Science & Technology Review

May 2007

National Nuclear Security Administration's Lawrence Livermore National Laboratory

Simulating Quantum Technologies

Also in this issue:

- The Graceful Aging of Plutonium
- Imaging Complex Biomolecules
- Raftlike Structures in Cell Membranes
- Teller's Legacy in Condensed-Matter Physics

About the Cover

Computer simulations are a valuable tool for learning about nanometer-size materials and accounting for the behavior of individual atoms and electrons. The article beginning on p. 4 describes quantum molecular dynamics methods developed by Livermore's Quantum Simulations Group to model material processes at the nanoscale. The group focuses on a wide range of materials research, from simulating basic phenomena, such as water and hydrogen under extremely high pressures, to evaluating potential materials for use in various technological applications. On the cover, a snapshot from a simulation of aluminum antimonide shows the atomic and electronic structure of the semiconductor material. Silver and gold balls indicate the positions of atoms in the crystal lattice, and the nearly transparent clouds characterize the electron density.

Cover design: Alexandria Ballard

About the Review

Lawrence Livermore National Laboratory is operated by the University of California for the Department of Energy's National Nuclear Security Administration. At Livermore, we focus science and technology on ensuring our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published 10 times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

Please address any correspondence (including name and address changes) to *S&TR*, Mail Stop L-664, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, California 94551, or telephone (925) 423-3432. Our e-mail address is str-mail@llnl.gov. *S&TR* is available on the World Wide Web at www.llnl.gov/str.

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Science & Technology REVIEW

May 2007

Lawrence Livermore National Laboratory

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Illustrator
Sabrina Fletcher

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Print Production
Charlie M. Arteago, Jr., and Cenveo GAC Indianapolis

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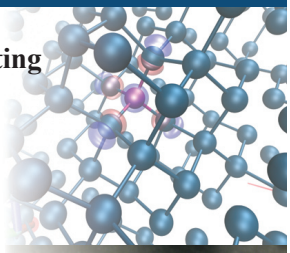
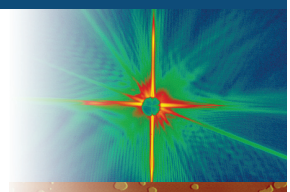
Features



Research Highlights



Teller Centennial Highlight

Departments

Lab's design selected for reliable replacement warhead

The Department of Energy's National Nuclear Security Administration (NNSA) announced that it has selected the design team from Lawrence Livermore and Sandia national laboratories to develop the reliable replacement warhead (RRW) for a portion of the nation's sea-based nuclear deterrent. RRW is a joint NNSA–U.S. Navy program to ensure long-term confidence in a more secure, smaller, and safer nuclear weapons stockpile. NNSA and the Navy will work together to generate a detailed RRW project plan and cost estimate for developing and producing the system.

In 2006, the Nuclear Weapons Council approved the RRW concept as a feasible approach for sustaining the nation's nuclear weapons stockpile. NNSA selected the Livermore–Sandia design because of the high confidence that it can be certified without underground nuclear testing. Several features of the design submitted by Los Alamos National Laboratory, also in partnership with Sandia, will be developed in parallel with the Livermore effort. As these features mature, they may be introduced into the warhead design as it progresses.

An important aspect of the RRW Program is its ability to exercise and maintain the critical skills of the country's nuclear weapons design, engineering, and production personnel. An integrated team of designers and engineers led by Livermore will work with the production plants to develop the nuclear explosive component of the weapon. Sandia will develop the nonnuclear components and ensure compatibility with the Department of Defense's Trident submarine-launched ballistic missile delivery system. The Navy will lead the overall project team.

Contact: K. Henry (Hank) O'Brien (925) 423-5017 (obrien6@llnl.gov).

Deciphering tissue-specific signatures in human genome

A collaboration led by Ivan Ovcharenko, a bioinformatics scientist in Livermore's Computation Directorate, has translated DNA sequence data into functional signatures corresponding to specific tissues of the body. Researchers from Lawrence Berkeley National Laboratory, the Department of Energy's Joint Genome Institute, and the University of Chicago participated in the study. Results appeared in the February 2007 issue of *Genome Research*.

Every tissue cell has the same code that dictates and regulates how the genome's approximately 30,000 genes perform the organism's myriad functions. However, much of this orchestration happens outside gene boundaries in what is known as noncoding DNA. Previously considered "junk" DNA, these regions are home to critical regulatory elements such as enhancers. Enhancers can be found in many places—inside the genes they regulate, barricaded before or after the genes they control, or located millions of nucleotide bases, or units of DNA, up or downstream from the genes they regulate.

To track down these elements, Ovcharenko's team analyzed a massive experimental gene expression, or microarray, data set generated by the Genomics Institute of the Novartis Research Foundation. A sequence-pattern search deciphered the code of tissue-specific regulatory elements hidden in the noncoding part of the genome, and it identified the signatures for specific tissues. The team then merged three analysis factors to develop an enhanced identification score, which indicates the level of confidence that a signature's location is accurate and that it contributes to the identified gene-expression event. This method may ultimately help scientists screen gene mutation by parsing the more cryptic elements of the genetic code.

Contact: Ivan Ovcharenko (925) 422-5035 (ovcharenko1@llnl.gov).

Laboratory Science Entwined with Rise in Computing

LIVERMORE scientists have been using computer simulations to attain breakthroughs in science and technology since the Laboratory's founding. High-performance computing remains one of the Laboratory's great strengths and will continue to be an important part of future research efforts.

To meet our programmatic goals, we demand ever more powerful computers from industry and work to make them practical production machines. We develop system software, data management and visualization tools, and applications such as physics simulations to get the most out of these machines. High-performance computing, theoretical studies, and experiments have always been partners in Livermore's remarkable accomplishments.

The Laboratory's cofounders, Ernest O. Lawrence and Edward Teller, along with Herbert York, the first director, recognized the essential role of high-performance computing to meet the national security challenge of nuclear weapons design and development. Electronic computing topped their list of basic requirements in planning for the new Laboratory in the summer of 1952. The most modern machine of the day, the Univac, was ordered at Teller's request before the Laboratory opened its doors in September. The first major construction project at the site was a new building with air conditioning to house Univac serial number 5, which arrived in January 1953.

Edward Teller, whose centennial we are celebrating this year, greatly appreciated the importance of electronic computing. His thinking was guided by his interactions with John von Neumann, an important pioneer of computer science, and his prior experiences using "human computers" for arduous calculations. Teller was attracted to and solved problems that posed computational challenges—the most famous being his collaborative work on the Metropolis algorithm, a technique that is essential for making statistical mechanics calculations computationally feasible. His work demonstrated his deeply held belief that the best science develops in concert with applications.

This heritage of mission-directed high-performance computing is as strong as ever at Livermore. Through the National Nuclear Security Administration's (NNSA's) Advanced Simulation and Computing Program, two of the world's four fastest supercomputers are located at Livermore, and they are being used by scientists and engineers at all three NNSA laboratories. The prestigious Gordon Bell Prize for Peak Performance was won in 2005 and 2006 by simulations run on BlueGene/L, a machine that has 131,072 processors and clocks an astonishing 280 trillion floating-point operations per second. Both prize-winning simulations modeled physics at the nanoscale to gain fundamental insights about material behavior that are important to stockpile stewardship and many other programs at the Laboratory.

The article beginning on p. 4 features Livermore-designed computer simulations that focus on the nanoscale beginning with first principles: the laws of quantum mechanics. The use of large-scale simulations to solve quantum mechanics problems was pioneered in 1980 by Livermore scientist Bernie Alder in collaboration with David Ceperley from Lawrence Berkeley National Laboratory.

To predict how materials will respond under different conditions, scientists need accurate descriptions of the interactions between individual atoms and electrons: how they move, how they form bonds, and how those bonds break. These quantum molecular dynamics calculations are extremely demanding. Even with the Laboratory's largest machines, computational scientists, such as those in Livermore's Quantum Simulations Group, must design clever modeling techniques to make the run times feasible (hours to days) for simulating perhaps only 1 picosecond of time (a trillionth of a second).

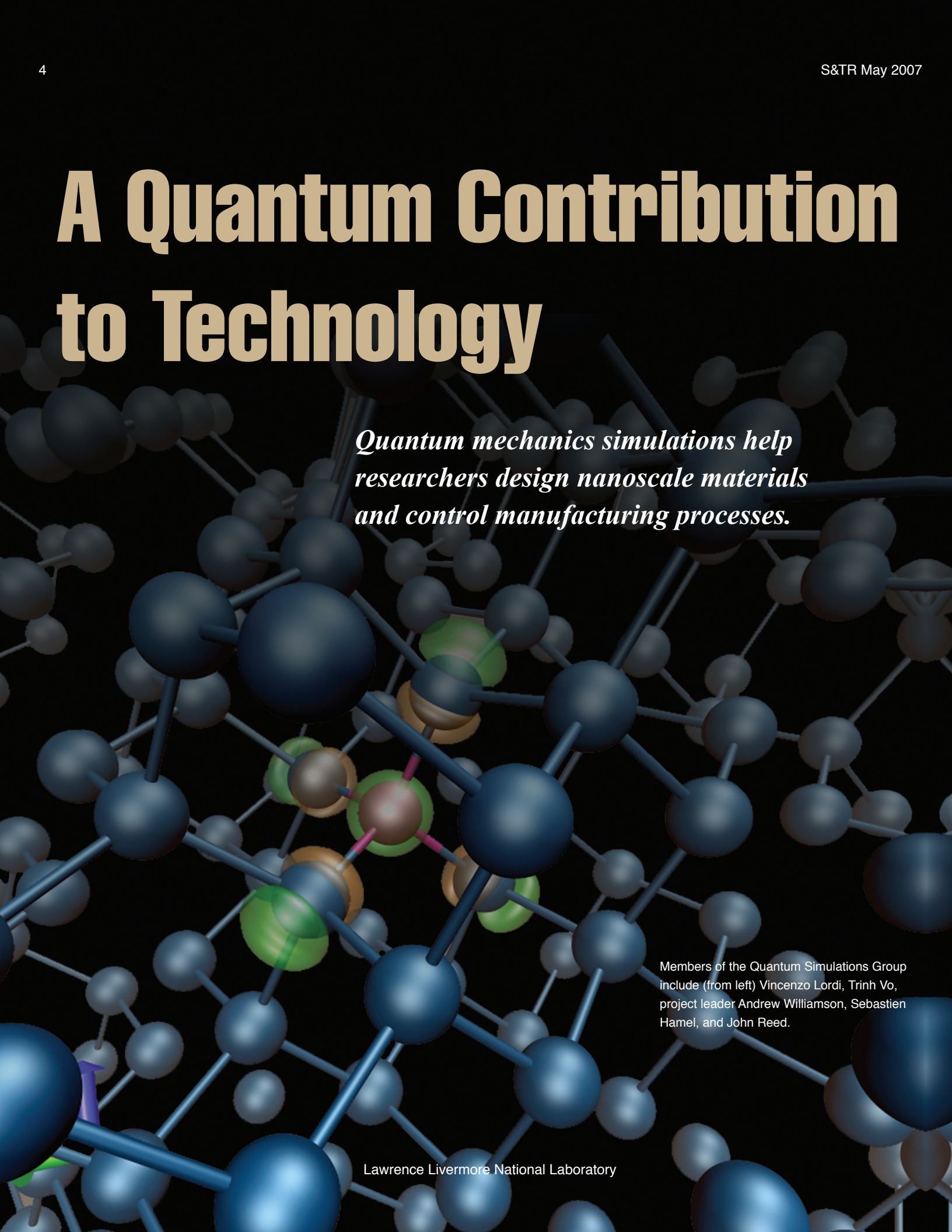
Outstanding science and technological applications go hand-in-hand in this work. As described in the article, our scientists are using quantum simulations to evaluate nanomaterials to reduce the size of gamma-ray detectors for homeland security, provide improved cooling systems for military applications, and help design even smaller computer chips. Yet another quantum simulation project is examining materials to improve hydrogen storage for future transportation.

These examples merely scratch the surface of the novel uses for nanotechnologies that scientists can explore through simulations. One can only imagine what possibilities might be uncovered in the future as computational power continues to increase and researchers become ever more proficient in nanoscale simulations and engineering. True to its heritage, Livermore will be at the forefront of this nascent revolution.

■ George H. Miller is director of Lawrence Livermore National Laboratory.

A Quantum Contribution to Technology

Quantum mechanics simulations help researchers design nanoscale materials and control manufacturing processes.



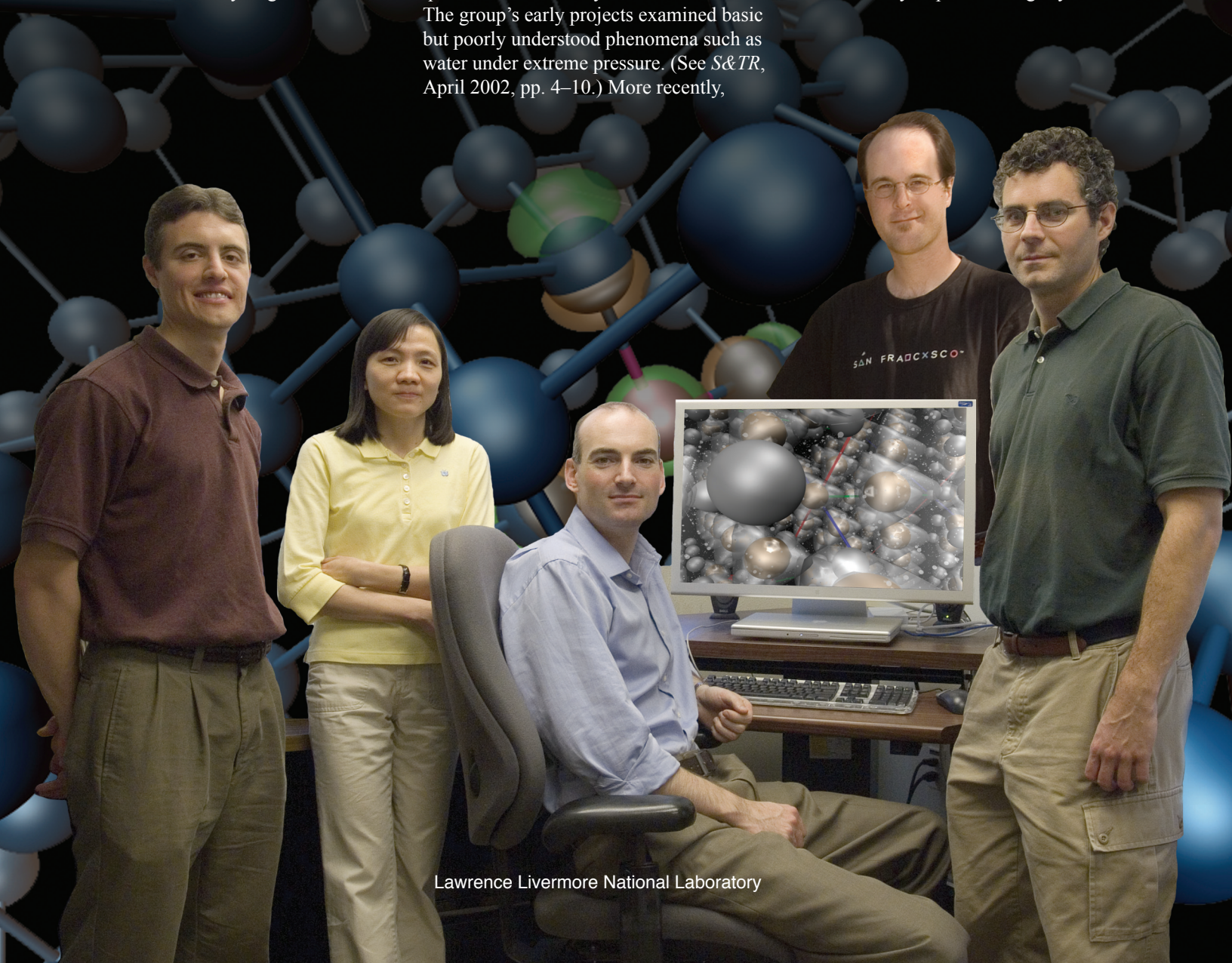
Members of the Quantum Simulations Group include (from left) Vincenzo Lordi, Trinh Vo, project leader Andrew Williamson, Sebastien Hamel, and John Reed.

