re-use. Performance metrics are identified for the entire energy system.
- On Task 1.2. PWR and VHTR physics models have been validated.
- On Task 1.3.1. Preliminary simulations have been performed to identify potential strategies for system optimization. Code system integration will be completed during summer of FY 2009 with the full implementation in the fall of FY 2010 for multiobjective high-fidelity optimization planned for the rest of FY 2010.

- On Task 1.4.1 (part I, preliminary studies). During summer of FY 2009, preliminary high-fidelity nuclear energy system optimization evaluations will be performed investigating scenarios leading to environmentally benign sustainable and secure energy sources.

Significance

This research is relevant to a variety of research programs led by DOE and Sandia, in particular, in the areas of modeling and systems analysis targeting high-fidelity analysis of nuclear systems, capturing their physics features and environmentally benign energy technologies for secure energy future. The focus on nuclear fuel cycles directly addresses the grand challenge of nuclear technology — nuclear waste management.

Water Behavior in Nanoporous Materials

135456
Year 1 of 1
Principal Investigator: R. T. Cygan

Project Purpose

The natural water cycle of the Earth includes the oceans, lakes, rivers, glaciers, groundwaters, and the atmosphere. In addition, a hidden, but still significant, amount of water is found in the minerals of the Earth's upper crust. Clay and zeolite minerals, found in sedimentary deposits and soils, include an extensive amount of molecular water that fills nanopores and nanochannels. Clay and zeolite phases are complex minerals that are characterized by the coordination of aluminum and silicon tetrahedra (for zeolites) or a combination of similar tetrahedra with aluminum octahedra (for clays). The ratio of aluminum to silicon, or the extent of similar heterovalent substitutions, will determine the negative charge that resides on the framework structure of these materials. When needed, cations provide charge compensation by occupying the nanopores defined by the topology of the zeolite framework and interlayer of the clay structure. In both cases, water molecules are ubiquitous and occupy the nanoporous structure, and exist with and without associated cations.

These materials provide a structurally controlled environment for the analysis of molecular water behavior in a confined configuration. Framework-water and water-water interactions (along with any interactions with cations) ultimately control many natural and technological processes. These fundamental processes are critical to improving modern technologies, such as the removal of contaminants in conventional water treatment processing. Cation exchangers, desalination membranes, gas purification, and catalysts are a few examples of how both zeolites and clays contribute to modern technologies. We will examine the behavior of nanoporous water in two unique materials using molecular simulation and inelastic neutron scattering. Palygorskite and sepiolite are naturally occurring clay minerals that have zeolite-like nanopores. Most important is that these phases provide pores that both strongly and weakly interface with the water molecules of the pore.

Summary of Accomplishments

We used inelastic neutron scattering, density functional theory, ab initio molecular dynamics, and classical molecular dynamics to examine the behavior of nanoconfined water in palygorskite and sepiolite. These complementary methods provide a strong basis to illustrate and correlate the significant differences observed in the spectroscopic signatures of water in two unique clay minerals. Distortions of silicate tetrahedra in the smaller-pore palygorskite exhibit a limited number of hydrogen bonds having relatively short bond lengths. In contrast, without the distorted silicate tetrahedra, an increased number of hydrogen bonds are observed in the larger-pore sepiolite with corresponding longer bond distances. Because there is more hydrogen bonding at the pore interface in sepiolite than in palygorskite, we expect librational modes to have higher overall frequencies (i.e., more restricted rotational motions); experimental neutron scattering data clearly illustrates this shift in spectroscopic signatures. Distortions of the silicate tetrahedra in these minerals effectively disrupts hydrogen bonding patterns at the silicate-water interface, and this has a greater impact on the dynamical behavior of nanoconfined water than the actual size of the pore or the presence of coordinatively unsaturated magnesium edge sites.

Significance

Our fundamental approach has applications to DOE Science and other Sandia missions. Confined and interfacial water controls corrosion, stability, friction, and transport response of materials critical to Sandia's nuclear mission and other defense applications; water determines component reliability and stockpile survivability. This project has relevance to Office of Science and Basic Energy Sciences (BES) goals, in particular to the emerging BES initiative in water treatment technologies.

Refereed Communications

N.W. Ockwig, J.A. Greathouse, J.S. Durkin, R.T. Cygan, L.L. Daemen, and T.M. Nenoff, “Nanoconfined Water in Magnesium-Rich 2:1 Phyllosilicates,” *Journal of the American Chemical Society*, vol. 131, pp. 8155-8162, 2009.

Ordered Nanoporous Materials for Plasmonic Devices and Sensors

135459
Year 1 of 1
Principal Investigator: M. D. Allendorf

Project Purpose

The objective of this project is to evaluate the potential of ordered nanoporous materials known as metal-organic frameworks (MOFs) to create devices and sensors whose properties are determined by the dimensions of the MOF lattice. Our hypothesis is that because of the very short (tens of angstroms) distances between pores within the unit cell of these materials, enhanced electro-optical properties will be obtained. Specifically, we expect tunneling rates through MOFs will be greatly enhanced if a few unit cells can be deposited in a bridging fashion across patterned electrodes. In addition, our preliminary work shows that, unexpectedly, surface-enhanced Raman (SERS) is observed when MOF films are infiltrated with silver. Transmission electron microscopy (TEM) images show that the average size of the silver particles thus formed is smaller than the 5 nm typically thought be the lower limit for SERS to occur. These experiments also reveal what appear to be silver nanowires passing through the nanopores of the lattice. Since nanoporous MOFs can have extremely high surface areas (more than a factor of 5 higher than the highest surface area zeolites) and have tailorable pore chemistry, the potential exists to create sensors that respond rapidly and specifically to analytes adsorbed within the pores. Alternatively, the dielectric (or potentially semiconducting) MOF could be used as the matrix for assembling highly ordered hybrid structures containing nanowires embedded in the lattice. Interesting electrical properties may result if a paramagnetic MOF is used. Finally, MOFs could be used as removable templates, which could be dissolved chemically in the presence of protecting groups such as surfactants to allow the creation of either nanoparticles or nanowires with extremely narrow size distributions determined by the size of the MOF nanopores.

Summary of Accomplishments

An investigation of two strategies for imparting electrical conductivity and/or plasmonic enhancement of Raman signals was completed in this one-year project. First, we completed a systematic investigation of silver nanocluster formation within metal organic frameworks (MOFs) using three representative MOF templates. The as-synthesized clusters have dimensions ~ 1 nm, with a significant fraction existing as Ag_3 clusters. Importantly, we show conclusively that rapid TEM-induced MOF degradation leads to agglomeration, explaining prior reports of particles larger than MOF pores. These results solve an important riddle concerning MOF-based templates and suggest that heterostructures composed of highly uniform arrays of nanoparticles within MOFs are feasible. In some cases nanowires appeared to form. Electrical measurements indicate no increased conductivity, however. Raman spectra of the Ag-MOF compared with the uninfiltrated MOFs exhibit some enhancement of the signal. However, the mechanism of this enhancement was not determined; the Ag particles are too small to produce plasmonic enhancement. One possibility is that interactions of the Ag clusters with the framework perturb the infrared spectrum.

A second, more preliminary, study was conducted in collaboration with the University of California, Berkeley to incorporate fulleride (K_3C_{60}) guest molecules within MOF pores. Several different MOFs with a range of pore sizes were selected to create van der Waals driving forces for infiltration. However, soaking crystals of these in solutions of fulleride dissolved in either toluene or THF did not result in any clear infiltration. This may be due to residual guest solvent blocking the pores, or to clogging by fulleride and/or solvent in the case of 1D channels. Although this limited investigation did not succeed in creating conducting MOFs, the new synthetic approaches tested provide a solid foundation for future efforts to use MOFs to construct nanoscale heterostructures.

