LDRD

Laboratory Directed Research and Development
2009 Highlights

Sandia
National
Laboratories

From the Chief Technology Officer

The Laboratory Directed Research and Development (LDRD) program is the sole discretionary research and development (R&D) investment program at Sandia. LDRD provides the opportunity for our technical staff to contribute to our Nation's future, to our collective ability to address and find solutions to a range of daunting scientific and technological challenges. The results of their work will shape the course of science and technology in the remainder of the twenty-first century and beyond.

From nuclear weapons to renewable energy, biodefense to cyber security, and computer science, to microelectronic engineering, LDRD projects support Sandia's national security missions, and hence, address the Nation's most-pressing challenges. This brochure offers an overview of 31 Sandia LDRD projects that were ongoing in FY 2009, and also highlights seven recent projects that were selected for an LDRD Award for Excellence. Both scientific excellence and potential for mission impact were considered in awarding projects the Award for Excellence. This brochure highlights only a small sampling of the LDRD program, providing a window into the program's S&T advances and their potential impact on National imperatives.

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About LDRD

Maintaining Sandia's world-class science, technology, and engineering capabilities and anticipating their evolution in response to future challenges are absolutely essential to the Laboratories' ability to address national security needs. Authorized by Congress in 1992, the Laboratory Directed Research and Development (LDRD) Program reflects precisely that congressional intent — to encourage and sustain preeminent science and technology by investing in high-risk, potentially high-payoff research and development. The program is designed to proactively anticipate the breadth and depth of research and technological development that oncoming challenges will require.

LDRD projects seek innovative technical solutions to our nation's most-significant challenges, often in collaboration with corporate and academic partners. LDRD allows Sandia to recruit and retain outstanding scientific and engineering talent in service to the Laboratories' five primary strategic business areas: nuclear weapons; energy resources and nonproliferation; defense systems and assessments; homeland security and defense; and science, technology, and engineering foundations.

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2009 LDRD Award for Excellence Winners:
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Cover Image:
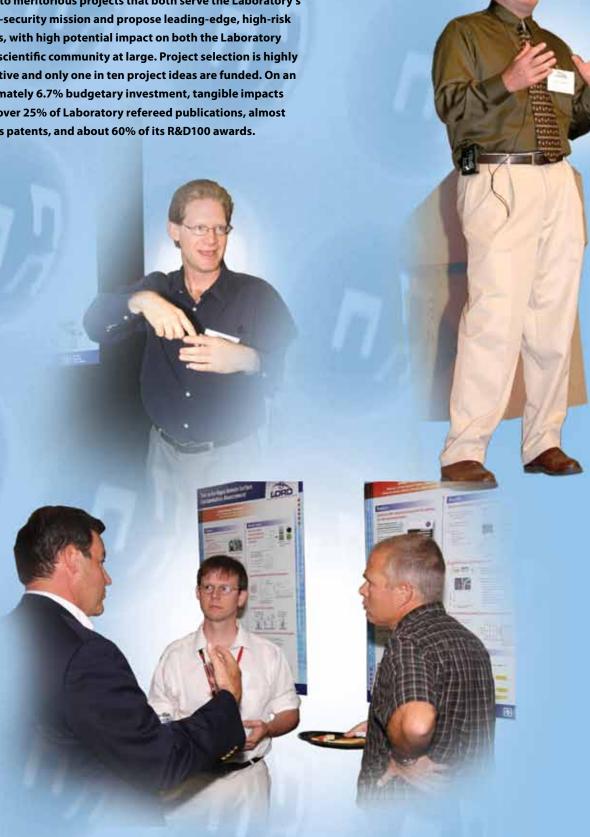**"A variety of colorized scanning electron micrographs of newly fabricated Metamaterials (see page 19)."**

The LDRD Program at Sandia:

Mandated by US Congress in 1992, the LDRD Program functions on a fixed percentage of Sandia's annual DOE/NNSA budget. From that budget base, the LDRD program allocates research funding to meritorious projects that both serve the Laboratory's national-security mission and propose leading-edge, high-risk activities, with high potential impact on both the Laboratory and the scientific community at large. Project selection is highly competitive and only one in ten project ideas are funded. On an approximately 6.7% budgetary investment, tangible impacts include over 25% of Laboratory refereed publications, almost half of its patents, and about 60% of its R&D100 awards.
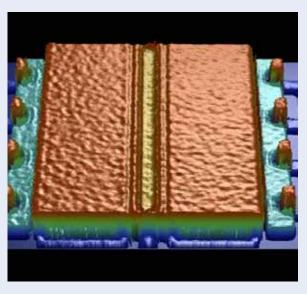
Developing Key Capabilities for Quantum Computing: Trapped Ion and GaAs Approaches Matthew Blain

This multifaceted project engaged numerous Sandia teams and disciplines in attempting to move significantly closer to the actualization of quantum computing, a technology that would revolutionize information processing both in civilian and defense arenas, by opening potential routes to currently intractable computational problems, and by giving the U.S. a vast advantage over its adversaries in the realm of code breaking.
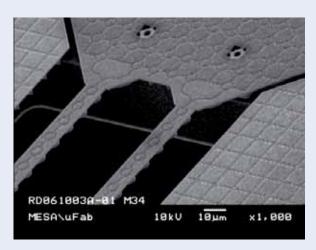
Because the trapped ions are among the most promising physical realizations of quantum bits (or qubits — the fundamental unit of code), the first emphasis of the work in this project was on developing linear micro-traps for the electrostatic confinement (trapping) of ions. In pursuing this work, the team applied the device physics principles and the engineering techniques for fabricating microelectromechanical system (MEMS) and complementary metal organic system (CMOS) devices, utilizing Sandia's Microsystems and Engineering Sciences Applications (MESA) microfabrication facilities.

Planar electrode configurations with overhung electrode structures allowed over-coating micro-trap electrodes and the chip surface with trap-friendly metals such as gold. The micro-traps also included a through-hole to allow for loading of ions and for 3-D application of the laser light necessary for the cooling and manipulation of the trapped ions. Packaging for the chip was also developed, and the chip was tested, successfully demonstrating its ability to trap ions.

To ultimately control multiple laser beams, a final project component fabricated MEMS tip-tilt mirror arrays using the Sandia Ultra-planar, Multi-level MEMS Technology 5 (SUMMiT V™). Finally, this project was able to demonstrate gallium arsenide (GaAs) quantum dot technology that could be used as the basis of semiconductor qubits. The knowledge gained in this project on quantum dot devices underpins a current Grand Challenge LDRD to develop a qubit in silicon using quantum dot technology. ■
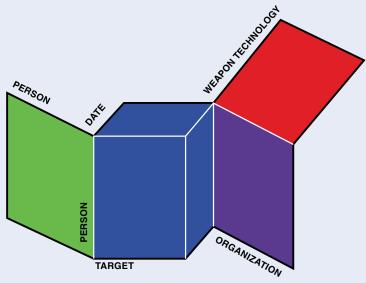

MEMS tip-tilt mirror.

Scanning electron micrograph of second-generation ion-trap chip fabricated during this project.

Data Mining on Attributed Relationship Graphs (ARGs)

Tamara Kolda

Intelligence analysts must somehow integrate and rank data from quite disparate sources, including newspapers, email, formal intelligence reports, records of telephone conversations, and others. Attributed relationship graphs provide one mechanism to accomplish the task of connecting these disparate sources into a useful whole. The graphs contain nodes and edges (connecting lines) whose attributes represent commonalities. Graphs enable understanding of the connections between vertices, which may represent individuals, webpages, documents,etc. In particular, ARGs explicitly identify the types of connections, so that one edge may be attributed as an "email," while another is a "phone call."