At the nanoscale, computer simulations are often the only way that researchers can learn about materials. Imagine the shaft of a human hair sliced about 50,000 times. One slice is about a nanometer, or one-billionth of a meter—a distance that can be spanned by just 3 to 10 atoms. This minute size range is the realm of nanoscale science, where materials typically measure between 1 and 100 nanometers (nm) across.

Accurate descriptions of nanoscale materials must account for the behavior of individual atoms and electrons: how they move, how they form bonds, and how those bonds break. In 1999, a Livermore simulation of such quantum behavior revealed the secrets of hydrogen fluoride mixing with water at high temperatures and pressures. The motion being modeled lasted just 1 picosecond (a trillionth of a second), yet the calculation required 15 days and the entire resources of Blue Pacific, which at the time was Livermore's fastest supercomputer. (See *S&TR*, July/August 1999, pp. 20–22.) In the years since, computers have grown far more powerful, imaging devices can record even smaller features, and nanoscale science is thriving.

Livermore's Quantum Simulations Group in the Physics and Advanced Technologies Directorate is a leader in modeling material processes using quantum molecular dynamics methods. The group's early projects examined basic but poorly understood phenomena such as water under extreme pressure. (See *S&TR*, April 2002, pp. 4–10.) More recently, quantum simulations revealed a new melt curve of hydrogen at extremely high pressures. (See *S&TR*, January/February 2005, pp. 4–13.) In 2006, a quantum simulation run on Livermore's BlueGene/L platform won the Gordon Bell Prize for Peak Performance.

More recently, the Livermore group has begun working on simulations for a diverse group of technological applications. For example, nanoscale materials could improve cooling technologies in military equipment and reduce the size of gamma radiation detectors being developed for homeland security. The Department of Energy (DOE) is funding research to dramatically improve storage systems



Lawrence Livermore National Laboratory

for hydrogen fuel on vehicles. In addition, computer chip manufacturers must ensure that their quality-control tools can detect defects in chips as their size continues to shrink. All of these applications require exploring materials at the nanoscale, a regime where simulations are often the most effective approach. "Nanoscale experiments are expensive," says computational scientist Andrew Williamson, a project leader in the Quantum Simulations Group. "At this scale, simulations can be more cost effective."

The computer codes for modeling dynamics at the molecular level are density functional theory and quantum Monte Carlo. Both types of code start from first principles—that is, with no laws other than quantum mechanics characterizing the system being studied. Density functional theory in quantum mechanics describes the electronic density of a molecular or condensed system. It can model atomic motion and the complex dynamics of material interactions. Quantum Monte Carlo also simulates these behaviors, but it uses a different technique. As the code's name implies, the computer essentially "throws the dice" millions of times to select possible answers.

Quantum Monte Carlo codes are more accurate than density functional theory codes, but they can be extremely demanding of computational resources. Williamson and his colleagues have developed a linear scaling technique that greatly reduces the computing time for quantum Monte Carlo calculations. Still, for most problems, density functional theory is the first choice.

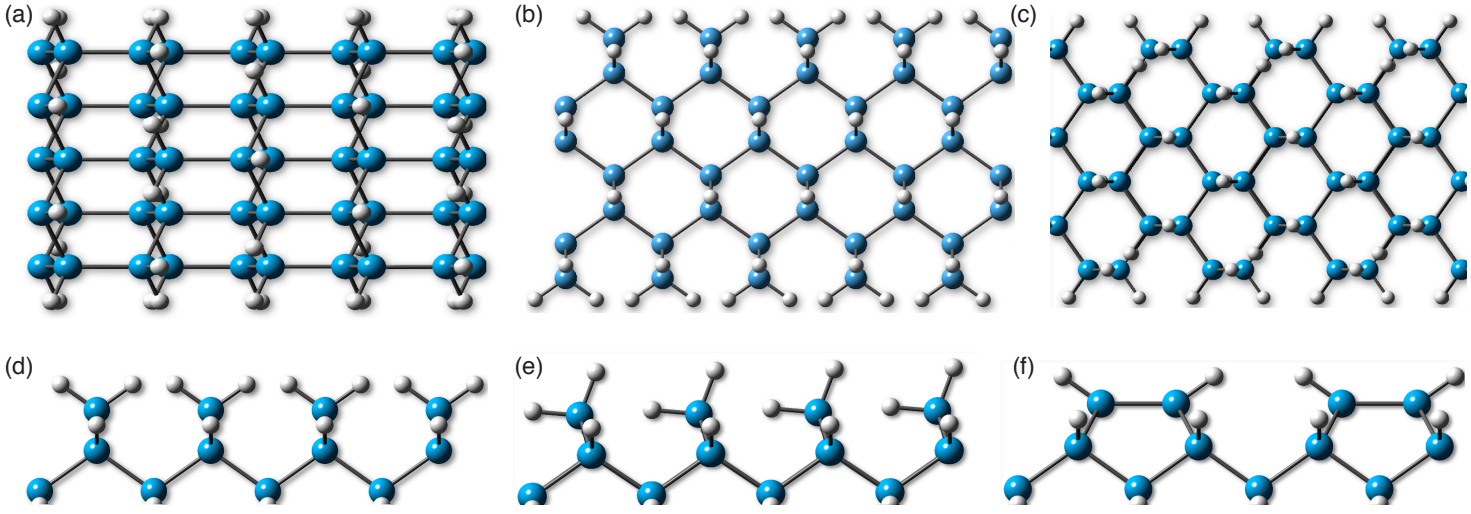
Refrigeration with Nanowires

In one project, researchers in the Quantum Simulations Group are evaluating new materials to provide cooling for military applications. Their simulations, which are funded by the Defense Advanced Research Projects Agency (DARPA), indicate that a highly efficient thermoelectric material may be achievable using silicon germanium (SiGe) nanowires.

Thermoelectric materials convert heat into electricity and vice versa. They have no moving parts and release no pollutants into the environment. A few niche markets have used them for decades to cool electrical parts or generate power. Researchers have considered using thermoelectric-based refrigerators to replace current heat-pump-based refrigerators that compress and expand a refrigerant such as Freon. However, despite extensive research, the efficiency of these materials has remained low.

A highly efficient thermoelectric material must exhibit a combination of properties that do not coexist in conventional materials. It must have the high thermoelectric power of semiconductors, the high electrical conductivity of metals, and the low thermal conductivity of insulators. By measuring these features, scientists can determine a material's efficiency or figure of merit, which is known as its *ZT*. The highest *ZT* achieved in the past 40 years is 1. A thermoelectric material designed to replace a conventional Freon-gas refrigerator must have a *ZT* of at least 3.

A semiconductor nanowire is an ideal thermoelectric material. Nanowires are so thin they are often considered to have only one dimension: their length. This extreme thinness restricts electrons and holes in a process called quantum confinement, which increases electrical conductivity. A nanowire's small size also increases the influence of its surfaces, reducing



Livermore's Quantum Simulations Group evaluated silicon nanowires with lattices grown in the (a) [111], (b) [011], and (c) [001] direction and with (d) symmetric, (e) canted, and (f) reconstructed surfaces.

thermal conductivity. To date, the best thermoelectric materials are superlattice nanowires with a *ZT* of 2.5 to 3.

For the DARPA project, Livermore scientist Trinh Vo, a postdoctoral researcher, developed simulations to compare the growth direction, surface structure, and size of silicon nanowires and determine the optimal properties for electrical conductivity. Vo studied silicon with lattices grown in directions known as [001], [011], and [111], and with symmetric, canted, and reconstructed surfaces. Starting with bulk silicon, she computationally constructed 1-, 2-, and 3-nm cylinders of silicon "terminated" with hydrogen on their surfaces. She then optimized their atomic structure using a density functional code called QBox. The [011] growth direction showed the highest electrical conductivity and thermoelectric power, two parameters that increase *ZT*.

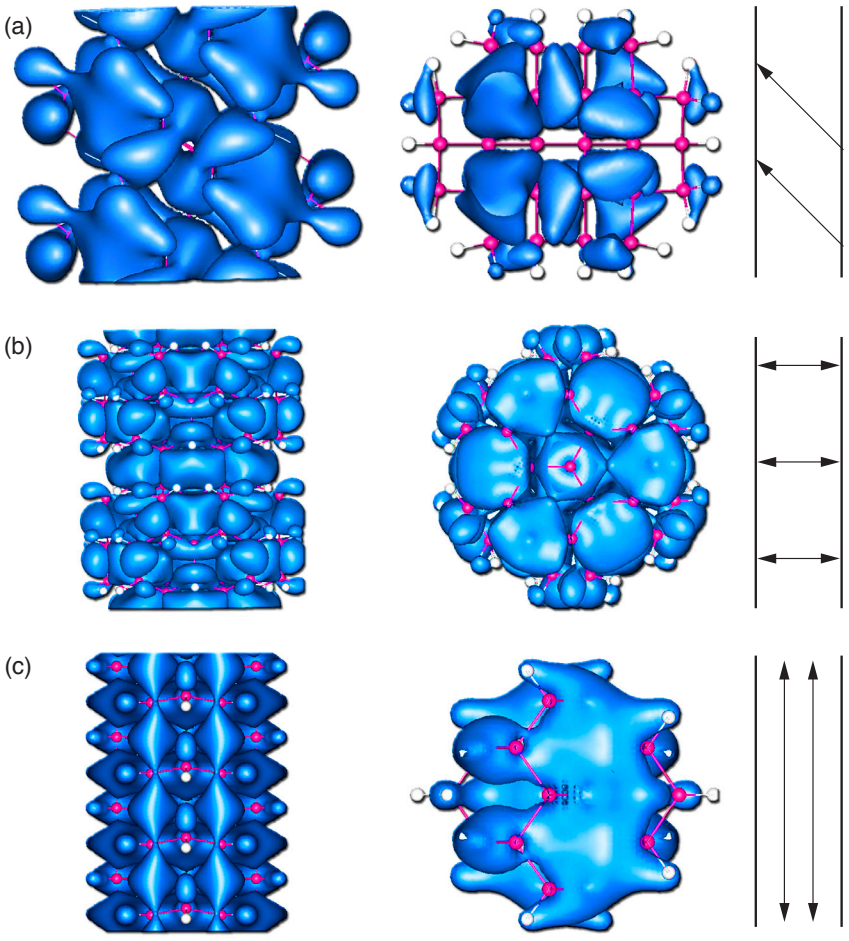
The effect of the wire's size was mixed. For wires with canted surfaces grown in the [001] and [111] directions, effective mass increased as the wire's diameter decreased. (As effective mass decreases, electrical conductivity increases and, thus, improves *ZT*.) However, for the [011] growth direction, where straight channels allow easy electron transport along the wire, effective mass remained the same regardless of the wire's dimension. "These findings indicate that we can tune the electron mass and mobility to optimize a wire's electronic conductivity," says Vo.

Canted nanowires grown in the [001] direction can achieve a *ZT* of 3.5 but require considerable doping with either phosphorus or boron. "I doubt that the wires could be doped strongly enough for this surface to work," says Vo. "Wires grown in the [011] direction will probably be the best compromise."

Although the low effective mass of silicon increases electrical conductivity, it also contributes to a high thermal conductivity. Thermal conductivity must be low for a thermoelectric material to be efficient. One solution is to change the material used for the wires. Vo's simulations indicate that a SiGe combination will reduce lattice thermal conductivity by as much as five times without affecting electrical conductivity. She is now working with Livermore scientist John Reed, who also is a postdoctoral researcher, to optimize wires made of silicon and germanium.

In collaboration with colleagues at the Massachusetts Institute of Technology (MIT), Reed is using classical molecular dynamics techniques to calculate the thermal conductivity of wires with various configurations of silicon and germanium atoms. The goal is to create a SiGe wire with the lowest possible thermal conductivity.

Optimizing the SiGe wire involves an iterative scheme. Reed extracts fluctuations in heat current from the results of his molecular dynamics calculations, and the MIT team inputs these data into a cluster-expansion-based optimization method. The cluster-expansion algorithm produces candidate structures. The



Simulations indicate that when canted nanowires have lattices grown in the (a) [001] and (b) [111] directions, the wire's effective mass increases as its diameter decreases. These configurations will increase electrical conductivity in thermoelectric materials. (c) When silicon nanowires are grown in the [011] direction, electron states are oriented along the wire. In this configuration, effective mass does not change when the wire's diameter changes.

thermal conductivities of these structures are then calculated by Reed's code and plugged back into the MIT optimization calculation. This iterative process can also be used to optimize the thermal properties of semiconductors similar to silicon and germanium.

"The cluster-expansion method could propose a configuration for silicon and germanium that is impossible to fabricate," says Reed. Consequently, potential configurations must be evaluated to ascertain whether they can be fabricated and doped appropriately, and whether they are stable.

A Better Radiation Detector

Quantum simulations are also helping researchers develop a lightweight, high-resolution gamma radiation detector. A portable detector that can identify specific threat agents while ignoring the many legitimate sources of radiation has been a long-term goal to enhance security in the U.S. and worldwide. Such units would allow security personnel at cargo ports, airport terminals, and border crossings to quickly and easily detect threat agents before they enter the country. Improvements in the detection of weapons-grade nuclear materials are also critical to the effectiveness of the U.S. nonproliferation program.

The challenge in designing a portable gamma radiation detector is that high-purity germanium, the best material to date, cannot be used at room temperature. It must be cooled to remove its inherent background noise so the detector can read the signal emitted by gamma rays. Because of the cooling required with current technology, a high-resolution germanium-based radiation detector is typically a heavy, fragile unit.