Significance

This work supports DOE's goal of scientific discovery and innovation to support key missions. Hybrid metal organic frameworks (MOFs) infiltrated with metal nanowires could be a precursor to defect-free solar-cell materials and quantum-computing devices. Silver nanodots within MOFs could serve as ultrasensitive gas detectors, a technology with homeland security, stockpile stewardship, and DOD uses. Enhanced gas sorption materials may also result, which have application to noble-gas isotope detection for nuclear nonproliferation. The specific results reported here confirm for the first time that the nanoscale pores defined by the crystalline structure of MOFs and related materials can function a template for nanoparticles, a fact that was in doubt prior to this work because of artifacts created during electron microscopic examination. This result opens the way to much more extensive use of MOF templates and for the first time, creates a template with both clearly defined dimensions and a chemically tunable environment to promote stabilization and confinement of particles. This development has implications not only for the applications described above, but also for catalysis, biological imaging using nanoparticles, and investigations of the toxicology of nanoparticles.

Refereed Communications

R.J.T. Houk, B.W. Jacobs, F. El Gabaly, N.N. Chang, A.A. Talin, D.D. Graham, S.D. House, I.M. Robertson, and M.D. Allendorf, "Silver Cluster Formation, Dynamics, and Chemistry in Metal-Organic Frameworks," to be published in *Nano Letters*.

Low Permittivity and High Tunability Composite (Ba,Sr)TiO_3 - Spinel Thin Films Utilizing Nanoscale Epitaxial Self-assembly

135568
Year 1 of 1
Principal Investigator: C. A. Apblett

Project Purpose

Future advanced radar and communication systems require the ability to quickly and efficiently change frequency for secure communications, imaging, and surveillance. Recently, tunable devices based upon ferroelectric thin films have been demonstrated with superior quality factors and switching speeds. Ultimately, these materials utilize device geometries requiring large tuning voltages. The high-voltage requirement may limit the application of these devices, particularly in applications where weight and space are limitations. Low-voltage tuning is possible utilizing an alternative geometry, however the high-permittivity of ferroelectric films makes impedance matching difficult. To circumvent this, we propose the development of nanoscale self-assembled composites of a tunable ferroelectric and a low permittivity insulator. In doing so, we will be able to develop tunable RF (radio frequency) and microwave devices that utilize low-voltage tuning while maintaining high quality factors and switching speeds. The ability to deposit self-assembled composites without multiple patterning steps will present a significant advantage in manufacturability and device reliability.

Summary of Accomplishments

Textured nanocomposite thin films were investigated in an effort to develop high dielectric tunability low permittivity materials for microwave applications. Methods to deposit these self-assembled $Ba_{0.5}Sr0_{.5}TiO_3$-$MgAl_2O_4$ (BST-MAO) textured nanocomposite thin films were investigated. Films have been deposited on (001)p-oriented $LaAlO_3$ single crystals and (001)-oriented biaxially textured nickel-tungsten tapes via chemical solution deposition. Films deposited on single-crystalline $LaAlO_3$ substrates possess greater than 98% 001 BST orientation. Films deposited on nickel substrates have orientation values ranging from 60% to ~ 90%. Field dependent dielectric measurements reveal a 75% reduction in capacitance with minimal change in tunability in a 50 mole percent composite film.

Significance

This effort supports multiple aspects of Sandia's nuclear security mission by enabling greater functionality in RF and microwave systems for applications such as fuzing radars, imaging and surveillance radars, and secure multiband communications. This will translate into improved communications security, jamming resistance, and overall system performance when compared to systems using alternate technologies to realize tuning. In turn, this increases the probability of success for the mission relying on the RF systems.

Nanostructured Material for Advanced Energy Storage

135569
Year 1 of 3
Principal Investigator: N. S. Bell

Project Purpose

Advances in energy storage technology are critical to the needs of the world as developing nations raise their standard of living, and energy consumption. In collaboration with the University of Florida we proposed to develop electrodes and electrolytic membranes for electric energy storage devices such as lithium-ion batteries and supercapacitors. The proposed devices will consist of electrospun ceramic and polymer based nanofibers in core or core-shell configuration. Electrospinning of ceramics is a new nanofabrication technique that has not been widely applied to electrode manufacturing. It promises large flexibility in chemistry, high level of nanostructure control, and very good manufacturing economics. We propose to develop polymer or ceramic nanofiber based membranes that are thinner, lighter, more conductive for ions, and more temperature stable than those currently in use.

Ceramic materials are of special importance, since they are able to endure higher temperatures and offer larger variety in electrical, optical, magnetic, ferroelectric, thermal and other properties than polymers. The confinement of these properties into one dimension challenges science and requires advancements in characterization techniques, modeling of properties, and opens novel applications of “old” materials. Nanostructuring of the electrode materials allows for using materials that have previously been discounted (e.g. Si, Ge, SnO_2, metal phosphates, MnO_2 or V_2O_5) either for having too slow kinetics or for degrading under repeated cycling (e.g., too large volume change). Characterization of these novel materials is performed using x-ray diffraction (XRD), scanning electron microscopy (SEM) and in-situ cyclic polarization in conjunction with atomic force microscopy (AFM), scanning tunneling microscopy (STM) and ex-situ (micro-Raman spectroscopy, Auger electron spectroscopy, and transmission electron microscopy [TEM]) techniques. A correlation between the structural, morphological, electronic and chemical properties of these interfaces and knowledge of how they evolve as a function of potential will allow identification of the mechanisms governing electrode performance and degradation.

Summary of Accomplishments

Electrospinning is usually a facile processing step that can potentially produce large quantities of fibers with diameters of tens of nanometers to micrometers. However, Teflon AF is difficult to electrospin due to its low dielectric constant and the low dielectric constant of the Fluoroinert FC-75 (~1.74) that Teflon AF is dissolved in when purchased. Two approaches were taken in producing Teflon AF fibers: electrospinning Teflon AF in Novec Engineered Fluids and core-shell electrospinning. We prepared 5 wt% Teflon AF 1600 solutions in the Novec fluids and electrospun them successfully. However, these fibers were tens of microns in diameter, and narrower fiber diameters were desired.

In core-shell electrospinning, concentric needles are used to deliver two solutions. An electrospinnable polymer solution is used as the core, and once an electric field is applied, this polymer solution drags the fluid from the outer needle to form the fiber’s shell. Aqueous solutions with varying concentrations of polyvinylpyrrolidone (PVP) and rod shaped alumina particles were attempted, but none were successfully electrospun individually or with a Teflon AF shell. An aqueous solgel/PVP solution was electrospun as the core material with as purchased Teflon AF 1600 and 2400 solutions as the shell. The Teflon AF 1600 solutions produced more uniformly covered fibers. However, the diameters of these fibers were still in the micron range.

In an effort to reduce the dimensions of the electrospun fiber, polyacrylonitrile (PAN) core solutions in dimethylformamide (DMF) were investigated. We were able to electrospin DMF solutions as the core with Teflon AF as a shell. The diameters of the PAN core and Teflon AF 1600 shell fibers were an order of magnitude smaller than what was accomplished with the other cores attempted and a previous report.

Significance

The project is relevant to the need for improved energy storage and batteries for a variety of national security missions from sensors to efficient alternate energy sources. Many application require standalone sensors that must function for long periods without maintenance. Wind and photovoltaic power sources also require energy storage. Improved lithium and other batteries and supercapacitors that may result from this project can help to meet this need.

Hazard Analysis and Visualization of Dynamic Complex Systems

135790
Year 1 of 3
Principal Investigator: K. V. Diegert

Project Purpose

Safety is often assessed after a design is created, thus reducing the possibility of designing safety into the system from the earliest stages of the development process and using safety to drive the design decisions as they are being made. Massachusetts Institute of Technology (MIT) has created a new model of accident causation (STAMP or systems-theoretic accident modeling and processes) that extends the current "chain-of-events" model to incorporate more types of accident causes, including accidents caused by software "misbehavior." A new, more powerful hazard analysis technique, called STPA (STAMP-based hazard analysis) has been devised with the new accident causation model as its foundation. STPA is based on the concept of controlling hazards during the design process rather than attempting to eliminate component failures (which are only one cause of hazards). STPA provides a powerful new way of thinking about accident prevention, but it has only been applied in a limited number of applications and has been used only in an ad hoc fashion. Additional research is necessary to define a methodology for its use that accommodates uncertainty and dynamics in complex systems. Research is also needed to investigate ways of visualizing and illustrating the analysis in a human-readable format to assist in performing the hazard analysis, to facilitate future system changes, and to minimize human error.

