Beauty, molecules deep

Sunshine to petrol
Witnessing a birth

Alliances
**What is LDRD?**

The Laboratory Directed Research and Development (LDRD) program provides Sandia the flexibility to invest in discretionary research and development that stretches the Labs’ science and technology capabilities.

LDRD supports Sandia’s four primary strategic business units: nuclear weapons; defense systems and assessments; energy, resources, and nonproliferation; and homeland security and defense. LDRD also promotes creative and innovative R&D by funding projects that are short term, often high risk, and potentially high payoff, attracting exceptional research talent from across many disciplines.

When the LDRD logo appears in this issue, it indicates that at some stage in the history of the technology or program, LDRD funding played a critical role.

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**On the cover:**

Nanoparticle-enhanced coatings are making their way to consumer products such as flat-panel TV screens. A consortium led by Sandia is addressing the associated technological barriers. See page 5.

*(Photo by Randy Montoya)*
Dear Readers,
When I came to Sandia in 1990, many wondered how the national labs would fare in a world in which some of the biggest threats to our nation have no geographic locations – threats like energy dependence and flagging U.S. competitiveness. One objective was to tap the intellectual capital amassed at the labs in ways that would boost the U.S. economy.

The labs soon discovered this wasn’t as simple as offering up the technological bounty to all takers. Good ideas don’t go far on their merits alone. Today we know alliances with industry, universities, and government agencies are essential to bringing products to bear on national security.

This month we look at the effects some partnerships are having on our nation’s welfare:

- A research and education institute turning students into tomorrow’s technology leaders (page 4)
- A consortium gaining ground in the burgeoning nanocoatings market (page 5)
- Fast-track programs giving warfighters needed new tools (page 10)
- A video game teaching soldiers to be both alert and diplomatic (page 17)

We also describe how a machine turns pollution back into fuel (page 2), reconsider an asteroid that visited devastation on Siberia a century ago (page 13), recount the first eyewitness account of a buckyball’s birth (page 14), and explore whether ancient Pueblo Indians drank beer before Europeans brought wine to the American Southwest (page 16). I hope you enjoy the issue.

John German
Sandia Technology Editor
Researchers are building a device intended to chemically reenergize carbon dioxide using concentrated solar power. The resulting carbon monoxide could be used to make hydrogen or serve as a building block of combustible liquid fuels.

The prototype device, called the Counter Rotating Ring Receiver Reactor Recuperator (CR5, for short), will break carbon-oxygen bonds in carbon dioxide to form carbon monoxide and oxygen in two distinct steps.

Liquid solar fuel is the end product – methanol, gasoline, or other combustible liquid made from water and the carbon monoxide. The Sandia research team calls the approach “Sunshine to Petrol” (S2P).

CR5 inventor Rich Diver says the original purpose of the device was to break down water into hydrogen and oxygen to fuel a future hydrogen economy. They soon realized that the CR5 also could break down carbon dioxide to distill carbon monoxide—a needed component of liquid fuel. They have shown proof of concept and now are completing a prototype device.

Team member Ellen Stechel says scientists have known for a long time that recycling carbon dioxide is possible, but many doubted it could be done economically.

“This invention, though probably a good 15 to 20 years away from being on the market, holds a real promise of being able to reduce carbon dioxide emissions while preserving options to keep using fuels we know and love,” she says.

“Recycling carbon dioxide into fuels is an attractive alternative to burying it.”

Sandia’s LDRD program supports the effort, which has attracted interest and some funding from the Defense Department’s Defense Advanced Research Projects Agency (DARPA).

“What’s exciting about this invention is that it will result in fossil fuels being used at least twice, meaning less carbon dioxide being put into the atmosphere and a reduction of the rate that fossil fuels are pulled out of the ground,” Diver says.

As an example, he says, coal would be burned at a clean coal power plant. The carbon dioxide from the burning of the coal would be captured and reduced to carbon monoxide in a CR5. The carbon monoxide would then be the starting point of making gasoline, diesel, jet fuel, or methanol.
After the synthesized fuel is made from carbon monoxide, it could be transported through a pipeline or put in a truck and hauled to a gas station, just like gasoline refined from petroleum is now. Plus, says Diver, it would work in ordinary gasoline and diesel engine vehicles.