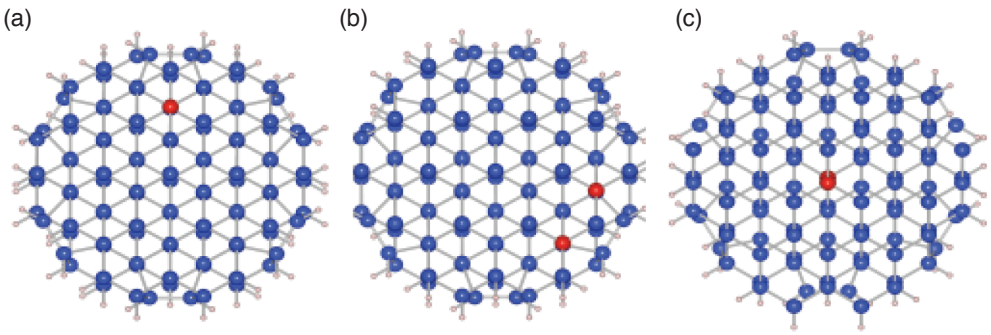
Researchers have proposed about 20 semiconductor elements and alloys as substitutes for germanium. Unfortunately, many of these materials have not performed as well as expected. Experimental investigations of every possible material would be prohibitively expensive. Now that computers can accurately predict material properties, computer scientists have joined the search for a new detector material.

When a semiconductor material interacts with gamma radiation, it produces electron–hole pairs that are detected as an electrical signal. A candidate material should therefore have highly mobile electrons (and holes) and long electron–hole recombination times to maximize the signal from each absorbed gamma ray. For use at room temperature, the material must also have an energy band gap large enough to preclude thermal excitations.

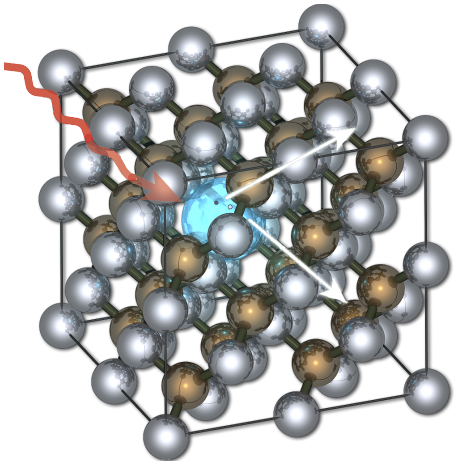
These features are controlled both by the intrinsic electronic properties of the semiconductor, such as its band structure and effective masses, and by the purity of the material. Structural defects in the material can trap electrons, reducing their mobility and increasing the probability of recombination, which in turn reduces the resolution of the detector.

Lawrence Fellow Vincenzo Lordi is performing first-principles studies to characterize the microscopic properties of materials and determine which ones are the best for semiconductor alloys. "Our research focuses on material impurities and ways to eliminate them," says Lordi. His simulations first provide an atomistic view of potential detector materials such as bulk gallium telluride and aluminum antimonide. Using density functional theory, he models the microscopic mechanisms by which defects degrade mobility. He then can calculate the intrinsic limits of mobility. Defects may be either native to the material or nonnative, for example, from a dopant.

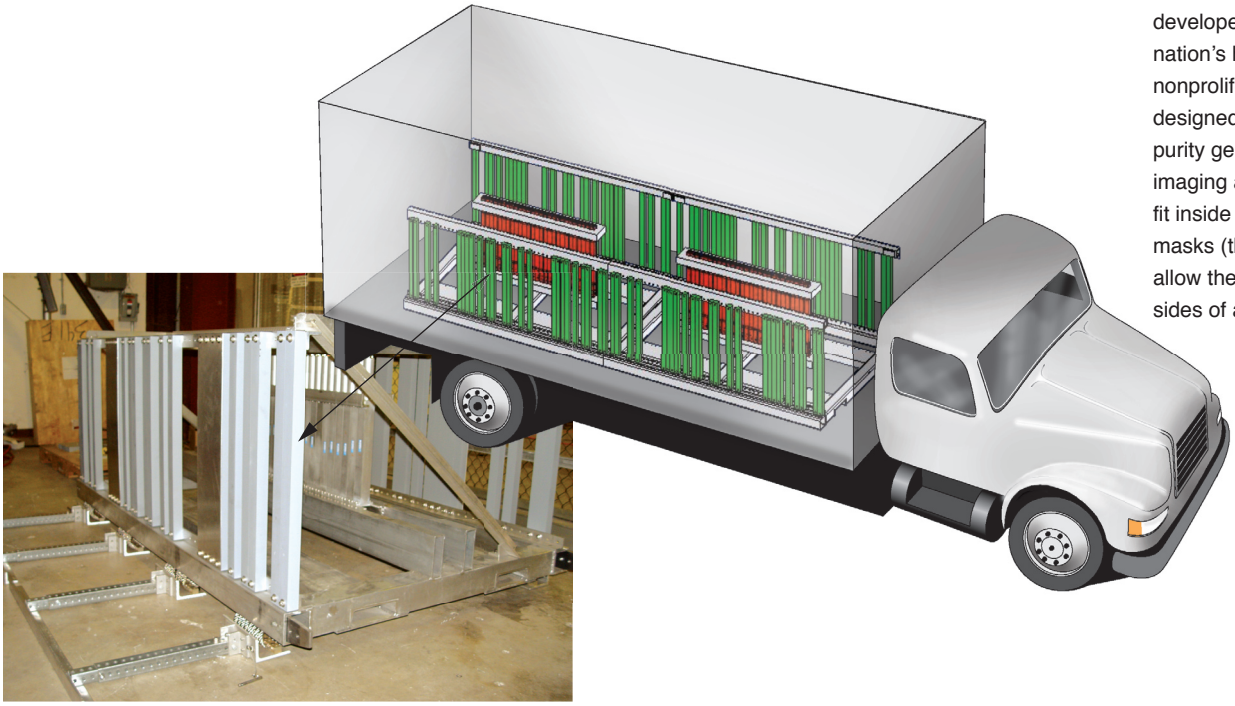
Kuang Jen Wu, a scientist in the Chemistry, Materials, and Life Sciences Directorate, is experimenting with



The cluster-based optimization method can be used to determine which configuration of silicon (blue) and germanium (red) produces the best thermal conductivity in a nanowire. (a) Germanium at one site increases thermal conductivity. (b) Having coplanar sites reduces thermal conductivity. (c) When sites are parallel to the wire, thermal conductivity increases.



This schematic of aluminum antimonide, a potential material for gamma radiation detectors, shows a defect (blue) in its lattice. Arrows indicate electron scattering.



High-resolution gamma-ray detection techniques are being developed to support the nation's homeland security and nonproliferation efforts. A detector designed at Livermore uses high-purity germanium for gamma-ray imaging and is small enough to fit inside a truck. Coded-aperture masks (the gray bars in the inset) allow the instrument to image both sides of a road.

aluminum antimonide, but the crystals produced to date have not been pure enough for use in a detector. Wu has tried annealing the crystals to repair some of the defects and is using Lordi's recent calculations to guide the annealing procedures.

Lordi and Williamson have also begun to develop a first-principles computational toolkit that will predict the structural, electronic, and transport properties of different semiconductor detector materials. The toolkit will evaluate a candidate material, determine the formation energies for a range of structural defects and dopants, and identify the most commonly formed defects. It will then predict how the concentration and distribution of defects will affect the material's electronic band structure, effective mass, and charge carrier mobility, lifetime, and scattering rate.

Ultimately, the toolkit will be used to create a database of fully characterized candidate materials for semiconductor detectors. With extensive information showing how the sensitivity of transport properties is affected by imperfections in a material's structure, the team can more easily identify promising materials. "The database will also allow us to evaluate methods to improve a material's performance by modifying the synthesis process," says Lordi.

A high-resolution room-temperature radiation detector has other potential applications in addition to homeland security and nonproliferation. For example, astrophysicists are interested in using these detectors to better study gamma-ray bursts, the most luminous events to occur since the big bang. Orbiting satellites now detect a gamma-ray burst somewhere in the universe about once a day.

Squeezing Hydrogen from a Sponge

Another quantum simulation project is looking at material optimization, this time to allow auto manufacturers to scrap the internal combustion engine and make the move to hydrogen-fueled vehicles. "Fuel storage is a major stumbling block to further development of hydrogen vehicles," says Williamson. "With current storage technology, a tank holding enough hydrogen to travel 480 kilometers would be much too big and heavy for a car." Scientists have been trying to solve this conundrum for more than 30 years.

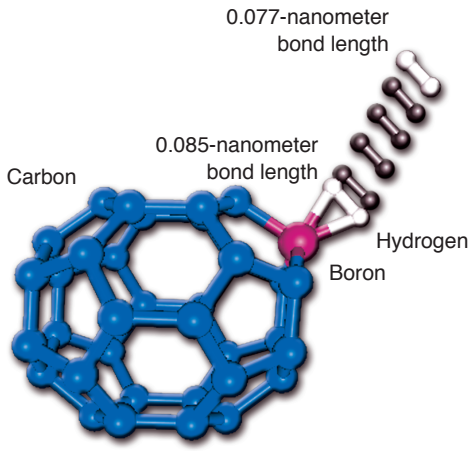
Williamson is working with researchers Julie Herberg and Ted Baumann from the Chemistry, Materials, and Life Sciences Directorate to determine if spongelike materials made of carbon can be used to soak up hydrogen and efficiently store it on cars. This project, which is funded by DOE's Office of Science, also includes computer scientists from the National Renewable Energy Laboratory (NREL) in Boulder, Colorado. Williamson likens the team's research to Thomas Edison's hunt for the best light bulb filament. Edison experimented with thousands of materials before settling on carbon.

The ideal storage material cannot react with hydrogen but must weakly bind to it so that hydrogen can be easily drawn off when a vehicle needs more power. In other words, the binding must be reversible. The optimal storage material will be very light so that more of the weight of the full tank is taken up by hydrogen, rather than by the tank itself. Before Williamson joined the project, the NREL scientists conducted experiments with boron and boron-doped carbon ($C_{35}B$) fullerenes. Their research showed that pure boron would have to be heated to release hydrogen, but $C_{35}B$ remains a possible choice.

These materials absorb hydrogen by the Van der Waals intermolecular force. This force, which is much weaker than a chemical bond, arises when molecules polarize into dipoles. These intermolecular forces may be feeble, but life as we know it would not exist without them. For example, the Van der Waals force provides just enough attraction to hold water molecules together in the liquid state.

Density functional theory does not capture Van der Waals forces. Instead, Williamson and his colleagues at NREL are using diffusion quantum Monte Carlo. By also incorporating Livermore's faster, linearly scaled version of quantum Monte Carlo, they have performed the first highly accurate quantum Monte Carlo studies of potential hydrogen storage materials. Calculations of the Van der Waals binding energy for hydrogen and carbon fullerenes doped with either boron or beryllium showed both materials to be adequate for reversible hydrogen storage. The team is now investigating other possible carbon-based storage materials, such as calcium-intercalated graphite.

These preliminary results will be augmented by a new coding capability. Williamson and the NREL researchers are modifying density functional theory to explicitly include the nonlocal correlation effect particularly tailored for the Van der Waals interactions. This new tool and diffusion quantum Monte Carlo complement one another and should firmly establish the binding energy and reversibility of hydrogen in candidate materials. Having these data is crucial because DOE is considering whether to continue research on carbon-based storage materials for hydrogen-fueled vehicles.



Livermore researchers calculated the binding energy of a boron-doped carbon fullerene to determine if it is a suitable material for hydrogen storage systems in vehicles.

Quality Control for Chip Manufacture

Each year, computers become faster and more powerful because chip manufacturers can fit more features on a silicon wafer. As silicon chips get smaller, they become more difficult to make. Manufactured chips now have features measuring 65 nm, and in the laboratory, features can be made as small as 25 nm. Experts predict that features will be less than 10 nm by 2015.

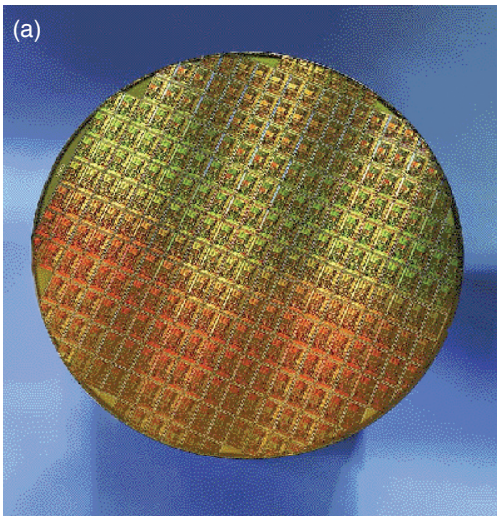
Silicon at 10 nm may behave differently than it does at 50 or 100 nm. At the larger, bulk scale, silicon's behavior follows the rules of classical molecular dynamics. At smaller scales, however, quantum mechanics rules behavior. The Quantum Simulations Group is working to better understand the optical properties of this important material. Postdoctoral researcher Sebastien Hamel is using quantum simulations in a project funded by Intel Corporation and KLA-Tencor to determine the transition point between bulk and nanoscale behavior.

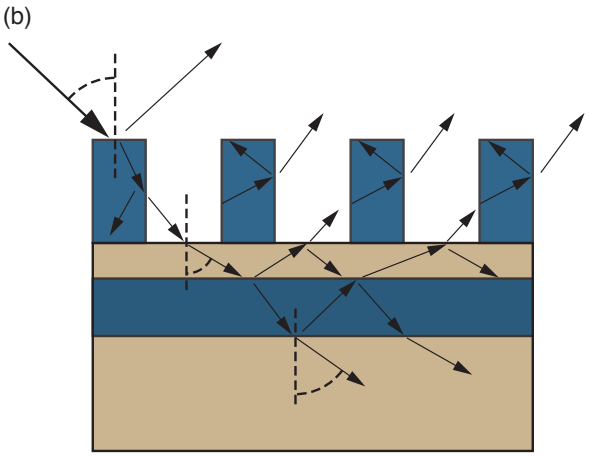
Semiconductor manufacturers such as Intel use optical scatterometry equipment made by KLA-Tencor to control the quality of their silicon wafers. In scatterometry, light shone on a wafer at a specific angle bounces off the wafer's features. Measurements of the scattered light reveal critical structural parameters of the wafer's nanoscale features. As feature size shrinks, KLA-Tencor must adjust its algorithms to account for the changed properties of silicon. At 65 nm, the refractive index of silicon is the same as that of bulk silicon, but at 10 nm, its refractive index is unknown.

"We know something about the properties of silicon nanowires and have plenty of information on bulk silicon, but we don't know much at all about silicon at dimensions in between," says Hamel. "We need to determine how characteristics such as width, height, and rounded corners will affect the material's properties. The big question is how small can a feature be and still behave like bulk silicon? Or at what point does quantum behavior kick in?"

In Hamel's simulations using density functional theory, he looked for the distribution of electrons and the material's dielectric response. He found that a slab of silicon only 2.5 nm thick responds the same as bulk silicon. Silicon nanowires are different because they have so much surface area. For them, 5 nm is the limit for bulklike behavior. In the Intel laboratories, researchers have produced features as small as 5 nm by 25 nm, which Hamel predicts will have a dielectric response the same as bulk material.