Overall Objectives:

1. Develop a framework and structured methodology for the application of STPA to address risks associated with uncertainty and dynamics in complex systems.
2. Investigate alternative visualizations of the analysis and its results in a human readable format.
3. Apply this framework to an existing application and evaluate its effectiveness in terms of the identification and mitigation of control flaws.

Summary of Accomplishments

The following methods were reviewed: a) fault tree analysis (FTA); b) AcciMap models; c) probabilistic risk assessment; d) event tree analysis; e) hazard and operability study (HAZOP); f) failure modes and effects analysis (FMEA); g) failure mode, effects, and criticality analysis (FMECA); and h) hazard analysis with critical control points (HACCP). These methods were examined to identify strengths and weaknesses compared to MIT's STPA.

STPA applications reviewed include: NASA Outer Planets Explorer (OPE), FAA Traffic Collision Avoidance System (TCAS), and others. In systems that may be complex in terms of software interactions, human interactions, or other emergent behavior, STPA's application of control theory is able to address weaknesses found in many of these methods.

A comparison of the methods revealed that STPA works better in the design phase, not only by identifying controls but also by incorporating system failures from interactions — as compared with component failures only. A short list of desirable attributes would include the following: a) ability to help identify hazards, not just analyze them; b) ability to handle system safety constraints distributed among several components; and c) ability to address system failures, not just component failures.

Significance

This work will develop hazard analysis methodology that could impact the quantification of nuclear safety risks, and other high consequence applications.

Simulation of Ion Beam Induced Current in Radiation Detectors and Microelectronic Devices

135791
Year 1 of 1
Principal Investigator: G. Vizkelethy

Project Purpose

Ionizing radiation is known to cause single event effects (SEE) in a variety of electronic devices. The mechanism that leads to these SEEs is current induced by the radiation in these devices. While this phenomenon is detrimental in integrated circuits (ICs), this is the basic mechanism behind the operation of semiconductor radiation detectors. To be able to predict SEEs in ICs and detector responses, we need to be able to simulate the radiation induced current as a function of time. There are some analytical models, which work for very simple detector configurations but fail for anything more complex. On the other end, TCAD programs can simulate this process in microelectronic devices, but these TCAD codes costs hundreds of thousands of dollars and they require huge computing resources. In addition, in certain cases, they fail to predict the correct behavior. We propose to create a simulation model based on the Gunn theorem. We intend to do it by developing a radiation-induced current module for the COMSOL Multiphysics® framework.

Summary of Accomplishments

We developed a method to apply the Gunn theorem in the COMSOL Multiphysics package to calculate ion beam induced current (IBIC) in semiconductor devices. As demonstration of the method we calculated the IBIC signal for various cases in a single Si detector, Si diode, and MOS (metal-oxide semiconductor) structure.

Significance

Sandia is charged with developing and qualifying microelectronic parts for space missions and for nuclear weapons. During development, it is important to understand the failure mechanism of the devices and how their radiation hardness can be improved. This project helps understand the basic processes that lead to the failure of devices due to radiation. In addition, the results of the project can contribute to a better understanding of the operation of radiation detectors and help improve them.

Processor Modeling for use in Large-Scale Systems Models

137299
Year 1 of 3
Principal Investigator: E. P. DeBenedictis

Project Purpose

The complexity of contemporary and future computer processors has changed the methodology and tools that have been traditionally used for performance and design space analysis. Multicore, multithreaded architectures cannot be designed solely using cycle-accurate simulation, which is commonly used as a design tool for next-generation processors. Cycle-accurate simulation is very accurate and robust, but prohibitively slow, with slowdowns on the order of 10^4. Therefore, new techniques and tools must be developed for the design and analysis of processors and processor systems.

Our collaborator, Presidential Early Career Award for Scientists and Engineers (PECASE) recipient Jeanine Cook of New Mexico State University (NMSU), has been developing a Monte Carlo-based processor modeling technique that can be used for performance analysis and prediction of contemporary and future processor architectures. These models abstract the execution pipeline into a stochastic model using both processor and application characteristics. To date, models of the IBM Cell BE (broadband engine), the Sun Niagara 1 and Niagara 2, and the Intel Itanium processors have been developed. This methodology is in its infancy and must be matured to enable the modeling of complex future architectures. Currently, these methods are only able to model in-order execution, single-threaded processors.

Summary of Accomplishments

We designed a method to model processors that support out-of-order execution. We developed some of the tools necessary to collect model parameters. We redesigned the existing model code for the Niagara 2 processor model to be object oriented, so that it is much more easily encapsulated and able to be integrated into a large-scale simulator such as Sandia Simulation Toolkit (SST). We wrote a paper on the Niagara 2 Monte Carlo processor model; this paper is currently in submission.

Significance

Microarchitecture simulation is important for the design of high performance computers. These types of computers will be used by advanced simulation and computing (ASC) and other DOE missions for nuclear weapons simulation, extreme scalability initiatives for scientific research, in manufacturing facilities like Microsystems and Engineering Sciences Applications (MESA) and the Center for Integrated Nanotechnologies (CINT). The tools developed will help evaluate designs that will become the basis of procurements, R&D contracts, and lab products.

The redesign of an existing model code has enabled us to integrate the Niagara 2 processor model into SST. This redesign will also be applied to the other existing processor models so that they can also be integrated into SST. Additionally, once complete, these new model implementations can be released for use by the community, to be used in performance prediction, algorithm development, and procurement.

The development of the out-of-order execution support for the Monte Carlo processor modeling method will be applied in this next year to the implementation of a processor model of the AMD Opteron, which is commonly used in Sandia supercomputers.

Application of Microeconomic Theory to Intelligence Remote Sensing

138274
Year 1 of 1
Principal Investigator: J. H. Ganter

Project Purpose

In previous research, we observed how remote sensor operators compare current situations with their mental models of pre-planned schedules and performance objectives. However, we also observed rapid transitions to ad-hoc modes where sensor costs and data benefits had not been weighed in advance. Exchanges of situational awareness information became negotiations between multiple sensor teams and end-users that improvised new coordinated actions on-the-fly. Predictions and feedback about suddenly varying needs, costs, and information value temporarily bypassed formal chains of command. What had appeared to be a closed, steady-state factory showed market-like, dynamical behaviors. This project will use microeconomic theory to re-examine observational data from cross-cultural, multisensor operations that include market-like supply-demand phenomena invisible to or inexplicable within current models like TCPED (task, collect, process, exploit, disseminate). We will develop new theory to explain why and how remote sensing allocates resources in distinctly different modes, which will clarify trade spaces and options for system engineering and management.

Summary of Accomplishments

We applied microeconomic theory to three case studies from the domain. We showed that principles of production, costs, markets, utility, and margin were applicable to phenomena in the domain and provide a novel perspective. We published a SAND report that has been distributed in the domain and is attracting interest from practitioners and policymakers.

Significance

National security sponsors grapple with not just up-front investments in sensors, but concerns about the back-end and downstream costs and benefits. Publication of evidence-based, holistic analyses could provide concepts and vocabulary to enrich these discussions and improve overall systems engineering and data utilization.

Parallel Digital Forensics Infrastructure

138301
Year 1 of 1
Principal Investigator: D. P. Duggan

Project Purpose

Digital forensics has become extremely difficult with data sets of one terabyte and larger. The only way to overcome the processing time of these large sets is to identify and develop new parallel algorithms for performing the analysis. To support algorithm research, a flexible base infrastructure is required. A candidate architecture for this base infrastructure was designed, instantiated, and tested by this project, in collaboration with New Mexico Institute of Mining and Technology.

Previous infrastructures have not been designed and built specifically for the development and testing of parallel algorithms. With the size of forensics data sets only expected to increase significantly, this type of infrastructure support is necessary for continued research in parallel digital forensics.