Problematically, however, these ARGs must also somehow be deconstructed or decomposed, so that the stored data they contain is more-readily available and useful for analysis. Matrix decomposition techniques have already been shown to be useful at such decomposition for single values, that is for graphs with a single type of edge. An example is the search algorithm that ranks the authority of web pages. Other algorithms can reveal the nexus of links among analyzed text and cluster related information across different languages, or probe emails for topical relatedness, and organize them on that basis.

Tensors, the product of three vectors, can be used to decompose higher-order ARGs with multiple edge types, which thereby store more relational data. This project sought to extend these techniques to higher

Conceptual illustration of multi-way linkages among heterogeneous data sets.

dimensions using such mathematical tensors. Such decompositions are also useful in chemometrics, signal processing, and neuroscience in addition to their importance to an intelligence analyst.

Two software packages emerged from this project, the Tensor Toolbox for MATLAB, a set of tensor decomposition algorithms, which has been downloaded, worldwide, and has over one-thousand registered users and Tamale (Tensor Multi-Attribute Link Explorer), developed to convert raw data (stored as text files or spreadsheets) and create an ARG. Toolbox users report using it for continuum mechanics, online monitoring of network data, acoustic signal research, studies of bird migration, biochemical analysis, and other fields. In addition, several spinoff LDRD projects in data analysis, as well as external funding were offshoots of this project. ∎

Infrastructure for Nondestructive Real-time Fingerprinting of Integrated Circuits

Todd Bauer

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 the physical protection of the system, but another 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.When provided with an input (challenge), a PUF provides an output (response) that depends on these manufacturing variations, thus providing a means of authentication.

This project developed technologies that impart trust during the deployment phase of a product's life-cycle.
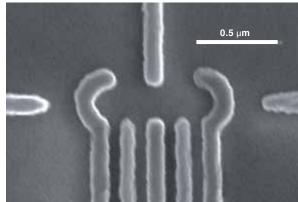
This short project, has prototyped field programmable gate array (FPGA)-based PUFs interrogated through the JTAG interface, and implemented and analyzed fuzzy extraction with error correcting codes (ECCs) to remove noise from a PUF output. It developed and analyzed the "List Infrastructure" required to detect and prevent insertion of or playback of maliciously fabricated authentication data. The team also analyzed integrated circuit (IC) materials and fabrication processes to minimize intra-device variation and maximize inter-device variation on an IC, with an eye toward implementing PUF-based authentication on an IC of its own design.

Engineering Few-electron-occupation Silicon Double Quantum Dots for Quantum Bits and Future Quantum Circuitry

Malcolm Carroll

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 challenges in quantum theory itself. The first step in engineering such a device is the realization of physical quantum bits (q-bits), 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 q-bits 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
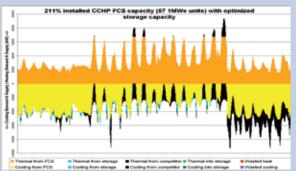

A physical q-bit.

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 q-bit modeling capability is operational and is being used to guide further design. In pursuing a second-generation q-bit, a silicon-germanium pathway is also being pursued, and significant external funding is in place to continue work after the end of LDRD funding.

Network Design Optimization of Combined Cooling Heating and Electric Power (CCHP) Fuel Cell Systems (FCS) and Distributed Energy Devices

Whitney Colella

This research develops novel design and control strategies for combined cooling, heating, and electric power (CCHP) fuel cell systems. Results indicate that CCHP power plants can reduce both fuel consumption and carbon dioxide (CO_2) emissions by up to 50%.

The project develops both chemical engineering and techno-economic-environmental models of CCHP fuel cell systems to optimize their design and control. These models consider both engineering and market conditions, and include the physics of advanced fuel cells, balance of plant components, and cutting-edge double-effect lithium bromide absorption chillers. The data from the models are independently validated with data from manufacturers and the literature. Several of the modeling strategies suggest that thermal storage can be economical, while cooling and electrical storage are less so. Both on-grid

Model of control strategy for FCS systems, including heating, cooling, and excess storage and discharge parameters.
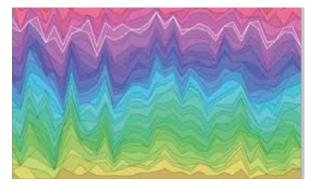
and off-grid scenarios are evaluated. The models identify the optimal dispatch of CCHP fuel cell systems and energy storage over time, indicate the possibility of overall CCHP efficiencies above 80%, and propose the best strategies for both cost savings and minimizing CO_2 emissions. Several DOE-funded projects have ensued as a consequence of the project's findings.

ParaText™: Scalable Solutions for Processing and Searching Very Large Document Collections

Daniel Dunlavy

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 between 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

One type of graphical representation depicting temporal relationships among documents.

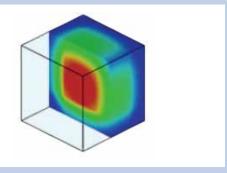and clustering, enabling assessment of emerging cyber threats. It has demonstrated its value in the area of nonproliferation. Combining ParaText™ text analysis with graph algorithms and visualization methods provides intelligence analysts with a broad range of document-analysis capabilities for assessing potential issues. In the arena of nuclear materials attribution, ParaText™ is capable of extracting meaningful patterns and trends, as well as providing information enabling rapid interpretation of nuclear-forensic signatures.

Automated Monte Carlo Biasing for Photon-Generated Electrons Near Surfaces

Brian Franke

The accurate assessment of radiation hardness of the electronic components in nuclear weapons and satellites has long been an area of Sandia expertise. Various methods have been applied to assess and predict the survivability of such components in high-radiation environments such as outer space. In simulating this class of problem, electron transport becomes particularly important near material boundaries. But electrons are computationally expensive to simulate, and there are certain problems that current methods have been unable to successfully approach with desired accuracy or efficiency. This project's goal is to produce an automated Monte Carlo-based technique for biasing radiation-transport Monte Carlo coupled electron-photon calculations, of the type arising from currents induced by radiation impinging upon electronics in high-radiation environments. Project success also demonstrates a more-general class of methods for improving the usability of Monte Carlo codes.

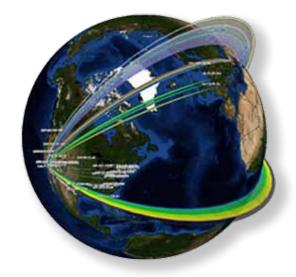**Example of a functional expansion algorithm tested in the project.**

The project has demonstrated a number of useful algorithms. Ultimately, the new method achieved a 10-fold speed-up in processing with more-accurate results. A key area in which these advances promise to exhibit application is in the cavity system-generated electromagnetic pulse (SGEMP), whereby x-rays, such as those produced by a nuclear device, strike a spacecraft, displacing electrons and producing large currents, usually with detrimental effects.

Network Discovery, Characterization, and Prediction

Philip Kegelmeyer

"Our adversaries are networks," is a key theme articulated by members of this project. The statement underlines the fact that there are countless networks of both people and information-processing devices in the world with goals that are adversarial to the interests of the U.S. and its allies. The problem for intelligence analysts is that these networks often only reveal themselves through a process of coalescence of parts, with relevant data from many sources, often temporally and geographically dispersed.

It is the fundamental proposition of this project that the characterization of networks requires methods for identifying hidden properties and relationships, and for analyzing the structure of a network to learn about its purpose and the roles of its components. In addition, analysts need a means to be able to predict the evolution of a network, its components and properties. To ensure usability, the algorithms developed in this project are assembled into carefully tested prototypes. In addition to the cyber-development team, a human factors team, led by a social scientist has worked closely with actual intelligence analysts eliciting both their needs and their responses to the
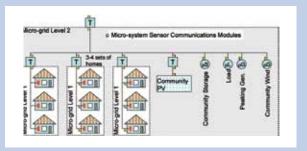

A representation of the global cross-talk among computers.

toolkit-in-development, such that refinements would reflect real-world applicability. In addition to the open source Titan toolkit (www.kitware.com/INfovisWiki), a significant input of work for others R&D funding has been attracted into the project.