His next research effort will examine the frequency dependence of the dielectric response—or absorption spectrum—of silicon nanostructures. The KLA-Tencor equipment uses a broad spectrum of light for the optical scatterometry experiments, but some parts of the absorption spectrum may be more sensitive to size than others. "KLA-Tencor wants to determine how





Manufacturers use optical scatterometry as a quality-control tool to ensure that semiconductor chips are free of defects. (a) A silicon wafer 30 centimeters in diameter is covered with thousands of minute features. (b) Scatterometry measures light as it bounces off a wafer's features. The scattering pattern indicates if a chip has been manufactured precisely as designed.

long the scatterometry technology will be effective," says Hamel. "At what point will chip manufacturers need a new quality-control technology?"

Quantum Coming of Age

The University of California recently selected Williamson as an Executive Management Discovery Fellow. Each year, the university chooses one fellow per campus and offers resources for these people to establish strategic partnerships and collaborations with industry, particularly small businesses, to spur the California economy. That a quantum simulations expert was selected as the Laboratory's Discovery Fellow reflects the growing importance of the quantum world in the private sector.

—Katie Walter

Key Words: density functional theory, hydrogen storage, optical scatterometry, quantum molecular simulations, quantum Monte Carlo, silicon chip manufacture, silicon nanowires, thermoelectric materials.

For further information contact Andrew Williamson (925) 422-8285 (williamson10@llnl.gov).

U.S. Weapons Plutonium

Advances in plutonium science enhance understanding of this mysterious element.

Aging Gracefully

ONE of the most important components of a nuclear weapon is the core or pit, a sphere of plutonium-239 that is compressed by conventional explosives to create a nuclear chain reaction. Understanding the performance of plutonium pits is crucial to Lawrence Livermore scientists and engineers who must ensure the safety and reliability of the nation's nuclear stockpile. Planning the future needs of the U.S. nuclear weapons complex also depends on confidence in the long-term stability of the pit and credible estimates for pit lifetimes.

Many physicists, metallurgists, and chemists have worried that the natural radiation produced by plutonium over many years might eventually damage the pit and compromise weapon performance. Although plutonium-239 has a half-life of 24,000 years, its decay rate is high enough to produce a significant amount of damage after only a few decades. In addition, many pits are in deployed weapon systems that are far older than their originally planned lifetimes. To maintain a system past its designed lifetime, weapon scientists need a more thorough understanding of plutonium as it ages.

"People have been studying metals for 3,000 years, but plutonium for less than 70," says Livermore metallurgist Adam Schwartz. Conducting research on plutonium's electrical, chemical, and physical properties is also much more difficult than it is on other metals because plutonium is radioactive, highly toxic, and sensitive to changes in temperature, pressure, and composition. In addition, its properties do not always change in linear fashion.

For years, weapon scientists examined plutonium's bulk behavior by testing nuclear devices at the Department of Energy's Nevada Test Site. However, the nation stopped underground nuclear testing in 1992. In its place, the department launched a vigorous science-based stockpile stewardship program to evaluate and certify the safety, security, and reliability of the nation's weapons.

In 1997, as part of this program, the National Nuclear Security Administration's (NNSA's) Enhanced Surveillance Campaign began funding a $100 million study at Lawrence Livermore and Los Alamos national laboratories to examine how nuclear warhead materials age and determine the likely effects of aging on weapon performance and safety. Livermore's research teams include physicists, chemists, engineers, materials scientists, and computer scientists from the Chemistry, Materials, and Life Sciences; Physics and Advanced Technologies; Defense and Nuclear Technologies; Engineering; Computation; and Energy and Environment directorates.

On November 29, 2006, NNSA announced the results from this effort: "These studies show that the degradation of plutonium in our nuclear weapons will not affect warhead reliability for decades," said Linton Brooks, then administrator of NNSA. "It is now clear that although plutonium aging contributes, other factors control the overall life expectancy of nuclear weapons systems." The laboratories' research teams also determined that the minimum lifetime for most of the plutonium pits in the nation's nuclear weapon stockpile is at least 85 years—25 to 40 years longer than scientists had previously estimated.

JASON, an independent panel of scientists who advise the government on science and technology, reviewed the scientific studies used to assess pit lifetimes. The JASON reviewers concluded that the credible lifetime for most of the pit types is at least 100 years. They also noted that mitigation plans have been proposed or are being implemented for those types with less than 100 years of projected stability.

These findings are the latest chapter in a scientific effort that began in 1941 when plutonium was discovered. Since the Laboratory's founding in 1952, Livermore scientists have made significant contributions to the science of plutonium and its closely related elements, called actinides. (See the box on p. 14.) The

Plutonium Grudgingly Reveals Its Secrets

In 1941, Glenn Seaborg, Edwin McMillan, Joseph Kennedy, and Arthur Wahl synthesized plutonium, element 94, in a cyclotron at the University of California at Berkeley. Since then, scientists have identified 21 plutonium radioisotopes. The most stable isotopes are plutonium-244, with a half-life of 80.8 million years; plutonium-242, with a half-life of 373,300 years; and plutonium-239—the isotope of greatest interest—with a half-life of 24,110 years.

When plutonium-239 undergoes fission, the nucleus releases enormous energy. One kilogram of this metal is equivalent to about 22 million kilowatt-hours of heat energy. When detonated, it produces an explosion equal to about 4 kilotons of chemical explosives.

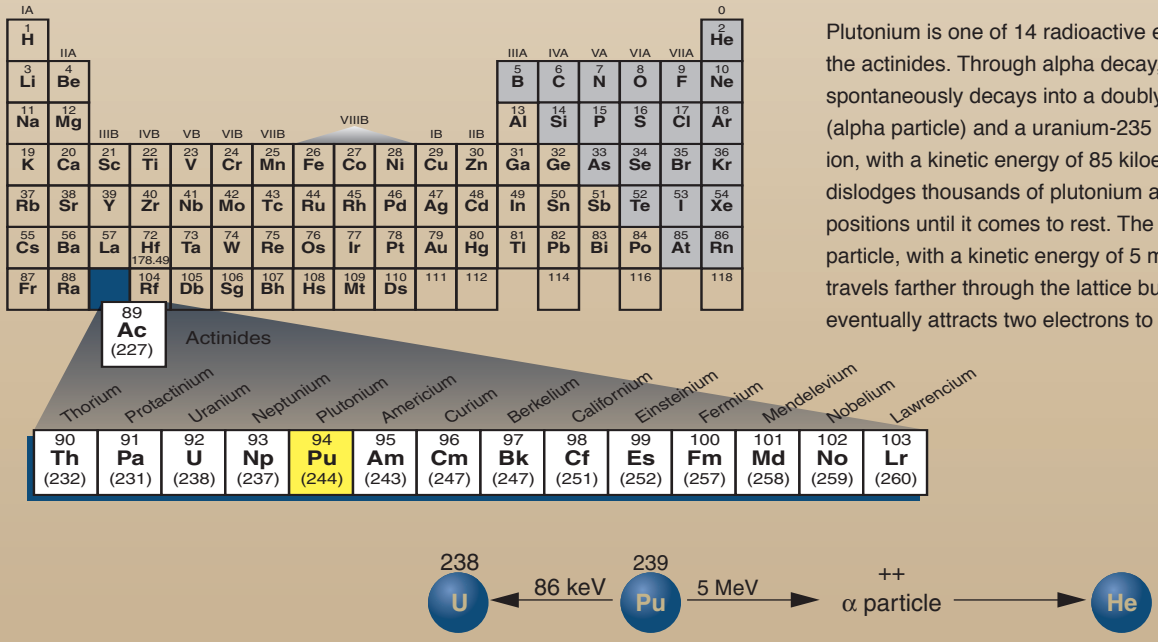
Plutonium is part of a series of 14 radioactive elements called the actinides, which all contain electrons in an outer shell called 5f. Plutonium's complexity derives from its position in the periodic table: the transition point at which 5f electrons change from forming bonds with other elements to being chemically inert.

Scientists consider plutonium the most perplexing element in existence. It joins with virtually every other element to make compounds, complexes, or alloys and forms up to 12 chemical bonds to molecules in solution, something no other element can do. Plutonium-239 goes through six solid-state phase transformations, more than any other element. Large volume and density changes occur as it transitions through these six phases to its liquid state at 640°C. Under pressure, it also exhibits a seventh phase.

An atom of plutonium-239 spontaneously decays into a doubly charged helium nucleus (alpha particle) and a uranium-235 ion. The uranium-235 atom has an initial kinetic energy of about 85 kiloelectronvolts. Before this atom comes to rest, it dislodges thousands of other plutonium atoms from their normal positions in the crystal lattice, thereby creating a large collision cascade. The alpha particle, which has an energy of 5 megaelectronvolts, travels farther. However, because it is relatively small, it creates fewer lattice defects.

Within 200 nanoseconds, about 90 percent of these displaced atoms return to a normal lattice position, a process called self-healing. If a defect does not self-heal, the lattice may have with vacancies, where atoms are missing, and interstitial atoms, where atoms are squeezed between other regularly spaced atoms. On average, each atom of plutonium is displaced once every 10 years.

After the alpha particle comes to rest in the lattice, it attracts two electrons from its surroundings to become a helium atom. This process creates about 29 helium atoms per year for every 1 million atoms of plutonium. The aggregation of helium atoms causes helium bubbles to form. Over many decades, this accumulation of helium becomes substantial, although bubbles stop growing once their diameter reaches about 1.4 nanometers. Why bubbles do not continue to expand is one of many questions that remain to be explained about this most mysterious of elements.



Plutonium is one of 14 radioactive elements called the actinides. Through alpha decay, a plutonium atom spontaneously decays into a doubly charged helium nucleus (alpha particle) and a uranium-235 ion. The uranium-235 ion, with a kinetic energy of 85 kiloelectronvolts (keV), dislodges thousands of plutonium atoms from their lattice positions until it comes to rest. The much smaller alpha (α) particle, with a kinetic energy of 5 megaelectronvolts (MeV), travels farther through the lattice but creates fewer defects. It eventually attracts two electrons to become a helium atom.

research has also benefited from studies conducted at the Laboratory's Glenn T. Seaborg Institute. (See *S&TR*, June 2000, pp. 15–22.)

As part of the NNSA study, Livermore scientists used some of the most accurate instruments in the world to measure the microstructural, physical, and chemical properties of plutonium and its alloys. In dynamic experiments such as gas-gun tests and static studies using diamond anvil cells (DACs), they examined how radioactive decay affects plutonium's structure, phase stability, and equation of state (EOS). They also measured the element's density and volume with unprecedented accuracy and reviewed data from past nuclear tests.

Advanced computational models of weapons physics and theoretical studies helped researchers design the experiments and provided data to complement the experimental results. In addition, calculations of design sensitivity determined the extent to which aging pits would affect performance of different weapon systems decades from today. By combining experimental and computational resources, scientists working on the NNSA study derived the most accurate estimates ever obtained for pit lifetimes.

Decay Generates Helium

The isotope plutonium-239 undergoes alpha-particle decay, in which a plutonium atom spontaneously disintegrates, turning into a uranium-235 atom while emitting a high-energy alpha particle (helium nucleus). The alpha particle and the uranium atom fly off in opposite directions, disrupting nearby atoms. As the alpha particle comes to rest, it picks up two electrons and becomes a helium atom. Weapon designers have long sought greater assurance that a pit would retain its size, shape, and strength in the presence of an ever-increasing amount of damage from alpha-particle decay.

One concern is that at some threshold, the accumulating damage might induce a change from plutonium's ductile delta phase used in nuclear warheads to the denser alpha phase, which is more brittle. Such a phase change could cause the crystalline lattice to crack and would likely degrade a weapon's performance. Helium atoms also might collect in large bubbles, weakening the part or otherwise changing its behavior.

Many scientists have also been concerned that a phenomenon called void swelling might occur. Studies of radiation damage in other metals, such as the steels used in nuclear reactors, show that helium buildup, in combination with vacancies in a metal's crystalline lattice, can produce voids in addition to helium bubbles. Voids cause most metals to swell in size, losing their critical shape and strength.

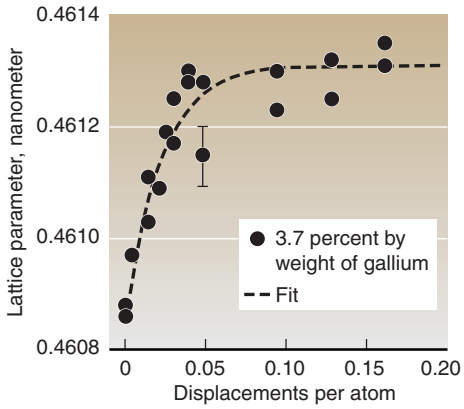
Results from the NNSA study indicate that the accumulation of helium would not significantly change the properties of plutonium in pits up to a century after they were manufactured. The helium bubbles appear to be distributed uniformly throughout the material, with only a small change in properties including a slight increase in volume.

The study also revealed no evidence of void swelling or other catastrophic damage in plutonium over several decades. "We now understand damage mechanisms in plutonium more precisely," says Schwartz. "The radiation damage is slow, and self-healing mechanisms occur in which atoms move back into the lattice from which they were displaced."

Schwartz notes that the behavior of aging plutonium is also important in dismantling nuclear weapons and disposing of pits from retired weapons. In addition, nuclear power plants produce plutonium as a by-product of burning enriched uranium fuel, and this waste must be secured against diversion or theft. The most likely methods for disposing of unwanted plutonium will be to burn it in a future nuclear reactor or sequester it underground in a geologic formation. With either approach, plutonium must be kept for many decades or centuries, and solid scientific understanding is required for its safe handling and storage. (See the box on p. 17.)

Accelerating the Aging Process

Researchers combined experiments and measurements to characterize samples of both old and new plutonium. The oldest weapons-grade plutonium made in the U.S. and available for detailed analysis was about 45 years old, taken from pits retired from the stockpile. The processes used to manufacture this plutonium differ somewhat from those used to make pits in today's stockpile. The oldest samples most directly comparable to current weapons were about 30 years old.