Summary of Accomplishments

The infrastructure implemented in this work provides a basis for continued work in the research, development, and testing of tools created to perform parallel digital forensics. The initial infrastructure is functional and was tested with some basic examples. A paper detailing its proposed use is being submitted for peer review to appropriate journals and the source will be available to researchers for their work in this area.

Significance

Information technology (IT) has infiltrated all aspects of DOE mission space and the ability to perform timely digital forensics on these systems is severely limited with today's algorithms. This work addressed the need to support development of parallel digital forensics research to improve the capabilities required as IT grows in size and complexity. Our ability to identify paths and methods of compromise into IT systems are critical as IT becomes an integral part of more of DOE's mission.

Correlation of Dimensional Measurement Uncertainties for Hybrid Measurement Systems

138635
Year 1 of 1
Principal Investigator: H. D. Tran

Project Purpose

In prior work, we demonstrated that a silicon micromachined artifact can calibrate tactile and vision-based dimensional metrology equipment with better accuracies and potentially lower costs. One remaining technical barrier is minimizing surface roughness of anisotropic etched <111> silicon planes over dimensions at the millimeter scale. Published research indicates that high concentrations of hydroxide combined with high temperatures and agitation of the etching solution lower the surface roughness, but this is typically over scales of fractions of a millimeter. The other factors which have not been considered are better alignment of the mask with the crystallographic planes of the stock silicon wafers, and longer etches to force alignment of the etched <111> planes to intrinsic crystallographic planes.

Our research will prove the ability to obtain low surface roughness over large spans in <111> anisotropic-etched silicon. This is a key technical barrier to adoption of anisotropic-etched calibration artifacts for vision-based dimensional metrology systems.

Summary of Accomplishments

We experimentally demonstrated fabrication of large areas of <111> planes with low surface roughness. We discovered that in anisotropic etching of large areas (order of mm or larger), undercutting of the masks can be a problem, as the mask material may break off, and deposit on the surface being etched. This leads to local surface roughness, which is not desired.

We have further refined fabrication processes.

We have shown that commercial coordinate measuring machines (CMMs) can obtain submicrometer repeatabilities in measuring these silicon dimensional standards. This establishes the path for commercial production and qualification of these dimensional standards.

Significance

The feasibility of using a silicon micromachined artifact for hybrid tactile and vision dimensional calibration has been established.

We have discovered methods to improve the surface roughness over millimeter scale areas on etched surfaces.

We have also identified potential private sector users for this technology. Adoption of the silicon micromachined dimensional standard by the private sector will lead to widespread availability commercially; this improves the ability of Sandia's suppliers to provide us with quality parts and components.

Success of this project will benefit both the economical and reliable manufacture of stockpile components, and also advance scientific discovery.

Electrochemical Solution Growth of Indium Nitride

138637
Year 1 of 1
Principal Investigator: K. E. Waldrip

Project Purpose

Indium nitride (InN) is a new, narrow bandgap semiconductor material with applications in photovoltaics, terahertz emitters, solid-state lighting, high speed power electronics, chem-bio sensing, and superconductivity, to name a few. Advancements in InN devices are hindered by the lack of a suitable substrate; native substrates would be the most ideal. However, InN cannot be grown in bulk by traditional methods; it decomposes into InN and N_2 at relatively low temperature at atmospheric pressure (about 500 °C) and requires extreme nitrogen overpressures (>200,000 atmospheres) near its melting point of 1700 °C.

The electrochemical solution growth (ESG) is an innovative, Sandia-developed atmospheric pressure approach to bulk growth that is particularly well-suited for incongruently melting materials. It relies on a novel synthesis pathway involving a unique electrochemical reduction reaction of nitrogen gas, combined with a unique combination of previously proven concepts in the fields of electrochemistry and crystal growth. It shows tremendous promise, and gallium nitride growth has been demonstrated numerous times. The work performed will focus on achieving growth of InN by autonucleation in the bulk solution first, and later on a crystalline template. If successful, future work will optimize crystal quality and volume.

The development of ESG is a high-risk endeavor that combines both developed and undeveloped concepts in a unique way. The impact of the ability to synthesize bulk InN economically will be far-reaching in applications of this material, and in the many other materials that ESG could enable that are currently unattainable. If successful, ESG could enable new applications in the areas of crystal growth, energy efficiency, and energy storage.

Summary of Accomplishments

This project allowed for a few key experiments, where we gained some understanding of the behavior of the group III cations (indium and the closely related gallium) in the molten salts by performing some electrochemical experiments. We performed one attempt at growth of InN; the characterization is in process by collaborators outside Sandia.

Significance

Economical InN could play a critical role in implementing efficient photovoltaics. ESG is a cross-cutting technology that can benefit the energy security mission through producing materials with advanced functionality that cannot be grown by other methods. ESG offers the potential to deliver economical, high-quality substrates and produce a new field of materials research.

Polymer/Inorganic Superhydrophobic Surfaces

138638
Year 1 of 1
Principal Investigator: C. J. Brinker

Project Purpose

Several potential work for others (WFO) sponsors have expressed an interest in Sandia's R&D100 Award winning hydrophobic coating for applications to visual augmentation systems and other areas. It would also have wider applications across the DOD. However, the durability of the coating has not been developed to the point where technology development can be supported by these sponsors. This LDRD project is to investigate improvements in durability. We propose to develop a coating capable of producing a thin superhydrophobic coating that is optically clear, but is more tribologically robust than current techniques. Other methods for superhydrophobic coatings with improved environmental resistance rely on high-temperature steps and harsh chemical treatments, making the coating applicable only to surfaces that can withstand these processes, and with significant loss in transparency of the coating. In contrast, our process relies on sol-gel and involves room temperature and exposure to alcohols, and produces an optical quality coating that has contact angles exceeding 170 ºC. However, our methods of achieving superhydrophobic surfaces involve a nanostructured surface with chemical treatments, and these geometries make the coatings very fragile. Aging of these surfaces is largely unstudied, but continued exposure to extreme environments may produce coarsening of the nanostructure and loss of superhydrophobicity over time.

We will study the effect of adding polymeric based agents which share moieties with the silica backbone and should therefore provide good interfacial strength. The polymer additives will increase the chemical stability of the coating, by changing the environmentally exposed surface to one with less chemical reactivity. The combination should allow for retention of superhydrophobicity and transparency while increasing the wear resistance of the coating.

Summary of Accomplishments

A broad array of operations was investigated to improve the properties of superhydrophobic aerogel coatings. Strategies were applied to both tetraethylorthosilicate (TEOS) and tetramethylorthosilicate (TMOS) derived aerogels. Both types of aerogel were found to respond similarly to attempts at improving the material properties despite processing differences. As well as building on previous work, involving the addition of polymers to fully processed coating solutions, a variety of new polymers were investigated for post-processing addition. Quartz crystal microbalance (QCM) measurements made on these coatings found that the effect of increasing polymer content was twofold. Shear modulus increased and contact angle decreased with increasing polymethylmethacrylate (PMMA) concentrations. Examining different molecular weights of polymer showed that lower molecular weight polymers provide the best combination of durability enhancement and optical clarity. Better understanding post-processing polymer addition could be improved by visualizing the material using scanning electron microscopy (SEM) or other microscopy techniques. Polymers other than methacrylates which posses a better combination of hydrophobicity and optical clarity could also be investigated. Pre-gelation strategies were also employed to modify the material. Techniques include both horn and bath sonication, and the successful incorporation of vinyl polymer groups into the silica aerogel backbone. Horn sonication was found to moderately improve the durability of the material. Incorporation of vinyl groups was used as a means for adding functionality to the silica backbone. The functionality could be utilized for improving durability by means of chemically grafting polymer to the silica backbone. Functionality could also be exploited for other novel effects and is an area of interest for further research.

Significance

This project ties to our scientific discovery, energy efficiency and defense missions. Improved durability will increase the range of applications suitable for this easily coated transparent superhydrophobic material. Applications include coatings for windshields, optical windows, and other coatings that can rapidly shed water. Coatings that prevent wetting and salt buildup allow operation in highly corrosive or aggressive environments.