Team member Jim Miller says that while the first step would be to capture the carbon dioxide from concentrated pollution sources, the ultimate goal would be to snatch it out of the air. An S2P approach that includes atmospheric carbon dioxide capture might ultimately produce carbon-neutral liquid fuels.

“Our overall objective with this prototype is to demonstrate the practicality of the CR5 concept and to determine how test results from small-scale testing can be expanded to work in real devices,” Miller says. “The design is conservative compared to what might eventually be developed.”

Diver says the CR5 prototype, located at Sandia’s National Solar Thermal Test Facility in Albuquerque, should be completed soon. Initial tests will break down water into hydrogen and oxygen. That will be followed by tests that similarly break down carbon dioxide into carbon monoxide and oxygen.

The research team has proven that the chemistry works repeatedly through multiple cycles without performance loss and on practicable cycle times.

“We just have to do it all in one continuous working device,” says team member Nathan Siegel.
Nanotech 101

A radically different type of science education intended to accelerate innovation and involve more U.S. students in the study of nanotechnology is the goal of the National Institute for Nano Engineering (NINE), formed recently by Sandia and 17 leading American universities and technology companies.

The partnership is driven by concerns over the health of U.S. science education, as highlighted in the 2005 National Academies report “Rising Above the Gathering Storm.” The recently enacted America COMPETES Act supports the establishment of technology innovation and education institutes.

“This group came together based on a sense of urgency and recognition that academia, American industry, and government need to work together to develop a new partnering model that will lay the foundation for the nation's future in science and engineering,” says Rick Stulen, Sandia Vice President for Science, Technology, and Engineering.

The Sandia-led group has gathered industrialists, college professors, administrators, and students to develop a novel approach to teaching nano-engineering that will complement and extend the more standard techniques of education.

Students from collaborating institutions, ranging from freshmen to advanced graduate students, form integrated research teams that solve real science and engineering problems at scales where the rules governing the behavior of atoms and molecules preside.

Fifteen projects funded by Sandia’s program are under way involving as many as 50 students. The research is being done both at Sandia facilities and at participating institutions.

NINE students work on nano-engineering problems.

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NINE research will be conducted at partner facilities such as the Center for Integrated Nanotechnologies Core Facility at Sandia/New Mexico.
At the truly tiny scale of nanoparticles, attractions and repulsions among atoms and molecules often overwhelm the more ordinary forces at play in the larger-scale world. A pair of particles, for example, nudged close enough together, might snap like magnets into one.

Such nanoscale forces, driven in some cases by the momentary orientations of electrons, become a problem when the goal is to keep particles evenly dispersed in liquid — a challenge for manufacturers who want to make products featuring nanoparticle-enhanced films or coatings. Nanoparticles suspended in solvents at high densities tend to clump while the coating is drying, negating the benefits of their nanosized ingredients.

Improving the processing and manufacturability of such coatings and thin films is the primary goal of a research collaboration that began last spring among Sandia and a half dozen companies. The Nanoparticle Flow Consortium includes 3M, BASF, and Corning, among others. Sandia serves as the hub for the three-year, $2 million cooperative research and development agreement.
Nanoparticles make good building blocks for new and better materials because the materials can be, in essence, built from scratch at the molecular level. This allows chemists to take fuller advantage of principles of physics and chemistry to create materials with characteristics not available through traditional bulk chemistry methods.

Currently, however, most nanoscience takes place in research laboratories where very small amounts of matter are manipulated using specialized equipment. To manufacture consumer products, companies will need to master high-throughput, large-scale nanomaterial processing techniques.

The potential benefits are enormous. Embedding nanoparticles in coatings and films could result in materials with useful new properties: coatings that react to the environment, paint or glass that color-shifts like a chameleon, self-lubricating or self-healing surfaces, or antimicrobial coatings for hospital ventilation systems, for example.