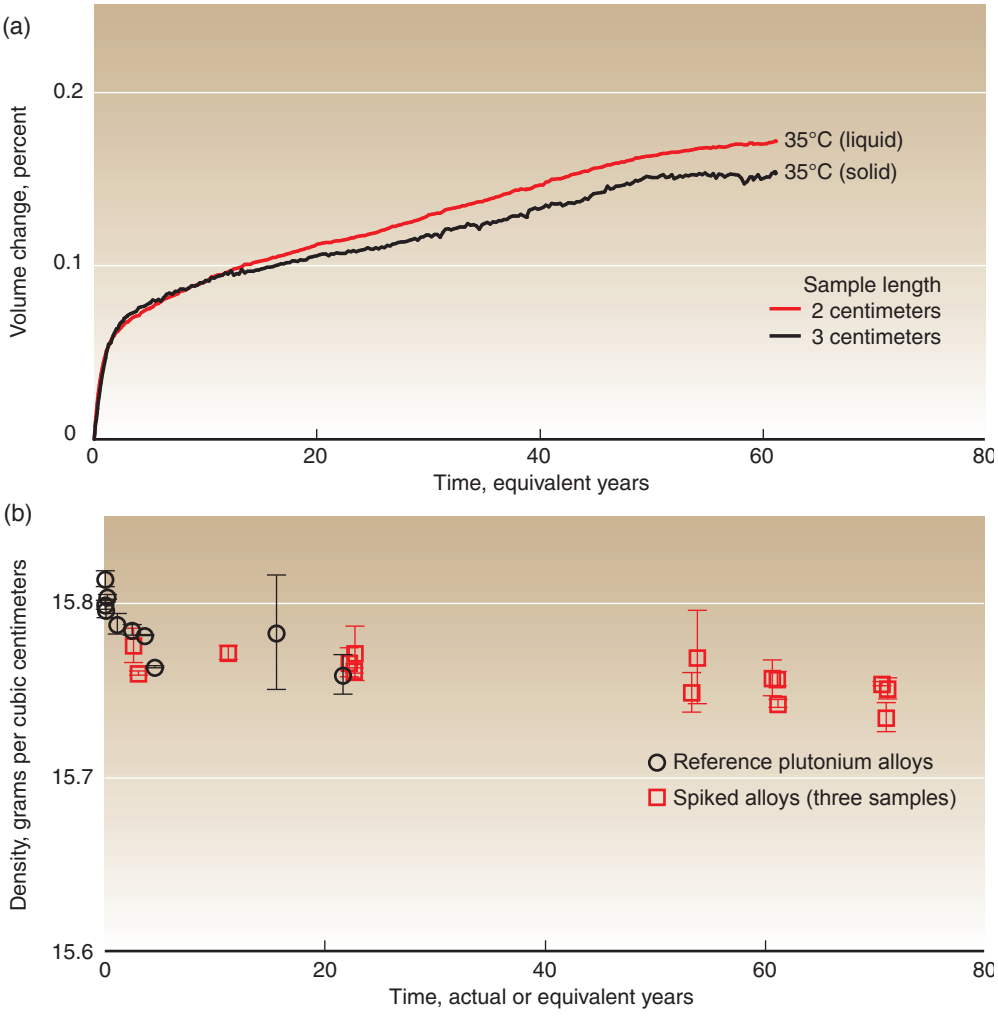
Alpha decay has a measurable effect on the lattice parameter, the distance between two faces of the crystalline lattice in delta-phase plutonium. The rate at which alpha decay knocks an atom from its original lattice position is measured in displacements per atom (dpa). In plutonium, 1 dpa equals 10 years. Experimental data show that early on, alpha-decay-induced radiation damage reaches a steady state where the rate of self-healing almost equals the rate of alpha-decay damage.

Plutonium is the most complex metallic element. Without a thorough scientific understanding of its behavior, some aging effects could appear suddenly. Scientists cannot merely extrapolate the effects found in samples from retired pits to determine the aging mechanisms over time. To simulate the properties of pits many decades into the future, Livermore and Los Alamos researchers accelerated the age of samples by adding isotopes with shorter half-lives. Using a recipe developed by Livermore physicist Bill Wolfer, the researchers "spiked" an alloy of weapons-grade plutonium-239 with 7.5 percent by weight of plutonium-238, which has a half-life of 87 years. Plutonium-238 is used to provide electrical power for deep-space probes such as the National Aeronautics and Space Administration's Galileo mission to Jupiter.

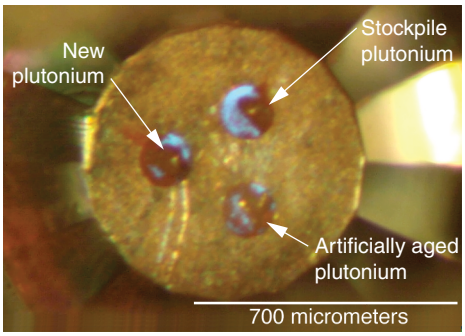
This spiked alloy accumulates radiation damage at a rate 16 times faster than weapons-grade plutonium alone. "Spiking gives us 16 years additional aging for every year of natural aging," says chemical engineer Karen Dodson, who has supervised the production of artificially aged plutonium. The oldest spiked samples, manufactured about 5 years ago, are now equivalent to 80-year-old plutonium. Because the damage rate is much higher in the spiked plutonium, those samples are maintained at a slightly elevated temperature to ensure that the self-healing rate is appropriately accelerated as well.

Livermore metallurgists made several batches of artificially aged plutonium alloys in a glove box under inert atmosphere to prevent oxidation. For each production batch, dozens of samples were machined at various sizes for the dynamic and static experiments. For example, samples measuring 2 and 3 centimeters long were manufactured for dilatometry experiments, which measure dimensions to extreme accuracy. Metallurgists also made reference samples that did not contain plutonium-238.

Chemist Brandon Chung is measuring property changes as a function of age for the various samples, including those that are artificially aged. He records changes in density, dimension, tensile and compressive strength, and hardness,



(a) Dilatometry measurements show a sharp rise and then an extremely slow increase in volume as plutonium ages over decades. (b) Immersion density experiments show a marked density decrease in both spiked and reference plutonium alloys, followed by a very slow, linear decrease.



Three plutonium samples, each 100 micrometers in diameter, are squeezed in a diamond anvil cell to determine how radioactive decay affects the metal's structure. The samples shown here include recently produced plutonium, artificially aged plutonium, and plutonium retrieved from a retired pit several decades old.

all properties related to the element's composition and crystalline microstructure.

His dilatometry and immersion density measurements on newly made spiked and unspiked alloys showed a limited period of significant volume expansion (and its corollary, density reduction), followed by extremely slow changes in volume and density. He found no indication of void swelling. "Plutonium ages at a much slower rate than we originally thought," says Chung, who will continue to measure the samples as they age.

DAC Applies the Pressure

Physicists Choong-Shik Yoo and Hyunchae Cynn conducted experiments on plutonium using DACs. In these experiments, a small mechanical press slowly squeezes a microgram or so of material between two small, flat-tipped diamonds, achieving pressures as high as 100 gigapascals. To better examine actinides under extremely high pressures, Laboratory researchers developed "designer" DACs, which have advanced sensors integrated into the cell. (See *S&TR*, December 2004, pp. 4–11.)

The two scientists conducted the DAC experiments at the Advanced Photon Source (APS) at Argonne National Laboratory. APS is the brightest x-ray source in the world and can reveal minute changes in crystalline materials. In this series of experiments, the Livermore team examined plutonium samples at different stages of the aging process. Samples included material recently produced, artificially aged, and taken from retired pits up to 45 years old.

The experiments used three samples of different ages in the same DAC. Each sample measured 0.1 millimeter in diameter and was secured within a metal gasket. The samples were heated either electrically or by a laser to several thousand kelvins. As pressure was slowly increased, the researchers tracked volume changes that occurred when samples transitioned from one phase to another. The APS experiments

Plutonium Futures Conference Growing in Popularity

One of the most important international forums for discussing the science of plutonium and other actinides is the Plutonium Futures Conference, held every three years since 1997. The conference highlights the latest research on the physical and chemical properties and environmental interactions of plutonium and other actinide elements.

Lawrence Livermore hosted the most recent conference in July 2006 at Pacific Grove, California. The program consisted of lectures, invited papers, and plenary sessions, which included policy makers and scientific leaders. U.S. and international scientists, engineers, faculty, and students from universities, research institutes, and nuclear complexes attended the conference, which attracted nearly 400 participants—many more than organizers had predicted.

Topics included the safe storage and long-term management of surplus weapons materials and large inventories of actinides generated by civilian nuclear power plants. Participants also discussed actinides in the environment; their properties, chemistry, quantum mechanics, and electron structure; and methods to detect them. "The technical basis for addressing these issues requires intensive and increasing understanding of the underlying plutonium and other actinide science and technology," says Livermore physicist and conference organizer Mike Fluss.

"Plutonium is the linchpin of any nuclear energy strategy," says Fluss. "It is a by-product from burning uranium. In future fuel cycles, engineers must find methods to dispose of it." The Department of Energy's recent nuclear energy initiative, called Global Nuclear Energy Partnership, proposes to reduce nuclear waste by using new proliferation-resistant technologies to recycle these fuels. According to Fluss, such an effort requires solid scientific underpinnings.

"The study of plutonium is a 21st century grand challenge for chemists, materials scientists, and solid-state physicists," says Fluss. "Each Plutonium Futures Conference presents an opportunity to bring these communities together." In particular, scientists believe that if they could fully understand the complex interactions of plutonium's 5f electrons, they could understand the electron behavior of any other element.

Lawrence Livermore hosted the 2006 Plutonium Futures Conference, which highlighted current scientific research on plutonium and other actinides. Nearly 400 participants attended from throughout the world.

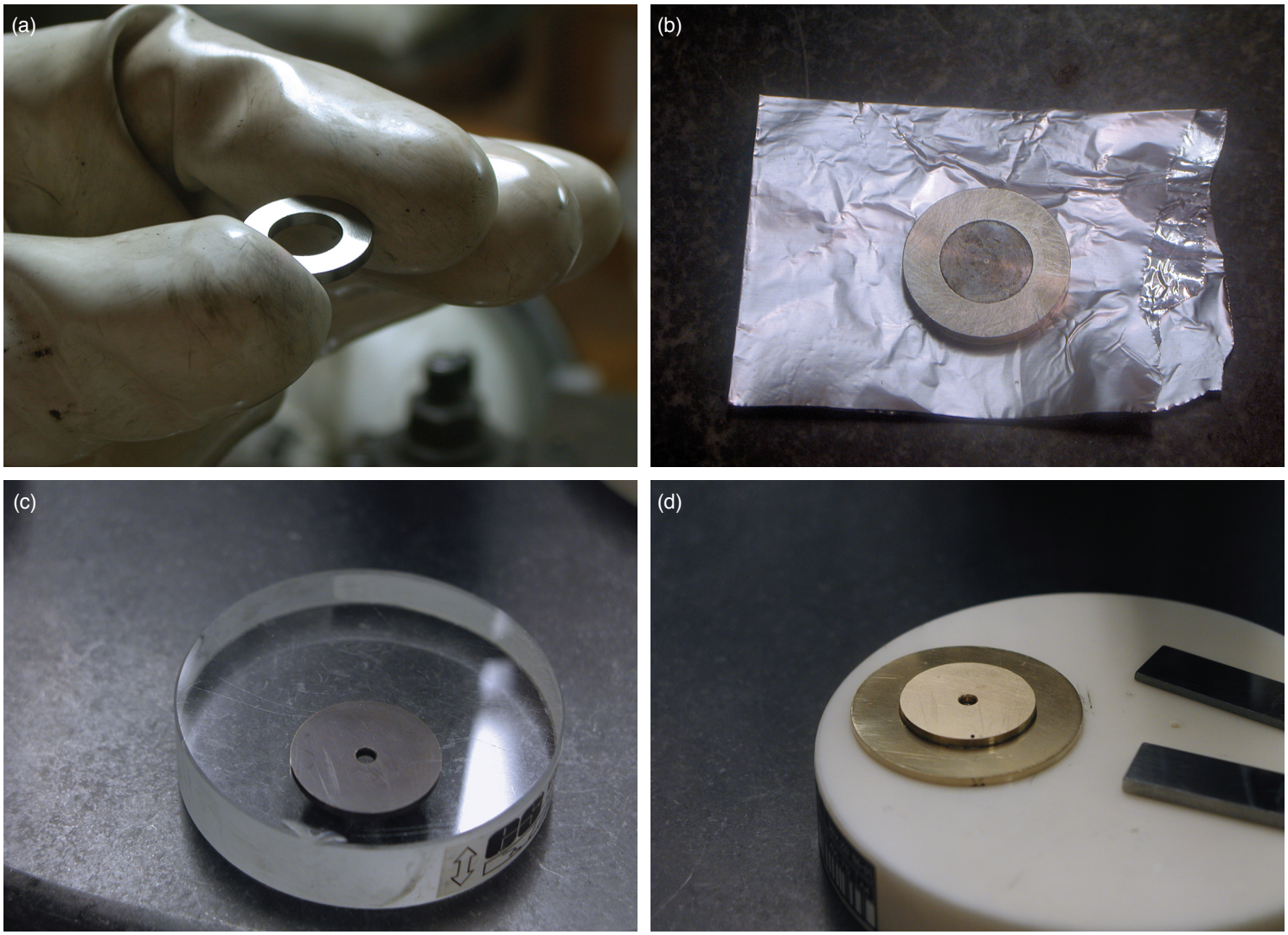
revealed no significant differences among the plutonium samples and no sudden or unexpected changes in properties. (See the bottom right figure on p. 16.)

Consistent Data from JASPER

Researchers at the Joint Actinide Shock Physics Experimental Research (JASPER) Facility acquired the first simultaneous dynamic comparison data for naturally aged plutonium obtained from retired pits versus newly produced plutonium. JASPER is a 30-meter-long, two-stage light-gas gun located at the Nevada Test Site.

Designed to gather EOS data on plutonium, the gas gun hurls projectiles at speeds up to 8 kilometers per second at plutonium targets. The impact produces an extremely high-pressure shock wave (about 600 gigapascals) in the target, raising its temperature to as high as 7,000 kelvins. (See *S&TR*, June 2004, pp. 4–11.)

For these experiments, targets were made of old plutonium pressed into a disk of new plutonium and machined extremely flat (to 1.5-micrometer variation). The disk had an outer diameter of 32 millimeters, and the old plutonium had an inner diameter of 19 millimeters. Nineteen pins



Researchers used the gas gun at the Joint Actinide Shock Physics Experimental Research Facility to simultaneously shock samples of aged and new plutonium. The sample assembly sequence shows (a) a ring of new, machined plutonium; (b) old plutonium pushed into the ring; (c) the concentric rings after being machined; and (d) the concentric rings after they are polished, coated with gold, and bonded to a larger ring of new plutonium.

placed in the two samples gathered shock velocity data.

JASPER engineer Matt Cowan explains that with this target design, the two concentric samples experienced identical shock waves at precisely the same time. "Testing the two samples simultaneously is better than conducting separate experiments because gun velocities are always slightly different," says Cowan.

The results unequivocally showed no statistically significant difference in the EOS of the new and old plutonium. "The experiments achieved EOS data with an accuracy never achieved before," says physicist Neil Holmes, chief JASPER scientist. "The DAC and gas-gun experiments produced entirely consistent data. One technique is dynamic, the other static, but the answers were the same."

Images and Modeling Aid Studies

To supplement the data from these experimental activities, Schwartz worked with staff associate Mark Wall to directly observe plutonium samples with an electron microscope. The ability to directly image the accumulation of self-irradiation damage is critical to understanding the element's aging process, says Schwartz. Using Livermore's 300-kiloelectronvolt, field-emission transmission electron microscope (TEM), he and Wall observed spherically shaped helium bubbles, each about 1 nanometer in diameter—too tiny to be seen with conventional TEM instruments. The bubbles form as helium-filled vacancies migrate and coalesce. (See *S&TR*, March 2001, pp. 23–25.)

Schwartz has not observed voids in aged specimens with the TEM, although he regularly finds high densities of nanometer-size helium bubbles. "Although the number of helium bubbles grows over time, the bubble size is limited," says Schwartz.