Refereed Communications

C.J. Homer, X. Jiang, T.L. Ward, C.J. Brinker, and J.P. Reid, "Measurements and Simulations of the Near-Surface Composition of Evaporating Ethanol-Water Droplets," *Physical Chemistry Chemical Physics*, vol. 11, pp. 7780-7791, September 2009.

An Investigation of the use of Ku-Band SAR Technology for Security and Emergency Response — Methods and Phenomenology

139707
Year 1 of 1
Principal Investigator: K. R. Czuchlewski

Project Purpose

Airborne synthetic aperture radar (SAR) imaging systems provide maps for situational awareness and reconnaissance of varied targets, especially where access is hazardous, or view is obstructed by smoke, clouds, or dust. SAR systems developed by Sandia for the DOE and various DOD customers are small in size, have reliable autonomy and are flexible. However, the civilian applications for SAR in the United States have been limited in scope. To address a pressing need of civilian emergency response organizations, this project investigates the utility of SAR imaging systems for responding to the impact of natural and manmade hazards. Sandia SAR images are 4-inch resolution at Ku-band, a very high resolution that facilitates terrain mapping and the identification of select manmade targets. Coherent change detection (CCD), a SAR image derived product, offers the capability for detecting changes between imaging passes at subradar wavelength resolution. This technique has been proven to identify subtle alteration of the landscape related to human activity, such as footsteps and irrigation. To better understand SAR emergency response applications, we will quantify radar phenomenology in imagery and CCD from various real-time airborne SAR imaging systems. We expect that a detailed analysis of these image products over damaged or altered structures and environments will enhance timely post-disaster situational awareness and assessment. Furthermore, we will evaluate the utility of CCD for identification of survivors and the monitoring of activity around high-value assets.

Summary of Accomplishments

We surveyed the current Sandia SAR imagery to identify the utility of Ku-band SAR for identifying certain key disaster-induced phenomena in an urban environment. We determined that, due to a combination of fine resolution and complex radar and scattering phenomenology, Ku-band is the optimal SAR frequency for identifying damaged roads, infrastructure and buildings in urban environments. In addition, we determined that cm-scale wavelength facilitates detection of subtle survivor activity in static imagery and CCDs.

Significance

Sandia's SAR group supports national security work for DOD and DOE. This work will extend the application suite of Sandia SAR imaging systems and analysis capabilities, especially for domestic security organizations that prepare for and respond to the impacts of natural hazards and provide security to high-value assets.

Development of a System for Identification of Data

139708
Year 1 of 2
Principal Investigator: J. Trent

Project Purpose

Loss of data confidentiality is a fundamental risk to any national security program. We have investigated new data confidentiality approaches that allow us to detect and investigate data leaks.

Electronic files can be copied infinitely and instantaneously. Electronic logs can be easily modified. Even if we are lucky enough to detect that the confidentiality of our electronic information has been compromised—a skilled attacker leaves no trace—finding the source of the compromise is all but impossible.

The purpose of this work is to create a comprehensive system for detecting and investigating information compromise. The goal of this system would be to address the complete document lifecycle, from creation to destruction. We have also investigated methods for tracking marked documents through Sandia's network. This work is being done in order to help protect sensitive information from digital theft.

Summary of Accomplishments

We have studied the types of document most commonly found on Sandia's networks and which are used to store and transmit the most critical information Sandia controls. We have analyzed the prototype system developed during FY 2008 and have identified what technical challenges still remain in implementing a system to detect data leakage. In order to address these technical challenges during FY 2010 we have designed a new approach based on the input of several subject matter experts.

Significance

The development of new techniques to protect and track sensitive data will benefit Sandia, DOE, and the greater government community while advancing the skills and state of the art at Sandia. If successful, this work will provide the larger government complex with a unique capability to protect classified information and investigate system compromise.

Scalable Circuits to Enable Performance Evaluation of High Performance Computing Algorithms

140159
Year 1 of 1
Principal Investigator: E. R. Keiter

Project Purpose

The Xyce parallel circuit simulator has demonstrated good parallel performance for certain subclasses of integrated circuits on traditional message-passing based supercomputers. However, there remains a rich and diverse set of unexplored options for parallel circuit simulation. Parallel simulation performance is determined by many factors: hardware platform, run-time environment, languages and compilers used, algorithm choice and implementation, and more.

Furthermore, emerging architectures, such as those based on graphical processing units (GPUs), as well as newer types of circuit analysis such as harmonic balance, remain unaddressed. Additionally there is no "characteristic circuit" meaning that no single algorithm can suffice for all circuit applications or for all types of circuit analysis.

For this proposal, we propose the development of a mini-application for parallel circuit simulation (a miniXyce), to enable algorithmic research and development for the next generation of computer platforms. The use of mini-applications (small self-contained proxies for real applications) has been demonstrated to be an excellent approach for rapidly exploring the parameter space. By adapting this approach for Xyce, we anticipate being able to rapidly explore new ideas, and weight algorithmic tradeoffs, much more quickly than with traditional application development. Furthermore the development of such an application will enable a much richer interaction between numerical algorithm researchers and application developers, as the source code will be kept to a manageable (small) size.

The development of such a mini-application (a "miniXyce") will not be without challenges. The goal of this type of application development is to find minimal, "characteristic" problems, while simple in some respects, sophisticated enough to retain the challenges of the original applications. As noted before, there is no single "characteristic" circuit problem, so the identification of key problem classes will be part of this work.

Summary of Accomplishments

Our long-term goal is to create a mini-application for prototyping parallel circuit algorithms, called MiniXyce. In the short-term, the focus of this work is to investigate alternative parallel algorithms, and how they can improve the performance of the device evaluation phase of the Xyce circuit simulator. Xyce, the original application, is already parallelized using a message-passing programming paradigm (MPI). Each individual device evaluation is carried out serially on each processor or compute node and then loaded into a globally distributed matrix. This is an effective strategy that allows Xyce to scale well across multiple processors. However, the compute nodes of modern parallel computers often contain multiple CPUs per compute node, and message-passing may not be the best approach for this type of architecture. For this investigation, we examined a more fine-grained parallelism based on threading. We applied the threading approach to a variety of circuits and conducted a performance study on 1,2,4,8, and 16 cores. The performance results indicate that, in all but one circuit, using multithreading in the device loads results in a speedup of the load time. Furthermore, in most cases the speedup increases with the number of cores. Even when the linear solver time dominates the cost of the simulation (which is the case for larger circuits), the total simulation time is still decreased by 30 percent. We conclude from the performance study that, if only threading parallelism is used (without message-passing), a significant speedup can be expected with Xyce. While mixed parallelism, using a combination of threading and message-passing was not explored here, it is reasonable to assume that the coarser-grained device distribution (via MPI) will be enhanced by the finer-grained device evaluation parallelism (via threading). We plan to explore this issue in greater detail with the mini-application, miniXyce.

Significance

Xyce is a capability that is used for nuclear weapons qualification of circuits in hostile environments. Xyce is also used for cognitive science neurological simulation at Sandia. As new parallel hardware architectures are developed, Xyce will require new algorithms and data structures to be computationally efficient and competitive.

Optical Nanoscopy Using Stimulated Emission Depletion (STED)

140642
Year 1 of 1
Principal Investigator: I. Brener

Project Purpose

There is great need in the microelectronics community for optical imaging techniques that achieve deep subwavelength imaging (recently termed optical nanoscopies). We would like to take the first steps to develop one particular technique called stimulated emission depletion (STED) microscopy, which has shown spatial resolutions of 20 to 30 nm. This technique will be used to image single optical nanoparticles smaller than 50 nm and their interaction with nanoscale metallic structures used for energy transfer.

This technique requires the use of two picosecond lasers: one laser is used for excitation of the fluorophores whereas the other is used for driving these fluorophores to the ground state through stimulated emission. The latter beam is also manipulated in order to produce a “doughnut” mode, that is, an optical mode with a dark region in the center. The combination of the nonlinear behavior of these processes and the spatial mode lead to a drastic reduction in spatial resolution below the Abbe limit.