The U.S. National Science Foundation estimates that by 2015, the worldwide nanotechnology market could reach a trillion dollars annually. Potential mass-produced, nano-coated consumer goods and materials on the horizon include improved flat-screen TV displays, stronger and more transparent glue, lightweight composites, specialized sealants for microelectronics devices, and new materials for sensing and medical devices.

“The amount of money involved is staggering,” says Randy Schunk of Sandia’s Multiphase and Nanoscale Transport Processes Department. The chemical, defense, aerospace, electronics, computing, health care, and other industries are expected to see nanotechnology advances worth tens to hundreds of billions of dollars each, he says.

The Nanoparticle Flow Consortium’s work will address two main technical challenges: stable dispersal of nanoparticles in solution during processing, and improved understanding of particles dispersed in materials under stress or flow and how these states are affected by nanoscale forces. Both were viewed by participants as limiting factors in manufacturing of nano-enhanced materials and thin films.
To address these issues, Sandia is developing modeling and simulation tools to understand liquid flow chemistry, nanoparticle dispersal stability, and particle control. Together with Sandia’s high-performance computers, the new software tools are expected to result in a predictive capability for nanoparticle processing – meaning materials and techniques with the highest chances of success can be designed on computers before they are ever tried in a laboratory. The modeling tools will be available to all consortium partners.

Resolution of these technical barriers may open doors not only to advanced coatings, but to layered bulk materials as well, says Schunk.

“Manufacturable implies practical,” he says. “Companies need to disperse these particles in liquid, then cast them, coat them, layer them, or paint them on something, often over large areas. Such problems aren’t necessarily going to be addressed in a research lab.”

Nanoparticle dispersal in liquid is a key issue for the companies involved in the National Institute for Nano Engineering (NINE), a national hub for nanoscale engineering and education (see page 4). NINE collaborators and students will benefit from the consortium’s work, he says.

The Nanoparticle Flow Consortium is modeled after a similar cooperative research effort that began at Sandia in 1996, the Coating Related Manufacturing Processing Consortium (CRMPC). The CRMPC included many of the same partners and resulted in a software package, GOMA 5.0, which far exceeded existing modeling capabilities for coating processes, Schunk says.
Zinc-oxide nanostructures created by Sandia researchers who, by controlling surface chemistry at each stage of formation, were able to orient crystals as they formed and produce a wide variety of crystalline structures. Structures with desirable electronic and optical properties would be useful for smaller, 3D-patterned microelectronic devices of the future. The program funded the work.

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Stacked-grain microstructure of a bismuth- and titanium-based ceramic created as part of an project to fabricate materials that can substitute for lead in electrical components. The research team applied physical shear stresses during material growth to produce ceramic materials with desired grain orientation and electrical properties.

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Self-assembled quantum dots produced as part of an project to improve the technology base for infrared detection of people and electronic equipment for both military and civilian security. Current IR photodetectors operate only at cryogenic temperatures and use mercury. The Sandia project has pursued IR detection using self-assembled quantum dots of less-toxic indium and gallium. The yellow dots are approximately 25 nanometers in diameter.

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Developing an infrared detector that automatically distinguishes humans from wildlife and other moving objects is the goal of a project that could minimize nuisance alarms in border security systems. The technique combines results from multiple image frames and employs computer algorithms that compare known human-motion behavior with motions captured in the image series.

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Larry Stephenson looks into the vacuum chamber of a molecular beam epitaxy machine at the Center for Integrated Nanotechnologies Core Facility in Albuquerque. The machine, in which crystalline materials with tailored semiconductor structures are grown, was filmed recently for a scene in the upcoming science fiction movie “The Game.”

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(MPhoto by Randy Montoya)
In a world where national security threats evolve more rapidly than ever before, the Department of Defense and Department of Homeland Security are facing new challenges: How will innovations that save lives quickly reach the warfighter, analyst, or emergency responder without breaking a stressed federal budget? Who will develop and make the next-generation products that meet rapidly changing national security needs?