Scalable Microgrid for a Safe, Secure, Efficient, and Cost-effective Electric Power Infrastructure

Anthony Lentine

Scalable micro-grid concept.

Although it is clear that future solutions to electrical energy generation must include such carbon-neutral alternative distributed renewable energy sources such as wind and solar, our current electrical grid is not able to accommodate large percentages of renewable sources whose power output is unpredictably dependent on the incident sunlight intensity or wind speed. The structure of today's grid is not appropriate for these resources, since it is unidirectional and passive, unable to balance distributed renewable power generation, storage and loads. Since fossil fuels (coal and oil) inherently store their own power, there are few controls on our existing simple tree-like power-distribution system. Important considerations also include the fact that wind-turbine-generated power is often remote in location, and transmission-line losses can be reduced by siting these power sources geographically close to where power is consumed.
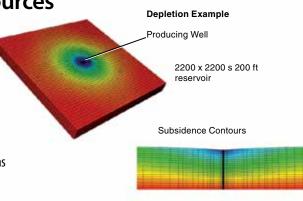
This project pursues a smart-grid design, based on local microgrids that are highly endowed with sensors distributed throughout the system to monitor power generation, control loads, and quickly respond to changes. The most-desirable situation would be power generation and usage in a small geographic area, with redundancy in information processing to avoid central failure points and enable pooling of local resources in the event of a failure. Models of such a grid architecture have been developed, and simulations are progressing.

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

Mike Stone

As part of the U.S. energy future landscape, subsurface activities such as mining, waste disposal, and reduction of carbon dioxide impact on climate change will require a better understanding of the dynamics of subsurface systems, from porous rock formations through fluid dynamics and microbial activity. This project is developing a coupled thermal, hydrological, mechanical, chemistry (THMC) modeling capability for massively parallel applications.

The project team implemented a coupled porous flow/mechanics and thermal/mechanical capability in the SIERRA Mechanics code and determined what additional functionality would be required. For example, a new nonisothermal, multiphase, multicomponent flow capability within SIERRA is being coupled to the geomechanics solver Adagio. Ongoing work is attempting to develop a robust coupling algorithm that addresses disparate

Depletion Example

Producing Well

2200 x 2200 s 200 ft reservoir

Subsidence Contours

Example of a model representation of a well undergoing depletion.

time and length scales in coupling geochemistry to subsurface flow. Several benchmark problems have been solved, for example, the ability to represent heterogeneous geomaterials in mechanics and flow simulations. Ultimately, the project will allow Sandia to address the broad range of multiphysics issues that arise in the energy cycle — from subsurface fuel extraction to waste disposal.
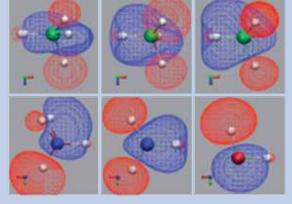
Multiscale Schemes for the Predictive Description and Engineering of Materials

O. Anatole von Lillienfeld

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. Consider for example, the reaction centers inside chloroplasts, which, inside the cells of a plant leaf, are able to harvest the sun's energy. In the leaf, special molecular complexes serve as the agents of this energy transformation. But suppose that non-biological materials could be designed that could carry out this process 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

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).

bridging statistical mechanics and electronic structure theory. 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.

Innovative Control of a Flexible, Adaptive Energy Grid

David Wilson

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

Model of "Real World" Microgrid able to simulate Lanai, Hawaii power-generation system to which intermittent energy sources were added.
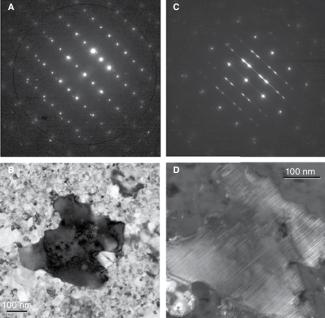
Hawaiian power generation systems that included diesel- and gas-powered electrical generators, to which this modeling endeavor added wind turbines. This scenario revealed several important operational findings, particularly that frequency variations occur due to wind intermittency, and may cause frequency 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.

Science at the Interface: Grain Boundaries in Nanocrystalline Metals Stephen M. Foiles

This project has deeply probed the effects of nanostructure on micro- and meso-structural properties in metals, with the ultimate aim of understanding how nanostructural boundaries affect material properties. With a focus on nanocrystalline nickel, the project pursued both experimental studies into grain morphology and modeling initiatives that employed Molecular Dynamics simulations of nanocrystalline grain growth, structure, and mobility.

Virtually every engineered material contains interfaces, both at free surfaces and internally, which are key determinants of that material's properties. The importance of these interfaces is magnified in nanostructured materials, in which interfaces are more numerous per volume of material. Microstructure — defined as the distribution of internal interfaces, defects, and phases — governs many properties of materials, including strength, toughness, conductivity, magnetic susceptibility, etc. Key among such interfaces are so-called grain boundaries, whose normal or abnormal structures can have marked effects these properties. Such boundaries possess a number of properties, including those of mobility and stiffness. Because microstructure is critical to materials performance, materials processing focuses on controlling and optimizing it. In polycrystalline materials, grain structure is a dominant feature of the microstructure. Since grain structure changes via motion of the grain boundaries, grain boundary properties play an important role in microstructural evolution.

High-resolution transmission and scanning electron microscopy (TEM/SEM) of these nanoscale grain-boundary features, together

Electron diffraction patterns (a and c) and transmission electron micrographs (b and d) of an abnormal nickel grain.

with atom-probe tomography observations at the atomic level, have complemented new simulation techniques to reveal several unexpected findings in this project, for example formation and growth of metastable phases, with an apparent effect on thermal stability. The research also discovered that the formation of lattice defects depends in a yet unexplained manner on the scale of the grain structure.
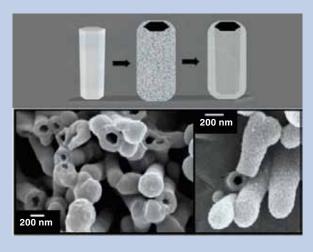
The project carried out a comprehensive survey of grain boundaries and their energies, finding that overall, there appeared to be no clear correlation between energy and the parameters typically associated with energy in the literature. These findings clearly call for a more general model for grain boundary energy. The project's results provide an extensive database of grain-boundary energies useful to motivate and/or test such a global model. ∎

Templated Synthesis of Nanomaterials for Ultracapacitors

Bruce Bunker

A hybrid between a battery and a capacitor, 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. For example, a hexane thiol template complexes with dissolved ruthenium species and generates porosity during thermal processing leading to a nanoarchitecture 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.

Hollow-rod nanostructures that are ideal for promoting electrolyte access to the electro-active materials previously deposited.
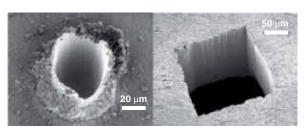
Mathematical models are used to analyze the results of these electrochemical syntheses, and conversely, once performance parameters are established, the models can predict nano-architectures that maximize performance. This research has indicated that highly desirable energy storage parameters of ultracapacitors — their rapid storage and release of charge — can be achieved relatively inexpensively and by several alternative routes.

Interfacial Electron and Phonon Scattering Processes in High-powered Nanoscale Applications

Patrick Hopkins

Short-pulse laser heating of thin films induces a large electron-phonon nonequilibrium.

Material interfaces in nanoelectronic devices are regions where imperfections can lead to interatomic mixing that can have serious impacts on heat transfer processes. This is particularly true in high-power nanodevices found in modern weapons and sensor systems. This so-called electron-phonon scattering at interfaces can be a limiting form of thermal resistance. With the increased power requirements in these systems, it is critical to develop a fundamental understanding of the thermal processes occurring across material interfaces.