Summary of Accomplishments

A STED system with a wavelength of 780 nm as the depletion beam was built. This beam is derived from a mode-locked Ti-sapphire laser and it is the most economical and fast way to show a proof of concept. We achieved enough supercontinuum (with wavelengths as short as 600 nm) in a short piece of photonic crystal fiber. Follow-on work will be needed to address the optical alignment (spatial and temporal overlap of all the beams, confirmation of a doughnut mode using a vortex phase mask) and a final STED demonstration.

Significance

Currently, there is no far-field optical nanoscopy tool at Sandia. We have several nanophotonics projects where we study energy transfer between fluorophores and plasmonic nanoparticles for energy applications and nanoscience research. This capability will benefit our DOE scientific discovery and energy security missions by providing a unique tool to image nanoparticles, cellular processes, etc. with a spatial resolution of tens of nanometers.

Responsive Nanocomposites

141076
**Year 1 of 4*
Principal Investigator: T. J. Boyle

Project Purpose

The creation of environmentally responsive nanocomposites will result in materials which are much more robust and stable. To produce such nanocomposites requires that the surface interaction between functionalized nanoparticles and the matrix be better understood and controlled. This project will attack this mission related problem of interest by invoking a multidisciplinary approach based on predictive computational models and experimental verification using a series of well-controlled complex nanomaterials dispersed in a variety of elastomeric or soft materials. We will determine the proper chemical species and length of the functional groups and the required surface coverage density of morphologically and compositionally varied nanomaterials dispersed in these matrices. Our initial response stimuli will focus on temperature or hydration since these are two major areas of interest to Sandia's missions as well as our industrial collaborators. The project will be initiated by building on Sandia's expertise in the synthesis of size- and shape-controlled nanomaterials of varied compositions and functionalizations, nanocomposite self-assembly, and computational modeling of nanocomposites aided by collaborations with Columbia University, Cornell University, the University of Florida (U Florida), Harvard University, the University of New Mexico (UNM), Northwestern University, the University of Texas, Austin (UT-Austin), the University of Washington and industrial partners with expertise in nanocomposite testing. Together a model for nanocomposite mixtures that possess "active" or "applied" responses to temperature or hydration environmental changes will be developed.

Summary of Accomplishments

Milestone 1. Initiate academic research contracts.

Contracts were submitted that will begin in the next fiscal year to U Florida, UT-Austin, UNM, Cornell, and Columbia for student support.

Milestone 2. Synthesize nanomaterials and initiate computational calculations.

Molecular dynamics simulations of amorphous silica nanoparticles coated with $Si(OH)_3(CH_2)_9CH_3$ oligomer chains in decane and squalene are underway. In decane the coating is uniformly distributed while in squalene the coating is much less uniform.

We designed a series of synthetic routes to create new copper nanostructures using soft templating strategies.

Using established literature preparative routes, we attempted to generate a series of nanojacks with an emphasis on MnO and FeO materials.

We prepared graphene oxide and reduced graphene oxide both as solid aggregates and dispersed as stable colloidal solution to functionalize the graphene oxide with chemical handles.

We started the synthesis of several magnetic nanoparticle systems. These are based on the synthesis of $M_xCo_{3-x}O_4$ spinels (where M = Co, Ni, Mn, Fe, Cu).

*This 36-month project will span four fiscal years

We initiated atomic force microscopy (AFM) studies of hydrogel cantilevers submerged in water as a potential means of characterizing the responsive hydrogel pillared surfaces to be prepared at Harvard.

We prepared core shell plasmonic nanoparticles, anticipated to be thermally and optically responsive, for further self-assembly into polymer films and pillars.

We initiated studies of solvent annealing as a means to restructure ordered nanoparticle/polymer monolayers.

Significance

Accelerating the property control of nanocomposite materials will contribute greatly to a number of DOE missions (nuclear and energy) as well as the nation at large. The improved tailored-nanocomposite materials are expected to be designed to be stronger, lighter, more resistant to aging, or any other desired property in a predetermined manner. All mission-critical systems that employ polymeric materials will benefit from this understanding.

Thermokinetic/Mass-Transfer Analysis of Carbon Capture for Reuse/Sequestration

141078
Year 1 of 2
Principal Investigator: C. L. Staiger

Project Purpose

Capture of CO_2 from the atmosphere is increasingly seen as an enabling technology for net neutral recycling of carbon dioxide, and as a potentially important tool for mitigating climate change. The technical feasibility of atmospheric carbon dioxide capture has not yet been unambiguously quantified though. We propose to establish the boundary conditions and performance metrics of atmospheric CO_2 capture by: 1. Analyzing the thermodynamic and kinetic controls over CO_2 uptake and release by sorbent media, 2. Quantifying air flux constraints over achievable mass transfer, and 3. Developing a detailed preliminary process model for CO_2 capture from air. The thermokinetic analysis of sorbent performance will provide a technical basis for selecting and optimizing new capture or separations media. The examination of the physical constraints over engineered air fluxes will result in the development of a portfolio of wind control approaches that might be applied. The process model will provide a starting point for improving component performance. The media, wind engineering, and process analyses should together establish the achievable performance window for all atmospheric CO_2 capture approaches for reuse, recycling, or sequestration. This will enhance Sandia's efforts to develop low-net-carbon hydrocarbon fuels and build Sandia's capability to provide a wide range of climate mitigation tools.

Summary of Accomplishments

A preliminarily thermodynamic analysis was performed to assess the feasibility of capturing CO_2 from the air. We have found that extracting CO_2 from air is only three times more expensive energetically compared to a more CO_2 concentrated (12 vol%) stream of power plant flue gas. A thermodynamic and equilibrium analysis of readily available CO_2 sorption media (e.g., metal oxides) was also initiated and is continuing to examine tradeoffs between adsorption and desorption temperatures, cost and CO_2 collection efficiencies. While some attention in the literature has been placed on developing media to sorb CO_2 from air, low-energy methods for processing large volumes of air required for CO_2 air capture have been ignored. Computational fluid dynamic simulations were initiated to examine the use and limitations of artificial vortices, generated from thermal gradients, for sustained air flows over CO_2 capture media. A simulation utilizing a base structure of 10 m in diameter and 10 m high containing a heated plate of about 5 m in diameter at the bottom of the base structure was performed. The plate was specified at a temperature 30 °C above ambient. At this low temperature differential a vortex five diameters in height can be created with intake velocities at the base of approximately 1.5 m/s and volumetric air intake of about 60 m^3/s. It is anticipated that future simulations would reveal much higher intake capacities at prototypic scales.

Significance

Establishing the fundamental thermodynamics and kinetic of atmospheric carbon capture will accelerate development of effective means of separating CO_2 from the atmosphere for beneficial reuse (i.e., fuels production, enhance oil recovery, algal biofuels, etc.) and sequestration. Both would contribute to the mission of achieving US energy security.

Improved High-Temperature Solar Absorbers for use in Concentrating Solar Power Central Receiver Applications

141359
Year 1 of 2
Principal Investigator: A. Ambrosini

Project Purpose

Concentrating solar power (CSP) systems use solar absorbers to convert sunlight to electric power. Increased operating temperatures of the central receiver CSP process are necessary to lower the cost of the solar generated electricity by improving power cycle efficiencies and reducing thermal energy storage costs. In order for CSP to meet an electricity cost target of $0.055/kWh, durable new materials are needed to cope with operating temperatures >600 ºC. Ideal absorbers must have high solar absorptance (>0.95) in the visible region and low thermal emittance (<0.05) in the IR region, be stable in air, and be low-cost and readily manufacturable. In the case of central receivers, little effort has been spent in this area. The current coating technology (Pyromark® high temperature paint) has a solar absorptance in excess of 0.95 but a thermal emittance greater than 0.8 which results in large thermal losses at high temperatures. In addition, because solar receivers operate in air, these coatings have long-term stability issues that add to the operating costs of CSP facilities. We propose to utilize solution-based synthesis techniques to prepare promising intrinsic absorbers (e.g. Si_3N_4-ZrB_2) and cermets and evaluate their efficacy as solar selective coatings. Success in producing more efficient solar selective coatings for central receivers can help reduce costs and bring us closer to cost parity with fossil fuels, a necessary factor for widespread implementation of alternative energy production technologies. Such implementation benefits the US from both a national security and climate change perspective.