Commercial firms are under similar time and budget pressures. Technology innovation is essential as they anticipate customer problems that require fast but comprehensive research and development programs. Firms in the aerospace and defense industries often face a double whammy: how to quickly bring innovations to market while meeting stringent military or regulatory requirements and specifications. Increasingly, these firms are seeking alliances with universities and national laboratories, whose R&D infrastructures are in place and whose multidisciplinary staffs allow them to tackle questions at all points along the product development cycle. Sandia has formed many military and industrial alliances, some of which extend back to the lab’s founding, that are helping firms develop new capabilities and enhance their own capabilities.

A few of the products created through alliances with Sandia’s Defense Systems & Assessments group are described on pages 11 and 12. Such alliances are the foundation for Sandia’s future as well as a wellspring for tomorrow’s national security technology.
Electric guns

Gunpowder has propelled projectiles for more than 900 years. Ranging a shell fired by high explosives is both a science and an art, due to variables such as the amount of explosives used and differing explosive chemistries. Range is limited by the strength and weight of the guns themselves.

Electromagnetic launchers, first proposed more than 25 years ago, are now feasible. Their advantages are more precise muzzle velocities, as the “charge” can be finely tuned; far greater range, as the shell can be accelerated the entire length of the launcher; and a smokeless, heatless launch, which helps to conceal the location of the launcher.

Lockheed Martin is developing both long-range launchers (many times the range of traditional guns) with very heavy payloads, and mortars for closer-in battles.

Welding without sparks

Boeing and Sandia collaborate under a broad cooperative research and development agreement signed in 2002 that covers 14 technical projects.

In one effort, Sandia adapted its computer modeling codes to understand the chemical processes at work during Friction Stir Joining (FSJ) operations. The technique, invented in 1991, is a method of joining metals that avoids the heat, filler material, and other potential problems of conventional welding. FSJ welds are created by frictional heating and mechanical deformation of the materials.

Another Boeing-Sandia collaboration is improving the analysis of fracture and failure in composite materials. Sandia developed the peridynamic theory of continuum mechanics, a potentially revolutionary advancement in the analysis of structural failures in materials because of its ability to model the growth, interactions, and effects of any number of cracks in complex geometries.
Smaller SARs that can fly on unmanned aerospace vehicles (UAVs) bring surveillance capabilities down to the company and battalion level.

Boeing has applied the code to problems in metallic materials and is collaborating with Sandia to extend the model to fracture in composite materials.

Boeing’s new commercial airliner, the 787 Dreamliner, makes extensive use of composite materials.

**Hitting high-value hideouts**

Holding at risk hardened, deeply buried facilities in rogue nations is a significant national security challenge, especially if they harbor components of a nuclear or chem/bio weapons program. A massive ordnance penetrator (MOP) is one way to breach blast doors, but MOPs could spread contaminants by its blast.

The Matrix trilogy of movies showed machines burrowing deep into the earth to penetrate and destroy the deeply buried home of unplugged humans. Through a DARPA program, Sandia is developing a weapon with similar capabilities, albeit less dramatic than circular saws whizzing at the ends of robotic arms. A number of corporations are interested in partnering with Sandia for phase II development.

**Seeing what the enemy can’t**

In any battle space, many actions are purposefully done at night, or under daytime conditions that hinder an enemy’s ability to see what is happening. Clouds, smoke, fog, dust, and heavy rain blind most optical and traditional radar systems. In World War II large night movements and aerial bombardments occurred frequently. Only a fortunate break in the clouds revealed the Japanese fleet steaming toward Midway.

The battle spaces in today’s asymmetrical warfare are much smaller. A new generation of radars promises to help soldiers see during these conditions. Synthetic aperture radars (SARs) use computational techniques to see over a hill or around a corner. Rockwell Collins, General Atomics, and ITT Corporation are working with Sandia to develop enhanced SARs based on differing payload sizes and advanced capabilities.
Small rock, big shock

Forest devastation in Siberia a century ago may have been caused by an asteroid only a fraction as large as previously published estimates, according to supercomputer simulations that more closely match the known facts about the Tunguska asteroid’s destruction than earlier models.

The research is funded by Sandia’s LDRD program.