Modeling and simulations done by Wolfer and others has aided the plutonium imaging and experimental effort. In one project, Wolfer studied whether the delta-phase plutonium–gallium alloy could eventually convert to a more stable phase, such as alpha, which is 25 percent more dense. His calculations show that self-radiation damage is, surprisingly, a key factor in stabilizing delta-phase plutonium.

According to Wolfer, gallium atoms in the delta-phase alloy tend to aggregate, which over time could contribute to a transition to another phase. However, plutonium decay disrupts any nearby gallium aggregation. "It's a dynamic but stable situation that contributes to plutonium's graceful aging," says Wolfer.

He and chemical engineer Alison Kubota are using Livermore's Blue Gene/L supercomputer to simulate collision cascades of uranium-235 atoms created from the alpha decay of plutonium atoms. The simulated reactions have a volume of 30 cubic nanometers and occur over a span of 10 picoseconds. The simulations, which use 32,768 processors and require 30 hours of computational time, depict an entire cascade of atomic collisions from one alpha-decay reaction.

Design Sensitivity

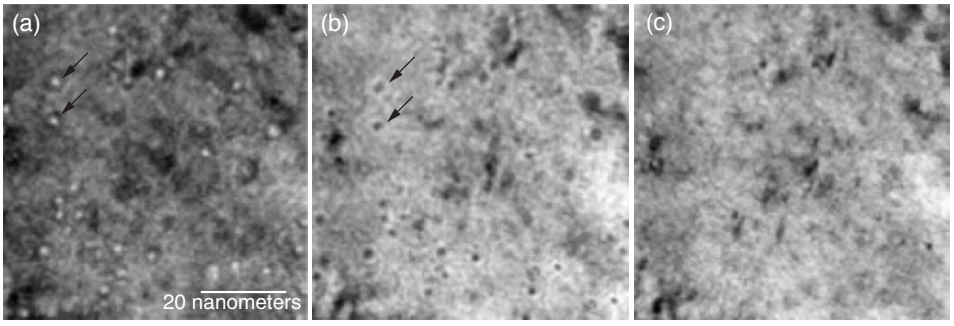
Data and models from this research improve the fidelity of design codes used to calculate the likely change in pit performance over the next few decades. Design sensitivity was then calculated for every weapon design in the stockpile.

"We take models that have been validated by nuclear testing, apply the documented effects of plutonium aging, and determine whether differences in the amount of aging affect the yield," says physicist Kris Winer. "Different devices have different performance margins, but we found that the effects of plutonium aging are very small."

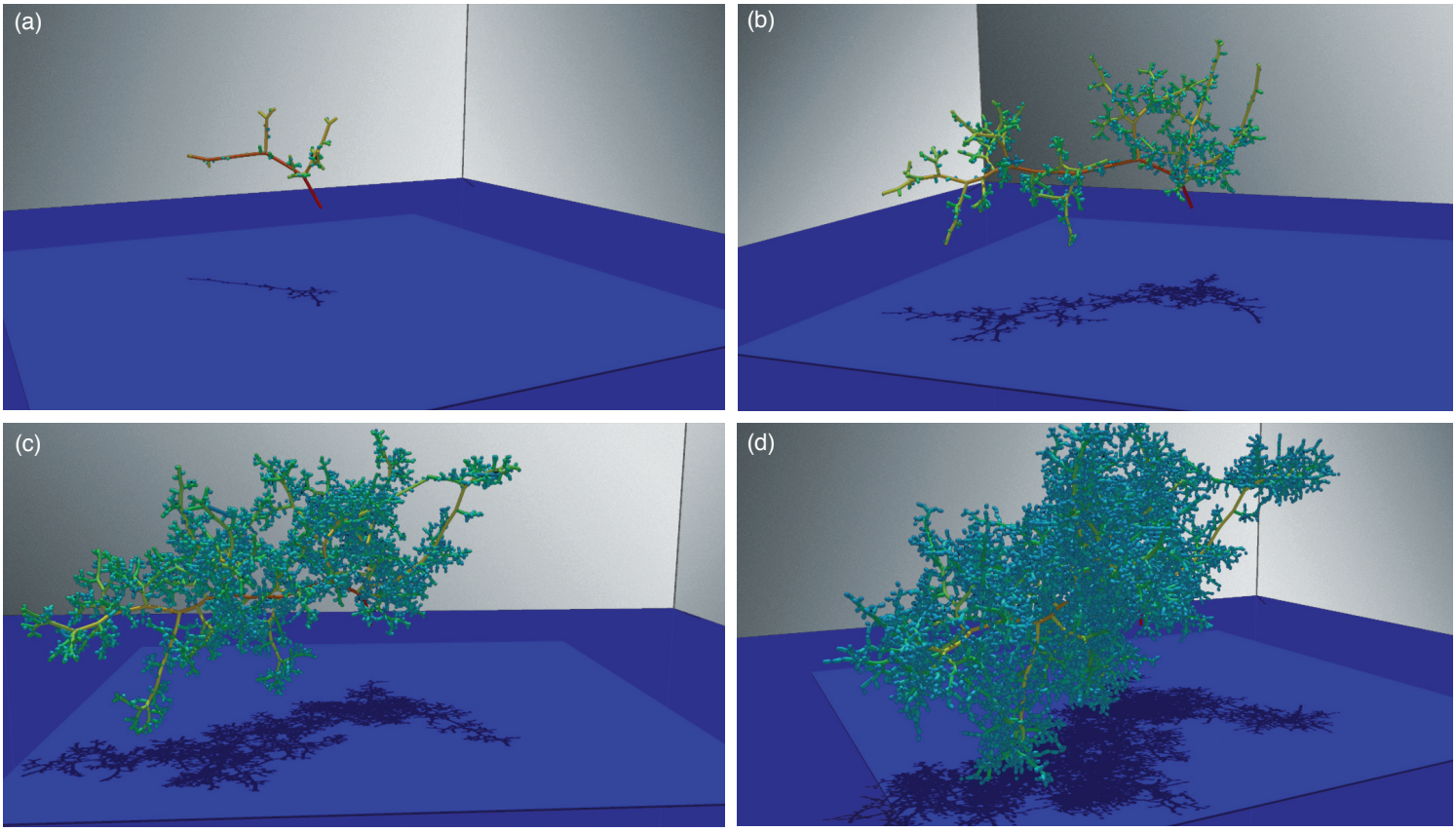
A small number of past underground experiments tested the same weapon design using plutonium samples at different stages of the aging process. "We compared the results of these detonations and determined what portion of the differences are caused by plutonium aging," says Winer. Again, these differences were small with large uncertainties.

An Informed Future

"Until NNSA commissioned this study, we didn't know with precision many of the details involved in plutonium aging," says Schwartz. "Now, we're finding out



Images of aged plutonium taken with a transmission electron microscope reveal helium bubbles measuring about 1 nanometer in diameter. (a) An underfocused image reveals tiny bubbles as a dark fringe surrounding a light dot. (b) In an overfocused image, bubbles appear as light fringes surrounding a dark dot. (c) A focused image shows no contrast from the bubbles.



(a–d) Frames extracted from a simulation run on Livermore's Blue Gene/L supercomputer show four steps in a collision cascade that occurs when a uranium-235 atom forms from the spontaneous alpha decay of a plutonium-239 atom. The newly formed uranium atom (in the red-colored region) begins to collide with plutonium atoms, forming a treelike structure. The entire simulation, which involved thousands of atoms, modeled a 10-picosecond process over an area of about 30 nanometers. Colors indicate energy levels, where red is high (85 kiloelectronvolts) and blue is low (4 electronvolts).

not only how plutonium ages but why. We still don't have all the details, but we have quantitatively improved our knowledge."

According to chemist Patrick Allen, leader of Livermore's plutonium aging study, "We now have a much better scientific understanding of several aspects of plutonium aging and so have greater confidence in the reliability of our pits and the stockpile." He points out, however, that nuclear weapon systems are extremely complicated, composed of thousands of different parts belonging to dozens of integrated systems.

"The pit is just one of a warhead's many components," he says. "Components such as high explosives and organic materials also require investigation so we can understand how aging affects their performance and stability as well."

The aging assessments of plutonium continue, as scientists track the properties of naturally and artificially aged samples. Additional data and analysis will allow them to refine minimum lifetime estimates for each stockpile system. In the meantime, experts can make more-informed decisions about America's nuclear forces and NNSA's future complex.

—Arnie Heller

Key Words: actinides, Advanced Photon Source (APS), alpha decay, diamond anvil cell (DAC), Global Nuclear Energy Partnership, helium, Joint Actinide Shock Physics Experimental Research (JASPER) Facility, nuclear power, plutonium, Plutonium Futures Conference, stockpile stewardship, uranium.

For further information contact Adam Schwartz (925) 423-3454 (schwartz6@llnl.gov).

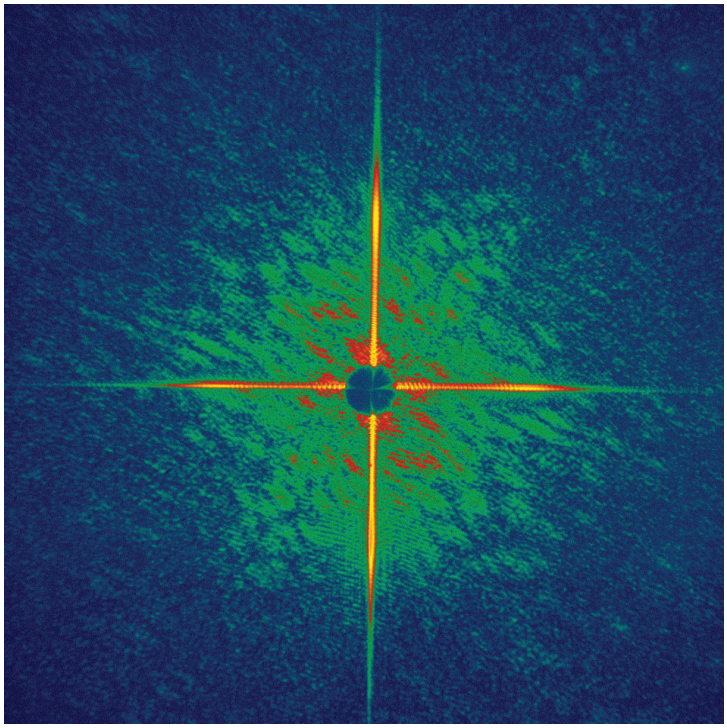
Imaging Complex Biomolecules in a Flash

VIEWING the detailed structure of a virus or protein to determine how that molecule interacts with others can help researchers better understand biological systems. Proteins, for instance, are essential parts of all living organisms. Some of them catalyze biochemical reactions that are vital to metabolism. Others help maintain cell shape or are essential in immune response and cell regeneration. These complex macromolecules can range from 400 to about 27,000 amino acids in length, and their structures are a three-dimensional (3D) tangle of precise folds and twists. Furthermore, proteins may shift between several related structures during their normal biological functions. Determining a protein's 3D structure provides important clues about its behavior and function.

Scientists usually recover 3D images of large macromolecules with x-ray crystallography, which uses x rays to bombard a crystal. As x-ray photons pass through the closely spaced lattice of atoms forming the crystal, some of them are diffracted. Recording this diffraction pattern can reveal information about the crystal lattice and its constituents, which helps researchers determine a material's molecular structure.

Unfortunately, with this technique, the targeted material must be in crystalline form, and not all biological macromolecules can be crystallized. For example, many drugs developed to treat diseases target proteins that bind to membranes, but these proteins resist crystallization. Having more detailed information about protein structures and behavior could significantly benefit treatment options and improve human health.

A team of Livermore researchers in collaboration with colleagues from the University of California at Davis, Stanford Synchrotron Radiation Laboratory, Uppsala University in Sweden, and the Deutsches Elektronen-Synchrotron (DESY) in Germany is working to solve this problem. Led by physicist Henry Chapman in Livermore's Physics and Advanced Technologies Directorate, the team is developing a method that will use the extremely bright x rays generated by the Linac Coherent Light Source (LCLS) at the Stanford Linear Accelerator Center to examine the hidden structural details of biological molecules.



An experiment with a prototype x-ray free-electron laser at the Deutsches Elektronen-Synchrotron in Germany produced this initial diffraction pattern.

Blasted to Bits

In the late 1980s, Livermore scientists demonstrated that x-ray lasers could be adapted for biological imaging. Those experiments used an extremely short x-ray pulse generated by a Nova laser beam and a diffractive optical x-ray lens to form images of cells. However, the pulses were not bright enough to produce high-resolution images of macromolecules. In addition, the lenses were not suitable for this application.

LCLS will solve this challenge when it comes on line in 2009. The world's first x-ray free-electron laser (FEL), LCLS will emit x rays in the form of a laser beam with a brightness 10 billion times greater than existing x-ray sources. Its 0.15-nanometer wavelength pulses, which are about 100 femtoseconds long, will provide the beam qualities needed to image single macromolecules at the atomic scale. Chapman is working with Janos Hajdu, a professor at Uppsala University and SLAC, to determine the optical requirements for the proposed experiments. Hajdu was one of the first to propose using such pulses for biomolecular imaging.

Another challenge for the Livermore team was to capture the faint patterns scattered from the sample before the macromolecule

or particle explodes—a time span of about 10 to 50 femtoseconds (where 1 femtosecond equals 10^{-15} seconds). To solve this problem, the Livermore team combined a graded, multilayer mirror with a charge-coupled device detector. "We have a signal-to-noise problem," says Chapman. "We must be able to detect a single photon scattering from a beam of a trillion photons." The multilayer mirror reflects the single photons of interest and filters out the unrelated photons and plasma radiation.

In designing the detector, the team applied the Laboratory's expertise in extreme-ultraviolet lithography. "Livermore has an exceptional capability for making complex multilayer mirrors," says Chapman. "The mirrors must allow scattered photons of a particular wavelength to pass through and block the others."

The detector must quickly record the diffraction pattern, before the focused x-ray pulse turns the sample into plasma. No x-ray experiments had been conducted in the relevant time and intensity domains, so the Livermore team used computer simulations to evaluate experimental setups. Modeling results indicated that nearly atomic-level resolution could be obtained by carefully choosing the pulse length, intensity, and x-ray wavelength.

FLASH First, Then Shrinkwrap

The team's initial experiments of the diffractive imaging technique used FLASH, a prototype soft-x-ray FEL developed at DESY. In these demonstration experiments, FLASH produced coherent FEL pulses, each lasting 25 femtoseconds and containing about a trillion (10^{12}) photons. Targets included latex spheres 100 nanometers in diameter and 20-nanometer-thick silicon nitride membranes with patterns cut through them by a focused ion beam. Experiments on both sample types were conducted in a vacuum chamber. The x-ray beam illuminated and passed through the sample and exited through a hole in the graded, multilayer planar mirror. Light scattered by the sample reflected off the mirror onto a charge-coupled device, which recorded the diffraction pattern.

The information encoded in this pattern is similar to that from a hologram and must be transformed into an image of the original sample. "To convert the signal data into an image, we must determine the phase of the scattered waves, but we can only measure the intensity of those waves," says Chapman. "We correlate intensity to the strength of the spatial frequencies in an image, but we still need the phases to properly sum the frequencies and form the image."