This project employs several transient thermoreflectance (TTR) techniques to probe electron-interface scattering of thin films after short pulsed laser heating. The results have demonstrated electron system energy losses due to the presence of interfaces,
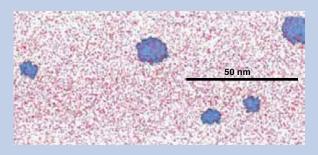
with the substrate-dependence of the scattering indicating that it is a thermal process. Higher temperatures, which can induce sub-conduction (d) band excitations can drastically affect thermal properties. Collaborations with the University of California (UC) Berkeley, Massachusetts Institute of Technology (MIT), Los Alamos National Laboratory (LANL) and the University of New Mexico (UNM) are permitting the study of thermal properties in a variety of systems, including semiconductor photovoltaics and nanowire contacts. A new phonon modeling technique has been outlined for one-dimensional thermal transport, pointing to phonon wave interference mechanisms that can possibly be controlled, potentially leading to thermal rectification.

Compositional Ordering and Stability in Nanostructured, Bulk Thermoelectric Alloys

Douglas Medlin

Thermoelectric (TE) materials are used in technologies for solid-state cooling and solid-state thermal power generation. A central materials research challenge, important to several Sandia missions, is to improve the intrinsic energy conversion efficiency of TE materials. This project is studying both theoretical and practical aspects of improving TE materials, using nanostructuring to decouple and enhance the thermal and electronic transport processes required for energy conversion. Based on recent advances demonstrating thermoelectric enhancement in bulk alloys possessing nanometer-scale compositional modulations, this project is seeking to better characterize and understand these factors in relation to the parameters known to affect the performance of these materials. An example is the presence of interfaces resulting from precipitated nanoclusters within a bulk semiconductor matrix.

The project team has synthesized bulk, nanostructured thermoelectric alloys, and using transmission electron
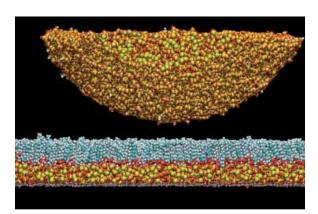

Atom probe tomographic reconstruction of embedded Ag_2Te (silver telluride) nanoprecipitates in a PbTe (lead telluride) thermoelectric matrix.

microscopy (TEM) and atom probe tomography, has characterized the synthesized materials to determine the mechanisms by which the internal nanostructures form and evolve. In the process, the project has developed a theoretical model to correlate this structural information with measurements of thermoelectric performance and to explain the mechanism of thermoelectric enhancement. Further analysis of the systematic variation of properties with the nanoprecipitate distribution will quantify the relationship between nanostructure and thermoelectric properties and will allow the model relating the relevant electronic and thermal transport properties to be refined.

Nanomanufacturing: Nano-Structured Materials Made Layer-by-Layer

P. Randall Schunk

Nanoparticle alloys can form at room temperature, when metal ions in solution are irradiated by either gamma rays or pulsed protons. Subsequent to the reduction of these ions to metal nanoparticles, they combine to form nanoparticle alloys. While theories of the formation chemistry exist, the chemistry is still incompletely understood. This project is investigating that fundamental chemistry, such that ultimately, better control of formation and composition of these alloys, particularly nickel-based, can be achieved in the absence of traditional mechanisms of alloy formation such as sintering. Underpinned by the defect-free possibilities of the cobalt-60 gamma-irradiation method, the alloys produced by this method are termed "superalloys," high-performance alloys with high strength and durability, resistant to both corrosion and to conditions such as high temperature and oxidation. They are thus ideal candidates for applications requiring such durability.

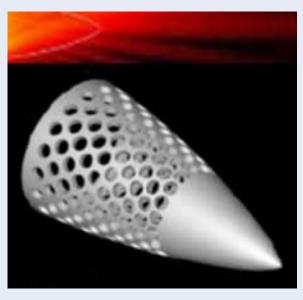**Molecular Dynamics analysis of friction and adhesion at the nanoscale.**

Silver-nickel and palladium-nickel superalloy nanoparticles have been created and characterized. Applications for such alloys include weapons casings, aircraft parts, satellites, power plants, and gas turbine engines. In addition, membranes to reversibly bind and release hydrogen will be required for hydrogen storage and utilization in hydrogen fuel cells. Nanoparticle superalloys may hold promise in that area as well.

Passive & Active Electromagnetic Frequency Selective Surfaces for High-Power Beam Applications   H. Jacques Loui

Pursuing novel territory through theoretical, numerical, and experimental approaches, this project's goal was to investigate and — to whatever extent possible — characterize and apply the physics of electromagnetic radiation (light) scattering from thick metal surfaces with periodic light-scattering unit cells. The goal was to create tunable frequency selective surfaces (FSS). Such structures would be able to collectively affect incoming electromagnetic radiation in a number of ways, based on specific configuration. Eventual engineering applications could ultimately be found in both defense-related and civilian arenas: Lensing, shuttering, RF antennas, and cloaking are but a few examples. An especially important application is found in Synthetic Aperture Radar (SAR).

In the design of these structures, varying their unit-cell geometry tends to control the device's frequency and angle dependence, while variations in the filling of the unit-cell apertures addresses the tunability of the structure with respect to its frequency selectivity. The project team discovered that the unit cell apertures through the thick metal offered improved response characteristics if, rather than quasi-cylindrical in shape, they were instead tapered at their midpoint, a modified hourglass shape

Significant effort had to be invested in characterizing ferrite, whose magnetic properties can vary among different samples, and an RF Gaussian

Model of a thick metal nosecone with periodic unit cells.

beam-measurement system was designed and built to experimentally measure properties. Numerical results supported the feasibility of this path. It was necessary to develop in-house numerical tools for this purpose, with the collaboration of the University of Washington. Academic collaborations played a large role in many aspects of the research.
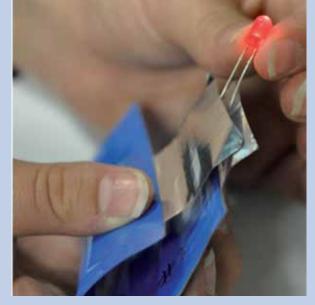
Essentially, this research has opened up a new direction for materials research at Sandia, in the areas of subwavelength scattering and radiofrequency ferrite-based innovations that should impel applications in several arenas, particularly the SAR program, which has flourished at Sandia for several decades. ■

A flexible battery supplies voltage to an LED.

Oxygen Insensitive Anodes: Towards a Printable Lithium-Ion Battery

Chris Apblett

This project is pursuing the development of new batteries that are both smaller in size and shape-conformant for a number of different applications, while retaining adequate energy density. It begins from the premise that choice of the right battery chemistry can allow the design and fabrication of batteries that do not need to be rigidly packaged in traditional configurations and that can operate in the presence of oxygen and water, which normally inactivate lithium batteries and necessitate the package.

In this instance, ionic liquids are used as electrolyte solvents because they have a low vapor pressure and oxygen solubility, thus conferring protection to ionic lithium (Li^+) while it is solvated in the electrolyte, carrying current between the $LiFePO_4$ cathode and the $Li_{4/3}Ti_{5/3}O_4$ anode. These electrodes are selected for their stability in open air, with their chemical potentials chosen to prevent either lithium oxidation or oxygen and water reduction. Methods for spray-coating and direct printing of both electrodes have been employed, thereby conferring shape conformance to a variety of situations. Together with the aforementioned oxygen tolerance, this enables the deployment of a battery that does not need a package. In turn, the elimination of the package and other inert battery components allows for a significant gain in energy density. Charge/discharge characteristics of printed batteries have exhibited good voltage performance, to a large percentage of the theoretical capacity, and life-cycle tests are encouraging, even though refinements likely remain.

A 100-nm membrane on a MgO carrier, exemplifying achievements in fabrication.