“That such a small object can do this kind of destruction suggests that smaller asteroids are something to consider,” says principal investigator Mark Boslough of the impact that occurred June 30, 1908.

The new simulations show that the center of mass of an asteroid exploding above the ground is transported downward, causing stronger blast waves and thermal radiation pulses at the surface than would be predicted by an explosion limited to the height at which the blast was initiated. Previous scientific estimates ignored the downward momentum of the asteroid’s mass.

“Our previous understanding was oversimplified,” says Boslough. “We no longer have to make the same simplifying assumptions, because present-day supercomputers allow us to do things with high resolution in 3-D.”

Simulations show that as the asteroid penetrates deeper into the atmosphere, increasing atmospheric pressure becomes more and more resistant and causes the asteroid to explode as an airburst.

Because of the additional energy transported toward the surface by the fireball, what scientists had thought to be an explosion between 10 and 20 megatons was more likely only three to five megatons.

“Any strategy for defense or deflection should take into consideration this revised understanding of the mechanism of explosion,” says Boslough.

Because smaller asteroids approach Earth statistically more frequently than larger ones, he says, “we should be making more efforts to detect the smaller ones than we have till now.”


Above: Fireball that might result from an asteroid exploding in Earth’s atmosphere, in a supercomputer simulation devised by a team led by Mark Boslough. (Photo by Randy Montoya)

Below: Simulations of the Tunguska asteroid taking into account downward momentum.

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Most everyone in science has heard of buckyballs, but no one had seen one being born until Jianyu Huang unexpectedly witnessed, under a microscope, the walls of a fullerene structure form into a sphere and then shrink into the well-known soccer ball shape.

Buckyballs – more formally known as buckminsterfullerene C-60 – are nanostructures formed by arrangements of carbon atoms that seem stitched or welded together, in appearance much like a soccer ball.

The carbon-carbon bonds give the buckyball great strength, and the spherical structure forms a relatively impermeable cage that conceivably could safely transport molecules of hydrogen for fuel, or tiny doses of medicine to targeted sites within the human body.
Atomic images of the inside of a nanotube show the formation of fullerenes, their reduction to C-60 buckyballs, and their dispersion.

But before their widespread use is possible, buckyballs have to be available in large numbers. To achieve that, better understanding of how they form is crucial.

“We have now the first direct, in situ, experimental proof of the hypothesis that these structures are formed by the heated ‘shrink-wrapping’ of carbon sheets,” says Jianyu Huang, who first watched the structures form under a specialized microscope.

The hypothesis: Heating bends single-atom-layer carbon sheets into nano bowls, and then adds more carbon atoms to the edges of the bowls until fullerenes — larger, less stable versions of the C-60 molecule — shrink to form stable and spherical C-60 molecules.

Buckyball codiscoverer (1985) and Nobel laureate (1996) Richard Smalley had hypothesized that buckyballs are formed in this fashion, but at his death in 2005 no experimental confirmation was yet available, and other methods of C-60 formation have been proposed.

Huang’s discovery happened unexpectedly. He was looking for flaws in nanotube durability. Transmitting electric current through the atom-sized tip of a scanning tunneling microscope (STM) — itself inside a transmission electron microscope (TEM) — he had heated a 10-nanometer-diameter multiwalled carbon nanotube to approximately 2,000 degrees Celsius when he saw the exterior shells of giant fullerenes form from peelings within the nanotube.

High-resolution two-dimensional images of the process taken by a CCD camera attached to the microscope showed the fullerenes reducing in diameter, linearly with time, until the structures became the size of C-60. Then the buckyballs vanished.

Simulations created at Huang’s request by Boris Yakobson’s team at Rice University showed that heating could reduce fullerenes by emitting carbon dimers (pairs of atoms) until they reached the basic buckyball shape. Further removal of carbon pairs collapsed the structure.


Interpretation of the research was paid for by Sandia’s Center for Integrated Nanotechnologies (CINT) and the program. CINT is a joint effort of Sandia and Los Alamos national labs and is supported by the DOE’s Office of Science.

“I used to study metals,” says Huang, who grew up in a remote Chinese farming village and now utilizes the most complex instruments at CINT. “But carbon nanomaterials now are much more interesting to me.”