One diffraction pattern consists of more than a million data points, which translates to more than a million unknown phases that must be determined. However, because many configurations will yield the same pattern, researchers needed a method to determine which one is correct.

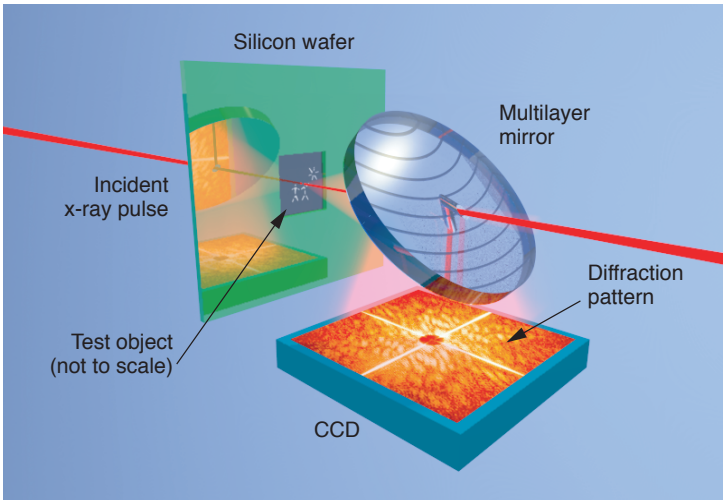
To solve this problem, the team used Shrinkwrap, an iterative transform algorithm based on methods used for astronomical imaging. Developed at Livermore by Stefano Marchesini, Shrinkwrap recovers an image in an iterative process, starting from some simple constraints. "Basically, we assume that the object is isolated with nothing around it of interest," says Chapman. "All spatial frequencies must then cancel outside the object's boundaries, adding up to zero."

Shrinkwrap iterates back and forth between the image and its calculated diffraction pattern, imposing the constraints in both spaces. Initially, the algorithm chooses a loose estimate because the object's boundary is unknown. As the iterations proceed, Shrinkwrap refines the boundary constraint and conforms to the object's shape. "The tighter the algorithm wraps around the object, the better it estimates the details and thus the boundary constraint," Chapman says. "Plus it does not require previous knowledge of an object's boundaries."

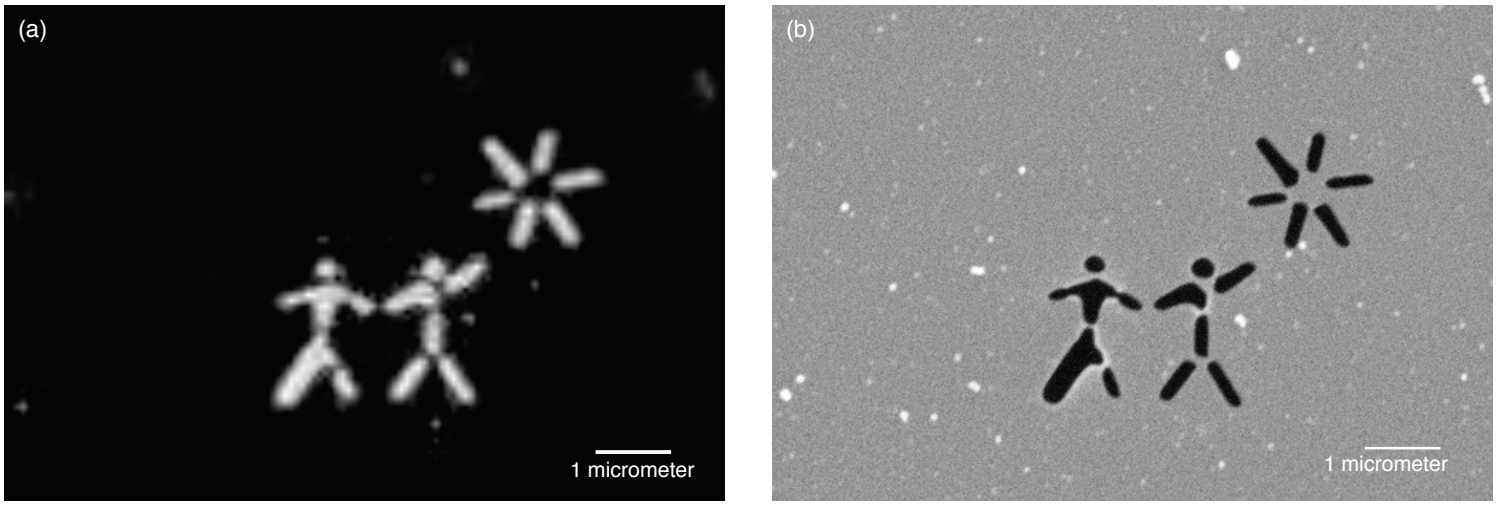
To test the technique, the team carried out many reconstructions, each time starting from random phases. Because of photon noise in the data, no solution can exactly satisfy all of the constraint sets. However, demonstration tests showed that by the final iteration, each image is clearly recognizable when compared with the micrograph taken of the object.

Seeing into the Future

This research, which was funded by Livermore's Laboratory Directed Research and Development Program, resulted in the first diffraction patterns to be created with an ultrafast pulse of soft x rays and transformed back into the original image. Featured on the December 2006 cover of *Nature Physics*, the images are thought to be the fastest ever formed. Chapman and his colleagues



In a diffractive imaging experiment using an x-ray free-electron laser, the x-ray beam is focused to a spot 20 micrometers in diameter. A multilayer mirror reflects the diffracting x rays onto a charge-coupled device (CCD). The powerful direct beam passes through a hole in the mirror to a beam dump.



The Shrinkwrap algorithm transformed the diffraction pattern shown on p. 21 into (a) an image of the targeted object, which can be compared to (b) a micrograph of the target. The pulse from the free-electron laser destroyed the object, but the destruction took longer than the pulse's 25-femtosecond duration.

are looking forward to testing the technique on LCLS, which will provide images with even higher resolution. Meanwhile, they continue to refine the process.

In March 2007, they injected submicrometer-size latex beads and biological cells into the beam using a technology developed at Livermore for use in the bioaerosol mass spectrometry system. (See *S&TR*, September 2003, pp. 21–23.) In addition, the FLASH machine is being upgraded at DESY so that it will produce even shorter pulses and wavelengths, which will reveal greater details at smaller dimensions. With LCLS and other hard-x-ray systems on the horizon, the time is coming when proteins, viruses, and complex biological macromolecules will give up their structural secrets, right down to the atomic scale.

—Ann Parker

Key Words: biological macromolecule, diffraction pattern, FLASH, Linac Coherent Light Source (LCLS), protein, Shrinkwrap algorithm, virus, x-ray free-electron laser (FEL).

For further information contact Henry Chapman (925) 423-1580 (chapman9@llnl.gov).

Lipid Rafts Observed in Cell Membranes

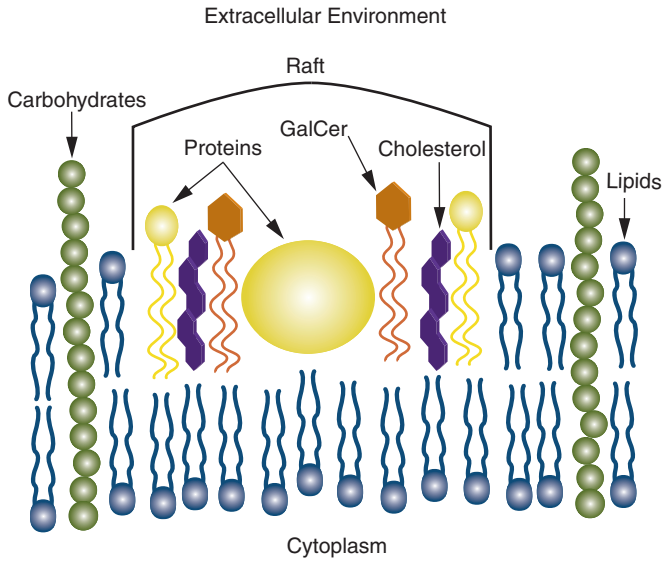
IMAGINE a raft so tiny that it floats inside the plasma membrane of a living cell. Thousands of nanometer-size rafts made of lipids may form, break apart, and reorganize in a typical cell membrane every second. Inside an already crowded membrane, the rafts can affect a cell's biophysical environment in ways that may be useful or detrimental. Lipid rafts may facilitate cell-to-cell communication, direct arriving proteins to their ultimate destinations, or regulate the uptake and transport of cholesterol by individual cells. Unfortunately, they also may provide docking sites for opportunistic viruses. A lipid raft 10 to 500 nanometers in diameter is the perfect size for free-floating viral agents such as human immunodeficiency virus (HIV) to bind with and infect individual cells.

Studying the evolution of lipid rafts can be extremely difficult. Lipid rafts are too small to see with optical microscopes, and they diffuse in milliseconds across the cell membrane. The rafts also respond unpredictably to tiny changes inside the cell and in the immediate extracellular environment. Although a 5-nanometer-thick cell membrane is just at the edge of direct observation using a transmission electron microscope, the more short-lived rafts can only be observed with advanced imaging techniques such as atomic force microscopy (AFM).

Researchers from Livermore and the University of California (UC) at Davis have teamed up to study lipid raft formation and growth. The team has for the first time observed lipid raft dynamics at the nanometer-size scale. Team members include Tim Ratto, a biophysicist from the Chemistry, Materials, and Life Sciences Directorate; Craig Blanchette, a participant in Livermore's Student Employee Graduate Research Fellowship (SEGRF) Program; and Marjorie Longo, a professor at UC Davis. (See *S&TR*, June 2006, pp. 4–13, for more about SEGRF collaborations across the Laboratory.) Other collaborators include UC Davis graduate student Wan-Chen Lin and Livermore physicist Christine Orme.

Experiments Provide Insight

Blanchette and Ratto are measuring the rates of lipid raft nucleation and growth in synthetic cell membranes, which are composed primarily of a fluid bilayer of lipids. Their work targets lipid constituents characterized by the liquid–gel phase separation (rafts consist primarily of gel-phase lipids). For this study, the researchers generated membrane systems that contain raftlike



Two opposed layers of lipids form the fundamental bilayer structure of the cell membrane. The outer layer is in contact with the extracellular environment. The inner layer touches the cell's cytoplasm. Carbohydrates traverse both layers of the membrane. Rafts are enriched with cholesterol and galactosyl ceramide (GalCer) and studded with proteins.

lipids, fluid-phase lipids, and cholesterol. Then they explored the behavior of rafts as the phase state of the cell membrane changes.

"Researchers no longer consider the cell membrane to be a static homogeneous lipid bilayer containing randomly diffusing proteins and other biological molecules," says Ratto. "The old model has been replaced by a more compartmentalized picture of the membrane in constant fluctuation. Certain lipid constituents phase-separate into these complex raftlike structures. We want to better understand how the liquid–gel relationship and the rafts themselves help mediate the cell membrane's response to environmental cues such as invasion by a pathogen."

Earlier research indicates that the phase separation of raft lipids is regulated by cholesterol, but little is known about the structural factors that create the distribution of cholesterol within multiphase lipid bilayers. Researchers now believe that cholesterol-enriched rafts signal, sort, and direct incoming proteins through biochemical pathways and can also act as attachment platforms for host pathogens and their toxins.

An example of the attachment function is the sexual transmission of HIV, which appears to occur via rafts enriched in galactosyl ceramide (GalCer). A carbohydrate-bearing type of lipid, GalCer collects in the extracellular leaflets of rafts—portions of the rafts that extend beyond the cell membrane into the extracellular environment. Local clustering of GalCer in raft leaflets may facilitate the initial adhesion of bacteria or viruses, including HIV type 1, through interactions between proteins and GalCer. In this way, the cell becomes infected. Further study on

blocking the attachment function may help scientists understand how to protect the cell from pathogenic invasion.

The team examined the biophysics of raft nucleation and phase separation. "The mixtures in our study contained GalCer, cholesterol, and three different structures of fluid-phase lipids," says Blanchette. "We found that the fluid-phase lipid component dramatically affects the partitioning of cholesterol between the raft phase and the fluid phase."

The team also calculated formation-rate relationships between the raft phase and the surrounding fluid phase. The researchers then ran calculations as a function of domain symmetry (the raft-to-liquid relationship) and of cholesterol for various compositions. The measurements and calculations proved valuable in understanding the dynamic nature of rafts in membranes and the limiting time scale during which membranes experience significant raft nucleation and growth.

In comparing diffusion- and reaction-limited time scales, the team found raft growth to be reaction-limited. That is, the rate of raft growth depended on the "success" of collisions between lipid particles as they bind—not on diffusion.

Innovative Tools Aid Observation

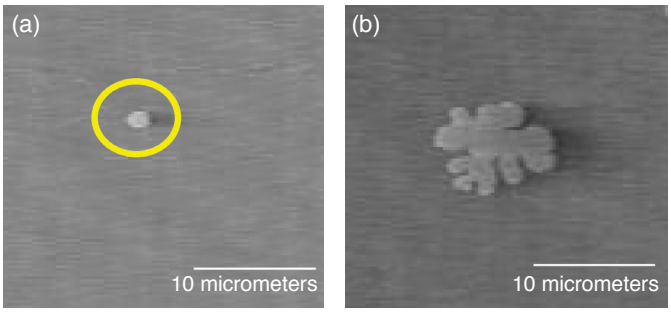
In another study, funded by the National Science Foundation, Ratto and Longo examined phase separation in bilayer membranes. Says Ratto, "Using the data on phase separation in supported bilayers, we can tailor experiments to display characteristics we want to study, either gel-phase lipid 'obstacles' surrounded by a fluid bilayer or fluid 'pools' bounded by an immobile gel bilayer."

The researchers used a technique called fluorescent recovery after photobleaching (FRAP) to confirm obstructed diffusion in cell membranes. This technique allows them to calculate diffusion across a plasma membrane. A pulse of laser light directed on a region of fluorescently labeled cell membrane temporarily bleaches the region until unbleached membrane molecules move into it.

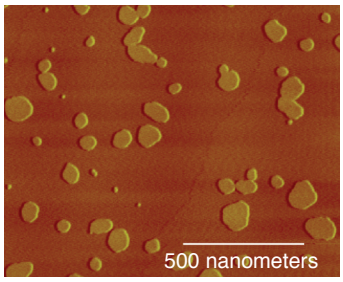
By comparing the bleached region to a region that has not been pulsed, they can calculate a recovery rate that provides information on two-dimensional diffusion. This rate characterizes the membrane's structure and the mobility of its lipids and protein receptors.

In these calculations, the researchers relied on correlations with relatively untested mathematical models of hindered diffusion. They then used the FRAP technique to test the models and predict the diffusion rate of molecules within a cell membrane.