High-temperature, Large Format Focal Plane Arrays For Emerging Infrared Sensing Applications

Jin Kim

This project is directed at materials research designed to evolve the next-generation of focal-plane arrays (FPAs), given that the current MCT (Mercury, cadmium, tellurium) technology is beginning to reach a performance threshold. Investigations into indium, arsenic, antimony (InAsSb) materials and into strained-layer superlattice (SLS) materials are expected to close the gap between theoretical and actual performance for next-generation FPAs. SLS materials are those with alternating layers of lattices of different materials, where mismatches in lattice spacing is accommodated by elastic strain. However, this can lead to material defects, which the project is seeking to identify, characterize, and control, as part of the initiative to utilize these materials productively.

The project is pursuing both better modeling approaches, as well as advances in epitaxy, fabrication, and material hybridization. Several codes have been developed to model performance of these new materials. Additionally, samples have been fabricated, in which membranes of 100-nm thickness (or less) have been suspended on holders that are transparent to terahertz probes.

Ultimately, the enhanced-performance FPAs are essential to mid- and long-wavelength infrared systems important to satellite-based, airborne, and ground-based systems for nonproliferation assessment, tactical surveillance, missile defense, and combat support.

A Zero Power, Motion Sensitive MEMS Wake-Up Device

Roy Olsson

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 than a few nano-Watts 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, processing such wake-up events consumes significant power, thus shortening the lifetime of these devices. Hence, a wake-up signal consuming

A 400-Hz, zero-power wake-up sensor.

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 and amplitudes, then combined into an array. A mass-prefabrication process has been designed with the assistance of 3D Finite Element modeling.
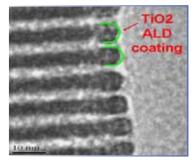
Understanding & Optimizing Water Flux and Salt Rejection in Nanoporous Membranes

Susan Rempe

Clean water is widely recognized as perhaps the most critical limited resource of this century. Although reverse osmosis membranes have been of great utility in purifying water of salts and contaminants, further modifications have begun to show diminishing returns. It is clear that new solutions to water purification are required in order to address the fundamental factors limiting efficient salt rejection at high water flux. Pushing water through RO membranes requires energy to maintain a pressure gradient, and new solutions addressing the energy consumption of purification devices are crucial.

Through study and modeling of biological membranes, this project's researchers hope to glean 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—sodium, potassium,

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).
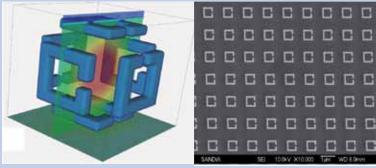
calcium, and others. This project's interest lies in determining whether inorganic chemical solutions to the problem of ion and water selectivity can be patterned based on their biological (organic) counterparts. Not only do researchers desire to purify water completely of its dissolved salts, but in some instances to find ways to allow certain salts to remain in the water, thus replicating naturally occurring mineral waters. Modeling has played an important role in informing material design, for example, employing parallel silica nanotubes as water channels.

Metamaterial Science and Technology

Michael Sinclair

Model (left) and electron micrograph (right of a novel metamaterial.

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 nano-fabrication — 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. The field is not new, for examples, metamaterials with radio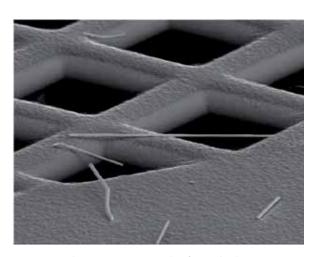frequency (RF) active properties are now incorporated into certain computer hardware peripherals. However, useful metamaterials in the visible and long-wavelength infrared (LWIR) portions of the electromagnetic spectrum do not exist. Hence, using a layered approach, where each layer is composed of a two-dimensional array of nanostructures, the project is seeking to manipulate these wavelengths in a low-loss fashion. Low loss of light is key, since this has been a problematic area. The project is developing new fabrication processes as well as new methodologies to analyze its fabricated metamaterials.

Understanding and Predicting Metallic Whisker Growth

Donald Susan

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 thus raising the possibility of shorting failures between conductors.

Scanning electron micrograph of tin whiskers on the surface of a support grid.

The project is characterizing the phenomenon using tools such as electron backscatter diffraction (EBSD), Focused-Ion Beam (FIB), transmission electron microscopy (TEM), confocal microscopy and others, studying whisker growth kinetics as a function of temperature. Additionally, computational modeling is being employed to predict whisker nucleation density and growth rate, thereby assisting in establish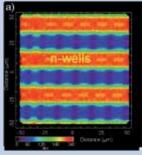ing the important parameters that determine whisker formation, so that it can be understood — ultimately well enough so that it can be controlled or eliminated. For example ESBD revealed that almost all whiskers are single crystals. The project team is collaborating with scientists at North Carolina State University to attempt to improve the accuracy and predictive value of its models. Thus far, growth rate and preferred growth direction are much better understood because of this project's investigations.
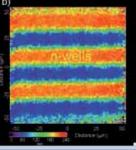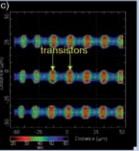
Heavy Ion Radiation Effects Microscopy
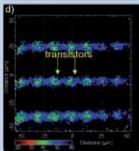
Gyorgy Vizkelethy

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 thickness through 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

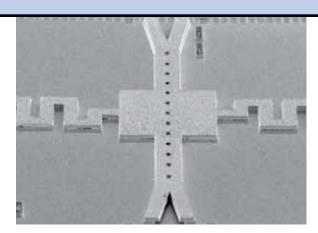**IPEM images illustrating penetration of the technique to reveal deeper-layer structure.**

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).

Terahertz Microelectronic Integration

Michael Wanke

See-through imaging through opaque materials for concealed weapons, high-specificity chemical detection of chemical signatures, lightweight, high-spatial-resolution radar and remote detection platforms, and secure high-speed communication links — these are just a few of the promises of a terahertz (THz) transceiver. This frequency range between infrared and microwave radiation has been difficult to utilize productively to this point in time, and has relied on fragile and expensive vacuum or gas tube components.

This project has demonstrated an integrated THz microelectronic transceiver using all solid-state components and fabrication methods compatible with modern semiconductor processing, A quantum cascade laser, waveguide and other components were successfully located on the same chip. The project team demonstrated all the THz components needed for THz integrated
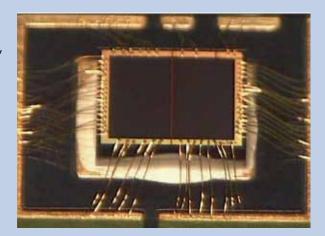

Scanning electron micrograph of on-chip waveguides.

circuits, achieving low propagation and bend losses. Full integration, reliability, and relatively low-cost fabrication are all outcomes of these successes. In addition, the project team developed unique device-modeling codes. The full integration of components paves the way for a whole spate of potential applications, rendering it likely that a practical THz technology can, ultimately, be fielded outside the laboratory. This would enable, for example, see-through inspection imaging, explosives spectroscopy, and applications in astrophysics and space programs.
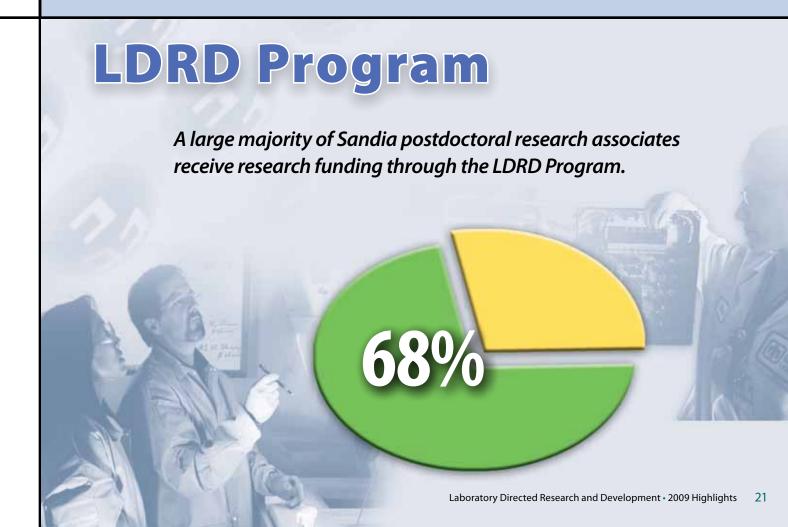
Radiation-Hardened Point-of-Load Power Conversion