Summary of Accomplishments

To date, we have begun to develop film deposition methods onto stainless steel (SS304L) coupons using spin- and dip-coating techniques. We have screened both commercially available materials (polysilazane, Co_3O_4, ZrB_2) and lab-synthesized spinel oxides for their optical and structural properties. Preliminary durability tests have been initiated as well as a survey of possible materials amenable to thermal spray coating. A more detailed discussion and table of results have been uploaded to this renewal proposal.

Mixtures of Co_3O_4/polysilazane were deposited via dip- and spin-coating. The coatings showed increased solar absorptivity (compared to uncoated SS304), however the thermal emittances also increased. Increasing the thickness of the coating by performing multiple dip coats increases the solar absorptance and thermal emittance values. Samples were cured at 800 °C for 5h to replicate concentrating solar central receiver conditions; neither absorptivity nor emittance values were affected, but some thicker films did crack.

Several spinels, AB_2O_4 (A,B=Ni, Co, Fe, Cu), were synthesized by solution methods, deposited via spin coating, and sintered. Preliminary results indicate that the $NiCo_2O_4$ and $FeCo_2O_4$ show promise, with absorptances approximately 0.9 and emittances below 0.7. The samples seemed to survive sintering at 800 °C for 6-12 hours intact, although their optical properties decreased by about 10%. Co_3O_4 and $Cu_{(x)}Co_{(3-x)}O_4$ were further investigated by dip coating from molecular precursors. Increasing the film thickness leads to an increase in absorptance but also to an increase in emittance. Several of these films were aged at 500 °C in air atmosphere for 5 days. Absorbance and emittance values remained essentially the same, indicating that the films exhibit good stability to thermal aging.

Significance

Cost parity with fossil-based power generation is a critical factor for widespread implementation of alternative energy production technologies. If successful, this work addresses the energy security and environmental missions of the DOE and the nation by improving the cost and efficiency of concentrated solar power for carbon neutral electricity generation. Success in solar selective coatings for central receivers can also be leveraged for other types of CSP, such as parabolic troughs.

Three Pathways to Enhanced Energy Storage

141370
Year 1 of 2
Principal Investigator: K. R. Zavadil

Project Purpose

This project will evaluate three novel strategies to enable a five-fold improvement in battery performance. This work is proposed in response to a need for transformational changes in electrochemical energy storage devices (EESDs) for both transportation and stationary applications; applications that require specific energy and power densities that currently cannot be realized in a time or cost-efficient manner. We contend that the path toward transformational advances lies in addressing three critical issues that promise to individually produce five-fold performance increases: 1) controlling passivation to better utilize the capacity available in developing materials systems, 2) development and control of novel electrodes structures that minimize charge transport lengths and reduce parasitic interfacial loss, and 3) new energy storage reservoirs with greater capacity.

High energy density electrodes are passivated in battery systems by decomposition of the electrolyte leading to the formation of a solid electrolyte interphase (SEI) which dictates the resulting performance of the system. We propose to test a concept of using inorganic modification to produce stable SEIs whose properties can be investigated to establish the ground rules for passivation of a broader range of electrode materials. Capacity gains can also be achieved by minimizing the charge transport lengths allowing for more of the theoretical capacity to be used in a storage material at higher rates and at higher cell voltages. We propose to test the concept of fabricating three dimensional electrode architectures based on extended pairs of electrode separated by tens of nanometer dimensions using templated synthesis. Alternate energy storage media based on multivalent electroactive materials represent an alternate approach to achieving stable, cost effective, and safe storage systems. We propose to test the concept of using the multielectron reduction of nitrogen to a nitride as an alternate storage scheme.

Summary of Accomplishments

- Controlled Passivation — SEIs by Design: A candidate lanthanide salt and solvent system has been identified for a demonstration of ultrathin film passivation for both carbon protective membranes (positive electrode coatings) and carbon intercalation hosts (negative electrodes) for a lithium ion system. Partial assembly of the experimental system, including an imaging method for monitoring deposition, has been completed. Discussion has taken place with laboratory personnel to ensure process compatibility to allow cell performance testing. A literature search was completed to evaluate the current status of tailored passivation strategies for Li and Li ion batteries. The project team is on track for completing an evaluation of lanthanide-derived SEI properties per project milestones.
- Nanostructured Electrode Architectures: Preparative work has been completed to enable the deposition of lithium onto porous carbon substrates. Porous carbon substrates are currently being prepared that will serve as the nanostructured negative electrode in the demonstration architecture. The team is on track for completing a demonstration of electrode architecture assembly per project milestones.
- Nitrogen as an Active Electrode Material: A review of nitrogen solubility in appropriately stable power source solvents has been completed. An inert atmosphere glovebox has been modified to handle nitrogen introduction into an electrochemical cell. The team is on track for completing a demonstration of nitrogen electrochemical activity per project milestones.
- Larger Scale Opportunities for 5X Performance: The project team has formed working groups to define existing technical barriers to achieving breakthroughs in two promising areas: 1) metal-air batteries

and 2) liquid fuels for electrochemical energy conversion. The purpose of this activity is to map the current project concepts onto envisioned larger scale projects that would yield breakthrough science and technology for electrical energy storage.

Significance

The proposed work addresses the energy security missions by enabling the reduction of petroleum imports, incorporation of large-scale intermittent renewable sources into our electricity grid, improvement in grid reliability and security, and reduction of carbon emissions. Generated new knowledge and tools will support homeland security mission needs for specialized power sources for weapons systems and for countermeasure sensor architectures.

Technologies for Concentrating Solar Power

141655
Year 1 of 1
Principal Investigator: E. S. Piekos

Project Purpose

Concentrated solar thermal technology for electricity generation can generally be classified into three main evolutionary branches: linear receiver (usually at the focus of a parabolic trough), dish Stirling, and power tower. Separately, all three technologies show great promise for providing renewable energy at large volume and reasonable cost in appropriate circumstances. However, there are limitations that preclude each of the three configurations from scaling appropriately to power military installations such as Kirtland Air Force Base. Recently, a novel hybrid concept was proposed that integrates aspects of dish Stirling and power tower technologies by leveraging optical waveguide intellectual property from the California Institute of Technology (Caltech)/ Jet Propulsion Laboratory (JPL). In collaboration with Caltech/JPL, this project provided initial research into this concept with the goal of assessing its performance and economics compared to conventional systems and refining the design.

Summary of Accomplishments

The proposed system was evaluated with respect to competing technologies to determine its relative merits. Several candidate receivers and thermodynamic cycles were examined with an eye toward exploiting its distinguishing features. An analysis of potential drawbacks, such as the secondary mirror temperatures and collector cost relative to conventional heliostats, was performed. The economic feasibility of the system, as well as mirror temperature, was shown to be strongly dependent on the attainable reflectivity and cleanliness.

Significance

Removing barriers to adoption of solar-electric technologies in general benefits DOE's energy security mission because it displaces generation based on fossil fuels that are often imported and, therefore, subject to manipulation by foreign entities. The scalability of the system proposed herein offers the additional benefit of providing an independent energy source for military bases, eliminating a potential means of disrupting their operation from outside the fence line.

Innovative Electric Power Grid Architecture for High-Penetration Distributed Renewable Energy Generation

141679
Year 1 of 2
Principal Investigator: A. L. Lentine

Project Purpose

Increasing renewable energy generation is a key element in gaining energy independence and decreasing global warming. Within ten years, distributed renewable generation (for example, solar photovoltaic), is expected to be cost competitive with centralized coal generation, yet the current electric power grid is ill-equipped to handle a large penetration of distributed renewable generation. This is largely because the control algorithms, hardware, and software do not exist to maintain stability of the power grid in the face of the variable supply of electricity from changing weather conditions. In addition, today's grid cannot safely and securely allow the bidirectional power transport in the distribution layer that optimizes efficiency and reliability in the absence of a strong grid connection.