The buckyball discovery was initially made by Huang on similar instruments at Boston College, and then interpreted at CINT.

“The STM probe inside the TEM is a very powerful tool in nanotechnology,” Huang says. “The STM probe is like God’s finger; it can grab extremely small objects, as small as a single atomic chain, enabling me to do nanomechanics, nanoelectronics, and even thermal studies of carbon nanotubes and nanowires.”

Beer before wine

Pot sherds collected by New Mexico state archeologist Glenna Dean and chemically analyzed by Sandia researcher Ted Borek suggest that food or beverages made from fermenting corn were consumed by native inhabitants of the American Southwest centuries before the Spanish arrived.

Dean, researching through her small business Archeobotanical Services, says many archeologists believed – possibly mistakenly – that the Spanish first introduced alcohol to local inhabitants when they brought grapes and wine in the early 16th century.

“By this reasoning, ancestral pueblosans would have been the only ones in the Southwest not to know about fermentation,” she says.

Historical evidence suggests fermented beverages existed for surrounding native groups before Spanish contact. The Tarahumara Indians in northern Mexico to this day drink a weak beer called tiswin, made by fermenting corn kernels.

To check her hypothesis that pueblosans may have done the same, Dean presented Borek with three types of samples: pots in which she herself brewed tiswin, tiswin-brewing pots used by Tarahumara Indians, and pot sherds from 800-year-old settlements in west-central New Mexico.

Using gas chromatography and mass spectrometry to analyze vapors produced by mild heating of pot samples, Borek checked for the presence of similar organic species.

“We see similarities,” says Borek. “We have not found that smoking gun that definitely provides evidence of intentional fermentation. It’s always possible that corn fermented in a pot without the intent of the owner and that it wasn’t meant to be drunk.”

Analysis is now under way to highlight patterns of organic species that might provide a more definite result.

Borek did the work through Sandia’s New Mexico Small Business Assistance program, which allows the Lab to apply a portion of the gross receipts taxes it pays the state each year to provide technical advice and assistance to New Mexico small businesses.
Some 20,000 soldiers a year may soon be trained in interpersonal skill building and cross-cultural awareness using a new video game created for the Defense Advanced Research Projects Agency (DARPA).

Developed by researchers from Sandia and BBN Technologies, the adaptive-thinking game and training methodology prepares warfighters for difficult situations in places such as Afghanistan and Iraq.

“We are talking about interpersonal communication, negotiation skills, and interpersonal rapport,” says project lead Elaine Raybourn. “The goal is to make soldiers better thinkers and communicators under stress.”

The tool is conceptually similar to a multiplayer game Raybourn developed several years ago, now used at Ft. Bragg, N.C., to train members of the U.S. Army Special Forces.

The new game developed for DARPA will allow as many as 64 people to play on networked computers simultaneously. Instructors can create custom scenarios or jump in to change the game’s direction at any time.

When DARPA came to Sandia it already had a training game in the works designed by BBN Technologies. It focused on physical challenges, such as encounters with improvised explosive devices and convoy ambushes.

“DARPA also wanted a nonkinetic adaptive thinking piece for the soldiers, to learn how to negotiate with tribal leaders, for example,” Raybourn says. “When things go wrong, troops have to learn to shift how they think in environments that are potentially dangerous.”

The modules are comprised of a socio-cultural overlay for a geographical area that is linked to key events and roles of host nation civilians.

Experts who helped design the game included an instructor from the Fort Lewis Battle Command Training Center (Fort Lewis, Wash.), as well as two former Sandia employees with military backgrounds.

DARPA plans to distribute the product to the Army and eventually the other armed forces. It also will be made available free to the U.S. military services and federal law enforcement agencies through DARPA’s website.
Firms in the aerospace and defense industries often face a double whammy: how to quickly bring innovations to market while meeting stringent military or regulatory requirements and specifications. Increasingly, these firms are seeking alliances with universities and national laboratories.

Jerry Langheim
Strategic Alliances, Defense Systems & Assessments, Sandia National Laboratories