Brandon Witcher

In the ever-evolving world of satellite electronics, power sources, power distribution, and lightweight components are an ongoing concern, with each new generation of satellite displaying novel requirements. In this project, the development, design, and fabrication of a new approach to the problem of space-qualified power distribution has been proposed, using point-of-load (POL) power conversion. This places individual power supply regulators close to their point of use in electronic circuitry, rather than attempting a more-centralized control of power. This is of particular importance for remote-sensing satellite data processing systems that, typically, require low voltages and will be called upon to process ever-increasing volumes of data as greater needs for persistent global awareness arise. If successful, POL promises to increase efficiency (reduce power losses) and, overall, reduce the size and therefore, the weight of cables required in satellite electronics. Reduced weight is a clear advantage for space vehicle launches and subsequent maneuverability.

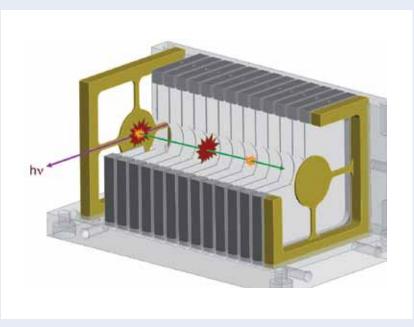**A chip mounted for radiation testing.**

This new approach requires space-qualified POL controllers and suitable radiation-hardened metal-oxide semiconductor field-effect transistors (MOSFETs). The project will design, simulate, and ultimately fabricate and characterize these components.

LDRD Program

A large majority of Sandia postdoctoral research associates receive research funding through the LDRD Program.

68%

Explosives Detection by Photo-ionization Ion Mobility Spectroscopy Thomas Reichardt

Efficient, effective detection of explosives and other chemicals and biological agents dangerous to civilian and military populations has been an ongoing priority for homeland security initiatives. An important technique for detection has been ion-mobility spectrometry (IMS). In this technique, an energy source is utilized to ionize suspected toxins, the mobility of their resultant ions in an electric field then becoming an identity signature.

Drawing of the photo-ionization/IMS instrument for explosives detection developed in this project.

In the past, ionization sources were radioactive materials, typically ^{63}Ni or ^{241}Am. However, these sources are inconvenient in many ways, producing unwanted effects, are continuous emitters, when pulsed emission is the desirable modality, and have regulatory issues associated with their transport. This project has pursued the alternative ionization approach of resonance-enhanced multiphoton ionization (REMPI) using a pulsed-laser source of ultraviolet (UV) radiation as the ionizing energy. Problematically, until the advent of compact diode-pumped solid-state laser technology, such lasers were far too large and inefficient to consider for anything even vaguely resembling a portable detector. However, this project has engaged its team's prior development of pulsed UV-laser sources to demonstrate the potential of a compact instrument coupling IMS with REMPI for the detection of explosives, first inside the laboratory, with the ultimate goal of developing portable device, with a design based on prior Sandia portable detection devices such as the µHound™.

Modification of existing sensors, and further laser miniaturization, as well as improvement of the electronics to enhance resolution and reduce noise were included in this all-encompassing project to draw closer to a fieldable technology. Ultimately, the project was able to demonstrate the coupling of IMS and REMPI to detect not only high-priority explosives like TNT, RDX, and PETN, but also to extend detection to chemical compounds previously undetectable by traditional IMS approaches. A compact laser source, suitable for REMPI and ultimate portability in a field instrument was also designed and evaluated by the project, which in addition to intra-Sandia applications, will find many others in intelligence, defense, and homeland security. ■

Overcoming Jitter Effects for Remote Staring Sensors

Katherine Simonson

An example of a local scene utilized to assess the robustness of the algorithms developed in this project: Change elements (motor vehicles) are boxed.

Staring remote sensors are a key element of our nation's information-gathering infrastructure, enabling persistent surveillance over broad areas of interest in support of a range of national security missions. One motivation for deploying such sensors is the real-time detection of significant scene changes that may impact security measures and responses. Timely and accurate change detection is particularly challenging when the platform on which the sensor is mounted is subject to jitter, as small shifts in sensor pointing can lead to large apparent intensity changes, particularly along scene gradients. Such "false alarms," can, in turn, overwhelm automated detection processors, or provoke unnecessary and potentially counterproductive responses. This project has developed advanced data-processing algorithms designed to facilitate change detection in high jitter environments.

Because the magnitude of "target" changes can lie far below the natural contrast levels in imaged scenes, simply thresholding observed frames is not an effective strategy. Instead, most approaches to change detection involve subtraction: To detect new energy at time t, an estimate of the "background" energy present in each image pixel prior to time t is subtracted from the frame observed at t. The resulting difference frame should highlight scene change.

This process requires highly precise frame registration, to within a small fraction of a pixel. Unfortunately, such precision generally cannot be realized in real-time (frame rates of 10 – 30 Hz) in the presence of significant sensor artifacts and high platform jitter.
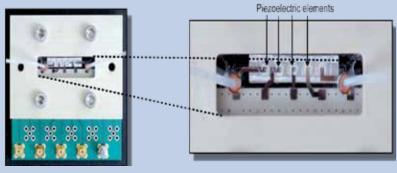
The real-time algorithms developed under this project do not require precise frame registration, relying instead on two statistical models — one spatial and one temporal — for variations in pixel intensity. At time t, each pixel's observed intensity is gauged with respect to the two models to determine whether the current observation is consistent with expectations. Depending on the type of targets sought, downstream logic using criteria related to area (detections covering at least a minimum number of contiguous pixels) or persistence (detection over at least a minimum number of frames) can decrease false alarms substantially. By collecting jittery visual data from local scenes (as well as a classified system), the team confirmed the robustness of the developed algorithms in challenging environments. ∎

Intelligent Front-end Sample Preparation Tool using Acoustic Streaming

Darren Branch

Biodetection systems that identify potential biowarfare agents are generally based on assessment of the internal macromolecules — commonly DNA, RNA, or proteins — that can provide unambiguous species identification. But to accomplish this in rapid fashion requires the lossless extraction of these intracellular or intra-viral molecules, and that has proven to be the rate-limiting step in most biodetection systems.

This project is approaching the problem of rapid, lossless extraction of DNA, without chemical treatment, such that the DNA can then be transferred to one of the many extant automated DNA detection systems. Key to this methodology is a combination of acoustic waves and microfluidics. Within a microchannel on a silica chip, acoustic pressure waves are utilized to lyse bacterial cells and release their contents. DNA capture is then accomplished by charge-switch beads, which

Photograph of the lysing system, showing the chamber containing the active piezoelectric elements.

bind DNA at lower (acidic) pH and release the DNA as pH is increased into the basic region. A second DNA extraction technique employs gold electrodes with a changing voltage to reversibly bind/release DNA.

The acoustic lysis of bacterial cells and the efficacy of both aforementioned DNA extraction cartridges have been successfully demonstrated.
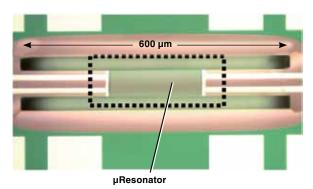
Featureless Tagging Tracking and Locating (FTTL)
(Pillar I: Microresonator Based Waveform Storage)

Karen Branch

This project's goal was to enable physically and electronically featureless tag systems capable of broad area search and precise geolocation. To accomplish this, the team identified three research "pillars" requiring technological advances: MEMS acoustic microresonator delay elements; featureless signaling waveforms, detection and geolocation algorithms; and antenna technologies required to obtain a very small tag.