We propose a new grid architecture very different from today's and well beyond industries' version of the "smart grid" of tomorrow. It will actively manage generation, storage, and loads in a distributed manner to avoid the vulnerabilities and single points of failure common to centralized control approaches. The control algorithms will rely on a low-power, high-security sensing network to route the required measured information to the control hardware. A new class of voltage control devices are needed at all points in the grid hierarchy that adjust voltage magnitudes and phases continuously in response to changing renewable generation, replacing the mechanical relays of today's voltage regulators and reactive power compensators that would quickly wear out under such conditions.

In this project, we will complete a preliminary high level design of the architecture, control algorithms, power electronics, communications, sensing, element models, and scaling analysis for this new grid paradigm. Existing microgrid based projects are not addressing many of these issues, specifically power electronics, reduced order models, similitude analysis, and applying the control theories at a large scale.

Summary of Accomplishments

Specific milestones called out in the proposal for FY 2009 include

- Generate a block diagram of a representative metropolitan/regional electric grid network to be analyzed.
- Complete a high-level control architecture block diagram for the representative grid network.
- Complete a high-level design of the sensing, communications, and control electronic subsystems required for the representative grid network.

We began the work on selecting a reference network. We identified the Public Service of New Mexico (PNM) grid network in New Mexico as a first choice in mapping the new grid network architecture onto an existing network. Other choices included Hawaii and a couple of military bases, where we have ongoing collaborations. We have started, but not yet completed mapping out the details of the reference network below the transmission layer.

Our control team members wrote a document that describes in detail the control methodology and application to controlling the grid. We have not mapped the control methodology and communications needs to specific hardware as called out in the second two milestones above, but the team will continue to pursue that element early in FY 2010.

Significance

Transitioning the grid from its current centralized structure to a distributed intelligent grid enables the transition of society from fossil-fuel based energy to a carbon-neutral, sustainable, and secure energy infrastructure. The proposed interdisciplinary program will utilize Sandia's leadership position in nonlinear control theories, high performance computing, semiconductor devices, energy systems, and secure communications to contribute to that goal.

Unpublished Summaries

For information on the following FY 2009 LDRD projects, please contact the LDRD Office:

Laboratory Directed Research & Development
Sandia National Laboratories
Albuquerque, NM 87185-0123

Project Number	Title
117763	Assessment of Vista Security Technologies
130703	Assessment of Software Streaming Technology
130711	Information Systems Analysis Using Agent Collectives
130713	Localized X-Ray Radiation Effects
130716	Miniaturized Integrated RF Systems
130796	Nanomaterials for Surety Application
130806	Material Development for Radiation Hardness
139073	Understanding Cloud Infrastructure and Capability
139582	Multi-Mission Defensive Space Control Payload
139864	Collaboration of Nontraditional Networked Devices
139865	Exploring Techniques to Analyze High-Level Structures from FPGAs
139866	Assessing Vulnerabilities in 3G Cellular Applications

Appendix A: FY 2009 Awards and Recognition

Award Description	LDRD Contribution
R&D 100 Award, *R&D Magazine*: Hyperspectral Confocal Fluorescence Microscope System	Project 67081, "3D Optical Sectioning with a New Hyperspectral Deconvolution Fluorescence Imaging System," and others
R&D 100 Award, *R&D Magazine*: Catamount N-Way Lightweight Kernel	Project 117785, "A Lightweight Operating System for Multicore Capability Class Supercomputers"
R&D 100 Award, *R&D Magazine*: NanoCoral™ Dendritic platinum nanostructures for renewable energy applications	Project 113490, "CO_2 Reduction Using Biomimetic Photocatalytic Nanodevices," and Project 130772, "Hierarchical Electrode Architectures for Electrical Energy Storage and Conversion," and others
R&D 100 Award, *R&D Magazine*: Ultralow-Power Silicon Microphotonic Communications Platform	Project 117822, "Integrated Optical Phase Locked Loop (IO-PLL) for Attosecond Timing in Microwave Oscillators," and Project 130727, "Silicon Microphotonic Backplane for Focal Plane Array Communications"
Award for Excellence in Technology Transfer- Federal Laboratory Consortium, 2009 - Novel Dendritic Platinum Catalysts for Fuel Cells	Project 130772, "Hierarchical Electrode Architectures for Electrical Energy Storage and Conversion"
Materials Research Society Fellow: *C. Jeffrey Brinker*	Project 105722, "Discovery, Integration, and Interrogation of Biotic/Abiotic Materials and Systems," and others
IEEE Fellow: *Weng Chow*	Project 117825, "Four-Wave Mixing for Phase-Matching-Free Nonlinear Optics in Quantum Cascade Structures"
Presidential Early Career Award for Scientists and Engineers: *Wei Pan*	Project 93511, "Bloch Oscillations in Two-Dimensional Nanostructure Arrays for High Frequency Applications," and others
Presidential Early Career Award for Scientists and Engineers: *Bert Debusschere*	Project 93558, "Computational and Experimental Study of Nanoporous Membranes for Water Desalination and Decontamination"
Robert B. Sosman Award - American Ceramic Society: *C. Jeffrey Brinker*	Project 105722, "Discovery, Integration, and Interrogation of Biotic/Abiotic Materials and Systems," and others
Young Leader Award - The Minerals, Metals & Materials Society (TMS), 2009: *Brad Boyce*	Project 117833, "Anomalous Suppression of Fatigue and Wear Through Stable Nanodomains"
Young Industrial Investigator Award - American Chemical Society, 2009: *Shawn Dirk*	Project 130797, "Novel Dielectrics with Engineered Thermal Weaklink"
Women of Color All Star, National Women of Color STEM Conference, 2008: *Elebeoba May*	Project 79749, "DNA-Based Intelligent Microsensors for Genetically Modified Organisms," and others
Outstanding Young Graduate Award - University of Virginia School of Engineering: *Patrick Hopkins*	Project 130818, "Interfacial Electron and Phonon Scattering Processes in High-Powered Nanoscale Applications"
Distinguished Service Award, The Minerals, Metals & Materials Society (TMS): *Neville Moody*	Project 105805, "Nanomechanics of Films on Compliant Substrates to Enable New Flexible MEMS and NEMS Devices"
Abbott Award, American Society of Mechanical Engineers: *Dan Segalman*	Project 105816, "Model Reduction of Large Dynamic Systems with Localized Nonlinearities"
Faculty Fellow Award, Virginia Tech: *Christopher Roy*	Project 130817, "Evaluation of Baseline Numerical Schemes for Compressible Turbulence Simulations"
Best Paper Award - IEEE International Conference on Data Mining , 2008	Project 117782, "Leveraging Multiway Linkages on Heterogeneous Data"
Best Paper Award - Journal of Rheology, 2009	Project 117790, "Surface Rheology and Interface Stability"
Best Poster Award - 58th Annual Denver X-Ray Conference	Project 117845, "Advanced Cathode and Electrolyte for Thermal Batteries"
Best Poster Award - Materials Research Society Fall Meeting, 2008	Project 105722, "Discovery, Integration, and Interrogation of Biotic/Abiotic Materials and Systems"
Best Poster Award - Materials Research Society Spring Meeting, 2009	Project 105893, "Compositional Ordering and Stability in Nanostructured, Bulk Thermoelectric Alloys"

Appendix B: FY 2009 Project Performance Measures

Measure	Number of FY 2009 Projects
Refereed Publications	**217**
Other Communications	**628**
Technical Advances	**114***
Patent Applications	**79***
Post-Doctoral Researchers	**98**
New Staff Hired from Post-Doctoral Researchers	**13**
Awards	**22**

*CY2008

Appendix C: FY 2009 Mission Technology Areas

Benefiting Mission Area	Number of FY 2009 LDRD Projects
DOE/Nuclear Security	**102**
DOE/Energy Security	**114**
DOE/Scientific Discovery and Innovation	**279**
DOE/Environmental Responsibility	**54**
Homeland Security	**126**
Department of Defense	**160**
Other Federal Agencies	**65**
Industry	**74**