In the area of the first of these project "pillars," the team is developing microelectromechanical system (MEMS) microresonator technology, progressing toward the goal of a 9-GHz device in X-band radar, with 50-MHz bandwidth, a 30-ns delay and insertion losses of less than 10 dB. If successful,
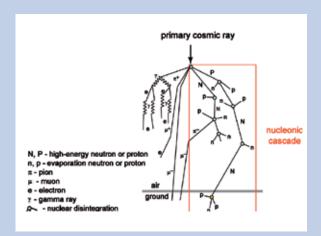
6.9 GHz Microresonator Delay Element.

the microresonator delay would eliminate up to 90% of the components required to form a radar tag. As part of this project area, improved aluminum nitride materials and supporting micro-inductor technology had to be developed, testament to the project's broad scope. The significance of a low power, low loss, wide bandwidth, high-frequency delay element goes beyond simply enabling FTTL. It also has the potential to impact other sensor areas such as spectrum analysis, cognitive radio, and ultra-stable clocks.

Nature's Neutron Probe: Measuring Soil Moisture and Snow at an Intermediate Spatial Scale using Cosmic-ray Neutrons

Darin Desilets

Predicting possible climate-change scenarios is a crucial aspect of beginning to cope with these changes in a productive fashion. Reliable field observations of annual variations in climate parameters are necessary to support modeling efforts that allow prediction. This project is measuring soil moisture and snow water equivalent depth (SWE) at an intermediate spatial scale, that is, larger than a single small area (or "point") sample, and smaller than the much larger area measured via satellite observations.

To accomplish this measurement, the project makes use of the cascade of subatomic particles (such as neutrons) that are formed as a consequence of naturally occurring cosmic rays colliding with the atomic nuclei in a variety of atmospheric gases. Since, at the earth's terrestrial surface, hydrogen nuclei are most important at controlling neutron fluxes from these collision processes, and since most hydrogen occurs as part of water molecules, the neutron fluxes at the surface can be used — via appropriately placed neutron detectors — to measure snow pack and soil moisture over a desired area.

Cascade of subatomic particles initiated by a cosmic ray striking the atomic nucleus of an atmospheric gas.

With measurements occurring at two field sites in New Mexico, the method has been validated. It is noninvasive and also independent of soil chemistry or terrain, and with portable, rugged detectors available, it promises to be a valuable technique for both climate modeling and hydrologic planning.

Deployable Pathogen Diagnostic System

Anson Hatch

Prototype of the field-deployable diagnostic system developed in this project.

Analysts predict that 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 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 can be performed simultaneously and with a short incubation time.
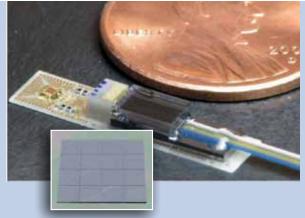
The portable unit is modularly constructed, and analytic cartridges can be quickly changed-out in the short term, but are also, ultimately, reusable. This robust system architecture has attracted significant interest from a number of potential users as the project matures and completes its developmental phase.

Highly Pixelated Hypertemporal Sensors for Global Awareness

Rex Kay

Remote sensing and surveillance of the environment and of outer space for full-earth persistent monitoring of transient events (e.g., explosions) potentially important to intelligence and to national security is best accomplished through focal-plane arrays (FPAs). These optical monitors sample the environment repeatedly and rapidly, such that even the smallest and most-transient event of interest will not be missed. In this Grand Challenge project, the team focused on development of the critical enabling technologies necessary to accelerate the realization of FPAs that will be key to persistent whole-earth monitoring.

The project's aim was futuristic, the goal to anticipate the future state-of-the-art in advance of specific needs. Hence the direction was clearly to maximize an opto-electronic functionality that would be extensible. In this context, it was also important to create full system modeling tools that would anticipate ongoing

Photograph of the slim, fully packaged technology, with micrograph of a 4 x 4 array opto-electronic wafer (insert).

rounds of development. In addition to optoelectronics, silicon circuitry, modeling, and packaging technologies were all key project activities.
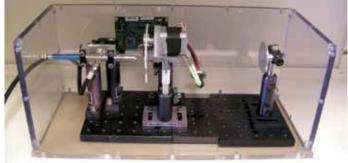
The tiled, scalable architectural unit is a 4 x 4-array wafer. The system has a very small footprint, is rugged, and paves the way for fabrication of larger FPAs, crucial to challenging national security remote sensing missions. Its advanced circuit architectures consumes small amounts of power and its optical fiber interfaces can move terapixels of data per second. Second-generation devices are currently being tested.

Two-pulse Rapid Remote Surface Contamination Measurement

Thomas Kulp

Remote sensing of surface contamination by toxic chemicals or dangerous pathogens is an important capability for both the military and for homeland security initiatives, in order to protect both warfighters in hostile territory and civilians who may be threatened by either accidental contamination or terrorism. This project is focused on a methodology for accurate detection of such surface chemical contamination — especially by chemical warfare agents (CWA) — at a three-meter or greater standoff distance. Existing detection approaches are all limited in performance. Such standoff detection covering large areas is efficient and protects responder personnel.

This project has developed a method using two successive laser pulses. By breaking a chemical bond, the first pulse dissociates the chemical agent to release a relevant detectable byproduct from the surface. The second laser pulse detects an emitted

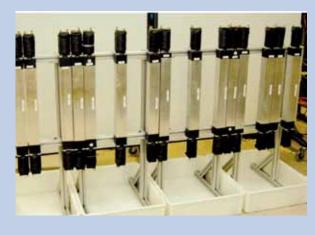**Experimental chamber built to test the project's two-laser-pulse methodology.**

fragment by its fluorescence signature. The method has been successfully demonstrated for detection of several chemical agents on a variety of surfaces, such as wood, cardboard and aluminum, in some cases, quantitatively. While optical emission caused by laser-induced breakdown spectroscopy can interfere with measurement, the project is exploring ways to minimize such interference.

Active Coded-Aperture Neutron Imaging

Peter Marleau

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, as 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.

Coded-aperture imaging works by the same principles as a pinhole camera only with multiple apertures. This approach has been used successfully in x-ray astronomy, but neutrons are harder to modulate. Meanwhile, double-scatter fast neutron imaging, the current state of the art, has limited detection efficiency. Hence 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

Prototype active coded aperture imager showing versatile modular design, each detector element filled with liquid scintillator and read out by photomultiplier tubes on either end.
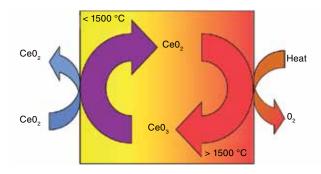
neutrons. This technique results in a better signal-to-noise ratio and efficiency of detection. A set of Monte Carlo simulation tools has been developed and calibrated by experimental results so that future detector designs can be tested. Preliminary results are promising, and this represents the first system of its kind that demonstrates fast-neutron imaging using an active mask.

Sunshine to Petrol

James E. Miller

Domestically produced carbon-neutral transportation fuel: meeting this challenge would be a huge boon toward attacking the problem of global climate change and ensuring the availability of energy to fuel the economy. The solution seems simple: Recycle the carbon dioxide that results from burning gas, oil and other fossil fuel sources by converting it back into hydrocarbons like ethanol, gasoline, and diesel that are used to power automobiles in the first place. Unfortunately, this "trick" is thermodynamically costly, requiring an uphill "push" from some other source of energy.

In this project, solar thermal energy is being applied to supply the required uphill push. Concentrated sunlight provides thermal energy to heat redox active metal oxides to high temperatures where they give up oxygen. The resulting reduced metal oxide is then capable of converting chemically stable and unreactive carbon dioxide (CO_2), to energy rich carbon monoxide (CO), an intermediate long used in fuel-producing syngas chemistry. This step regenerates the starting oxide. Monoliths of the active

Conceptual representation of using a redox active metal oxide and the thermal energy of the sun to generate carbon monoxide (CO) and oxygen (O_2) from carbon dioxide (CO_2) in a two-step cyclic process.
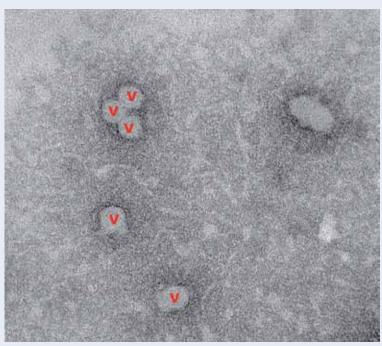
metal oxides have been developed for the unique reactor in which the cyclic reaction occurs. The process has exhibited ongoing improvements and the key issue for the future continues to be increased efficiency.

Optimized Coagulant Chemistry for Water Treatment

May Nyman

With potable drinking water supplies a major concern as a national security issue in this century and beyond, improved methods for ensuring drinking water purity are extremely important. Such methods must protect both against potentially toxic chemical pollutants and pathogenic bacteria and viruses, whether naturally occurring or introduced as a bio-warfare initiative by adversaries.

This project investigated a number of different hybrid precipitates of charged and amphiphilic (part hydrophilic, part hydrophobic) molecular colloids, for the purpose of discovering combinations that would be effective at trapping and precipitating both toxins and biological pathogens in water. Both anionic (negatively charged) polyoxometalates and cationic (positively charged) aluminum clusters were combined with surfactants of opposite charge, which resulted in a complex layered chemical structure in water. In the presence of viruses such as bovine enterovirus or human influenza A, project results showed that the virus particles (virions) were removed — precipitated by a physico-chemical enmeshment within the precipitate. The efficacy of virus removal was assayed via the polymerase chain reaction (PCR). Using NMR and dynamic light scattering techniques, the various precipitates were characterized structurally as well as in terms of their efficacy at viral removal.

Electron micrograph of viral particles (V) enmeshed in a surounding mollecular web of colloid.
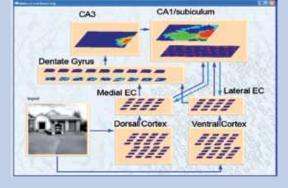
Chemistry was probed to a greater extent with the finding that substitution of a small percentage of gallium (Ga) into the ε-Keggin ion $[Al_{13}O_4(OH)_{24}(H_2O)_{12}]^{7+}$ creates a superior agent for viral removal, the improvement significant by comparison to the slight extra cost of synthesizing the material with a single Ga ion substituted for one of the 13 aluminum (Al) ions. This suggests a pathway for the ongoing improvement of water treatment processes, particularly in areas with a stressed water supply.

As municipalities and communities recognize the need to recycle and purify wastewater supplies, research such as this becomes ever more important for ensuring public health. ■

Modeling Aspects of Human Memory and Reasoning For Scientific Study

Michael Bernard

Schematic of the computational model of brain areas employed when someone facially associates a person with a particular location.

While great strides have recently occurred in the field of human cognition, there is no unified theory regarding the human thought processes involved in memory and reasoning, that is, the neural network dynamics in the brain that underlie such cognitive processing. 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, particularly the cortical-hippocampal pathways firmly implicated in declarative memory consolidation and retrieval. Collaborating with academic neuroscientists, this project is attempting to simulate this form of brain processing in memory consolidation, and to compare the results of human study participants and computational model at memory retrieval. The research is also aimed at a comparison of the activation of the different computational networks in the model with the brain regions known to be activated, as measured in human-subject studies from the brains of responding subjects. For example, 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.
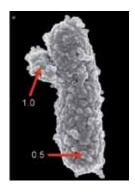
According to evaluations from the academic neuroscientists affiliated with the project, the Sandia research has produced a simulation environment able to accomplish these ends "with a biological realism greater than in any previously implemented model."

Development and Characterization of 3D, Nano-Confined Multicellular Constructs for Advanced Biohybrid Devices

Bryan Kaehr

The intricacies of cell-to-cell communication and the ability of living cells to remodel their environments underpin this project, which is investigating several ways to integrate living cells within environments that can, ultimately create a bridge to the use of living cells as sensors, integrators and manipulators of both organic and inorganic environments.

Several types of interfaces between cells and extracellular materials are being tested, primarily using the technique of dynamic mask multiphoton protein lithography. This strategy enables a diversity of biological micro-architectures to be fabricated, in the presence of cells, from several types of biologically active proteins, which retain their functionality, and which are tunable by altering conditions such as pH (acidity).

Electron micrograph of a rod-shaped bacterial cell (E. coli) asymmetrically coated with gold and platinum.

A fabrication facility has been integrated into the BSL2 certified laboratory at the Advanced Materials Laboratory, and preliminary work has shown that single bacterial cells can be confined in protein microchambers, in situ, resulting in unanticipated behavioral modifications.

In related work, this team has been able to use living bacteria as dynamic template upon which to segregate distinct metallic agents, effectively creating bimetallic motile microparticles, which are self-perpetuating. Ultimate possible applications of this ground-breaking research include micro-sensors and actuators, biocomputers, biomedical and bionic technologies.

Host Suppression and Bioinformatics for Sequence-based Characterization of Unknown Pathogens

Todd Lane

The level of sophistication for engineering DNA sequences has reached a point whereby adversaries can readily engineer a pathogenic microorganism designed to elude detection by conventional tools.

For such an unknown organism, current methods would rely on classic microbiological methods of culturing and growing the organism, processes that are very slow. By comparison, ultrahigh throughput sequencing (UHTS) of DNA (by which entire genomes [genetic information] are sequenced) is capable of rapidly analyzing DNA from such pathogens, so that it can be evaluated. However, extracting pathogen DNA against a large background of human DNA from cells is necessary before such DNA can be sequenced and analyzed. Rather than a needle in a haystack problem, this more-closely analogizes to finding a light-yellow fragment of hay in a similarly colored haystack.

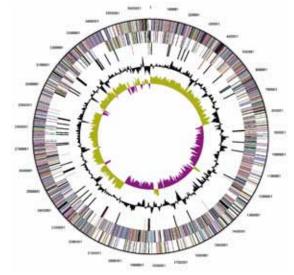This project is addressing the solution of selectively enriching this DNA mixture for the pathogen DNA, either by destroying human DNA or by finding other molecular biological methods to isolate the pathogen DNA, so that it can be selectively duplicated, and sequenced by UHTS. The project is comparing and evaluating experimental protocols by processing mock clinical samples, as well as evaluating a variety of software tools and methods designed to help identify pathogen DNA sequences for their similarity to those of known organisms.

Concentration of dye-labeled double-stranded DNA at a nanoporous polyacrylamide membrane.

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

Rajat Sapra

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 mismatch between the process of saccharification — the breakdown of the lignocellulose fibers in plant wastes to sugars — occurring most efficiently at 50–60 °C and fermentation, the biological process by which bacteria and certain fungi form the biofuel ethanol from these sugars, which normally occurs at about 30 °C. Additionally, saccharification of lignocellulose yields a mix of five- and six-carbon sugars, but many popular fermenting organisms are unable to use five-carbon sugars for fermentation to ethanol.

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

Circular chromosome of the thermophilic bacterium *G. thermoglucosidasius*.

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. Future work will aim at engineering a butanol synthesis pathway.

Sandia National Laboratories

NNSA National Nuclear Security Administration

LOCKHEED MARTIN