Using AFM allowed the researchers to distinguish a lipid raft from the lipid fluid on which it floats. They then combined the FRAP and AFM techniques to compare theoretical models with observed structures. FRAP was used to determine lateral diffusion rates across the bilayer, and AFM was used to characterize raft sizes and concentrations and to visualize nanoscale nucleations. After selecting the appropriate mixtures of lipids, Ratto and Longo produced circular raft domains with diameters ranging from micrometers to a nanometer and diffusion rates ranging across three orders of magnitude. This methodology shows promise as a means for testing theoretical models of generalized obstructed diffusion in thin films and for examining raft (obstacle) concentrations in cellular membranes.



In low-cholesterol environments, (a) lipid rafts nucleate symmetrically and then (b) develop asymmetrically. (Images courtesy of the University of California at Davis.)



Researchers used atomic force microscopy to capture this image of phase-separated lipid domains. The gel-phase domains (light) extend just 1.8 nanometers above the surface of the fluid phase (dark). (Image courtesy of the University of California at Davis.)

Longo and Ratto developed the means for later research teams to fashion experimental models for analysis using the Laboratory's nanometer-scale secondary-ion mass spectrometer (NanoSIMS), one of only five such instruments in the U.S. (See *S&TR*, December 2006, p. 3.)

Results from this collaboration between Livermore and UC Davis could help scientists develop methods to short-circuit a virus attack on cells, characterize structures within biological pathogens, and increase the sensitivity and flexibility of biological sensors. The field of cellular biophysics is advanced by their discoveries.

—Alane L. Alchorn

Key Words: atomic force microscopy (AFM), bilayer, cell membrane, cholesterol, fluorescent recovery after photobleaching (FRAP), human immunodeficiency virus (HIV), lipid raft, phase separation.

For further information contact Tim Ratto (925) 422-8739 (ratto7@llnl.gov).

Exchanging Insights on Quantum Behavior

Teller's Contributions to Condensed-Matter Physics

January 15, 2008, marks the 100th anniversary of Edward Teller's birth. This highlight is the third in a series of 10 honoring his life and contributions to science.

FOR Edward Teller, scientific research was a collaborative venture. He thrived on the exchange of ideas with other scientists. This approach allowed him to keep up to date on developments in many disciplines and helped him find connections between basic science research and potential applications.

Teller's work in condensed-matter physics shows the success of his collaborative style. Some of his research built on the ideas presented by his colleagues. In other projects, his insight led to a new understanding of atomic behavior in liquids, bulk solids, and material surfaces.

Solving a Quantum Puzzle

The discovery of quantum mechanics allowed scientists to unravel many of the paradoxes found in classical physics. One such paradox involved the magnetic properties of materials. All materials respond to a magnetic field, but in some substances, this response is weak. Classical physics predicts that the diamagnetic response, in which a material is weakly repelled by a magnetic field, does not exist. The classical computation of this effect always yields zero.

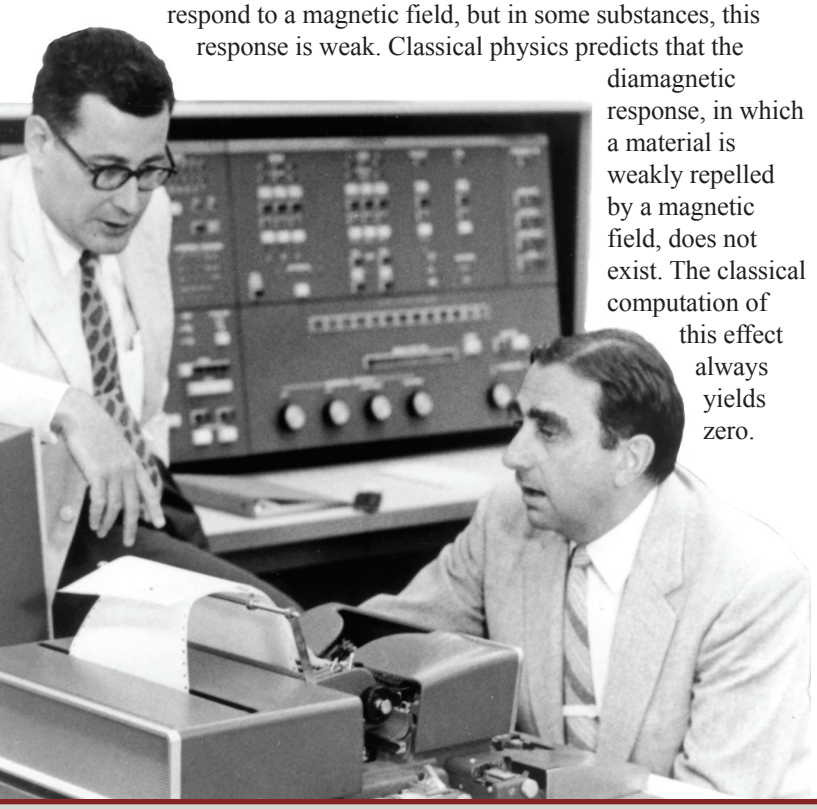
In 1930, Lev Landau, a physicist from Russia and friend of Teller's, applied quantum mechanics to address this paradox. Using the Schrödinger equation, Landau showed that an electron's orbit contributes to a material's diamagnetic susceptibility. He then computed this effect in a free-electron gas.

Werner Heisenberg, Teller's advisor from the University of Leipzig, suggested that Landau had not completely resolved the paradox and challenged Teller to explain the physical processes in the complex computations. The results, which appeared in the German journal *Zeitschrift für Physik* in 1931, presented a new way of looking at diamagnetism. In his study, Teller directly computed the electric current density induced by a magnetic field and showed how electron orbits at a material's outer edge contribute to Landau's solution. Physicists have since found this physical explanation to have several useful applications, for example, in determining the states of electrons in metals.

An Extended Model of Adsorption

Another important collaboration involved Stephen Brunauer, a fellow Hungarian and one of Teller's first students at George Washington University. Brunauer wanted to extend the Langmuir model—which describes the adsorption process for a layer of material one molecule thick—to multiple layers. An adsorbed material may change the overall behavior of an open surface, but it does not chemically react with the surface's molecular structure. For example, when condensation forms on glass, the water vapor molecules do not react with the glass, but rather form thin puddles of liquid phase. Understanding this adsorption process is important for applications involving catalysts.

Brunauer proposed that a surface's attractive force extends beyond the first layer of adsorbed material. Teller countered that the attraction would be too weak to hold multiple molecular layers. Instead, he proposed an adsorption model that accounts for the balance between an atom's simultaneous tendencies to attach and evaporate. To test Teller's hypothesis, Brunauer asked Paul Emmett, a physical chemist at the Department of Agriculture, to experimentally verify the model. The resulting Brunauer–Emmett–Teller equation of state, published in the *Journal of the American Chemical Society* in 1938, is still broadly applied in surface physics.



Harold Brown (left) and Edward Teller work on LARC, the Livermore Advanced Research Computer.

Teller and his wife, Mici, examine a model used to teach nuclear physics. In the background is the first page of the 1953 paper on the Metropolis algorithm.

How Polar Salts Respond to Light

In 1941, Teller led his colleagues Russell Lyddane and Robert Sachs to develop a rule describing the dielectric constant needed to explain how photons propagate in salts. Now called the Lyddane–Sachs–Teller relationship, this rule relates the very high and very low frequency-limiting values of a material's dielectric constant to the basic frequencies of salt's internal ion modes.

Published in *Physical Review*, the relationship can be used to explain insulating polar solids such as table salt, to determine the frequencies at which photons are reflected by the salt medium, and to study ferroelectric materials. The Lyddane–Sachs–Teller relationship is also analogous to nuclear vibrations—a connection that led Maurice Goldhaber and Teller to predict ubiquitous high-energy gamma-ray absorption resonances in nuclei.

Metropolis Accelerates Computational Science

Before Teller left Los Alamos National Laboratory to found Lawrence Livermore, he worked with Marshall Rosenbluth, his former student from the University of Chicago, to design the hydrogen bomb. The two physicists ran their equation-of-state calculations on the new Los Alamos computer being built by Nicholas Metropolis. At the time, scientists thought these calculations required an astronomical amount of effort, and a rigorous solution considering every possible microscopic state could not be computed for such a large system.

Teller and Rosenbluth realized that many points in phase space represent highly unlikely configurations, and random selection would thus be an ineffective sampling method. Instead, Teller imagined using a method that accepts or rejects a change in the system according to a probabilistic rule that mimics the system's dynamics.

Working with this idea, Rosenbluth designed an algorithm to select the samples. Teller's wife, Mici, began the computational work to encode the algorithm. Marshall's wife, Arianna, completed the code and carried out the calculations.

The result, now known as the Metropolis algorithm, has proven to be an extraordinary tool. Published in 1953 in *Journal of Chemical Physics*, this method has been used not only to calculate many properties of condensed matter but also to solve mathematical problems such as combinatorial optimization. In 2000, *Computing in Science and Engineering* chose Metropolis as one of the top 10 algorithms having the "greatest influence on the development and practice of science and engineering in the 20th century." The original 1953 paper has been referenced in more than 10,000 peer-reviewed articles, including a 1966 report on plasma equations of state by Livermore scientists Stephen Brush, Harry Sahlin, and Teller—their collaborator and mentor.

When Ernest O. Lawrence and Teller founded Lawrence Livermore in 1952, they encouraged Laboratory researchers to exchange ideas with their colleagues and those working in other disciplines. This tradition of collaborative, multidisciplinary science remains a hallmark of the research at Livermore.

—Carolin Middleton

Key Words: condensed-matter physics, Brunauer–Emmett–Teller equation of state, Edward Teller, Lyddane–Sachs–Teller relationship, Metropolis algorithm.

For further information contact Stephen B. Libby (925) 422-9785 (libby1@llnl.gov).

Each month in this space, we report on the patents issued to and/or the awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory.

Patents

Ultra-Narrow Bandwidth Voice Coding

John F. Holzrichter, Lawrence C. Ng
U.S. Patent 7,162,415 B2
January 9, 2007
This system removes excess information from a human speech signal, codes the remaining signal information, transmits the coded signal, and reconstructs it. The system uses one or more electromagnetic wave sensors and one or more acoustic microphones to determine at least one characteristic of the human speech signal.

Nucleotide Sequences Specific to *Francisella tularensis* and Methods for the Detection of *Francisella tularensis*

Paula M. McCready, Lyndsay Radnedge, Gary L. Andersen, Linda L. Ott, Thomas R. Slezak, Thomas A. Kuczmarski, Elizabeth A. Vitalis
U.S. Patent 7,172,868 B2
February 6, 2007
Nucleotide sequences can be developed specific to *Francisella tularensis* to serve as a marker or signature for identifying this bacterium. In addition, forward and reverse primers and hybridization probes derived from these sequences can be used to detect the presence of the bacterium.

Compact Accelerator

George J. Caporaso, Stephen E. Sampayan, Hugh C. Kirbie
U.S. Patent 7,173,385 B2
February 6, 2007
This compact linear accelerator has at least one strip-shaped Blumlein module that guides a propagating wave front between first and second ends and controls the output pulse at the second end. Each Blumlein module has three planar conductor strips, with one dielectric strip between the first and second conductor strips and a second dielectric strip between the second and third conductor strips. A high-voltage power supply charges the second conductor strip to a high potential, which is then switched to at least one of the first and third conductor strips to initiate propagating reverse polarity wave fronts in the corresponding dielectric strips.

Inline Evenflow Material Distributor for Pneumatic Material Feed Systems

Michael J. Thiry
U.S. Patent 7,178,750 B2
February 20, 2007
This apparatus reduces clogs in a pneumatic material feed line such as those used in abrasive water jet machining systems, by providing an even flow of material. A hollow housing defining the housing volume has an inlet connected to an upstream portion of the pneumatic material feed line and an outlet connected to a downstream portion of the line. A vent between the inlet and outlet releases excess air pressure from the housing volume. A diverter, that is, an impingement object, is placed at the inlet in the path of incoming material from the upstream portion of the feed line to break up clumps of ambient moisture-ridden material impinging on the diverter. One or more filter screens can also be located in the housing volume to further break up clumps and provide filtering.

Nonlinear Optical Crystal Optimized for Ytterbium Laser Host Wavelengths

Christopher A. Ebbers, Kathleen I. Schaffers
U.S. Patent 7,179,405 B2
February 20, 2007
A material for harmonic generation has been made by changing the crystal $LaCa_4(BO_3)_3$ also known as LaCOB to the form $Re1_xRe2_yRe3_zCa_4(BO_3)_3O$. In this form, Re1 and Re2 are rare-Earth ions 1 and 2 selected from the group consisting of scandium, yttrium, lanthanum, cerium, praseodymium, neodymium, samarium, europium, gadolinium, terbium, dysprosium, holmium, erbium, thulium, ytterbium, and lutetium; Re3 is lanthanum; and $x + y + z = 1$.

Awards

Livermore researchers **Kenneth Bogen** and **Edwin Jones** of the Energy and Environment Directorate received the **2006 Best Paper for Risk Analysis Award** in the decision sciences category from the **Society for Risk Analysis**. The award-winning paper, "Risks of Mortality and Morbidity from Worldwide Terrorism: 1968–2004," appeared in the February 2006 issue of *Risk Analysis*.

In analyzing 36 years of data, Bogen and Jones found that terrorism casualty patterns exhibit the same type of rare-event (worst-case) behavior as many types of extreme physical phenomena. With this information, they also estimated the lifetime risks of injury and death from terrorism events in different world regions.

A team of Laboratory researchers received the **Best Application Paper Award** at the **2006 Visualization Conference** held in Baltimore, Maryland, by the **Institute of Electrical and Electronics Engineers**. The winning paper, "Understanding the Structure of the Turbulent Mixing Layer in Hydrodynamic Instabilities," was coauthored by **Valerio Pascucci**, **Daniel Laney**, **Peer-Timo Bremer**, and **Ajith Mascarenhas** of the Center for Applied Scientific Computing and **William Cabot**, **Andrew Cook**, and **Paul Miller** of the Defense and Nuclear Technologies Directorate. In this study, the researchers used Morse theoretical techniques to extract bubblelike features from a large data set produced in a hydrodynamics simulation conducted on Livermore's BlueGene/L supercomputer. The new technique allowed them to analyze the complex topology that occurs in Rayleigh–Taylor mixing, which may play a central role in hydrodynamic instability.

Abstracts

A Quantum Contribution to Technology

Researchers in Livermore's Quantum Simulations Group have used quantum molecular dynamics modeling to solve many basic-science questions and are now turning their focus on examining nanometer-size materials for use in new technologies and in improved applications. One team is characterizing silicon and silicon germanium to maximize the thermoelectric efficiency of nanowires designed for cooling military technologies. Another project is studying semiconductor alloys that could replace high-purity germanium in radiation detectors. In collaboration with the National Renewable Energy Laboratory, Livermore scientists have developed quantum Monte Carlo tools to evaluate potential materials for hydrogen-fuel storage systems. These carbon-based molecules would act as sponges that store hydrogen fuel onboard vehicles. Quantum simulations are also helping researchers determine the effectiveness of quality-control tools used to analyze nanoscale features on silicon chips as chip sizes decrease.

Contact:

Andrew Williamson (925) 422-8285 (williamson10@llnl.gov).

U.S. Weapons Plutonium Aging Gracefully

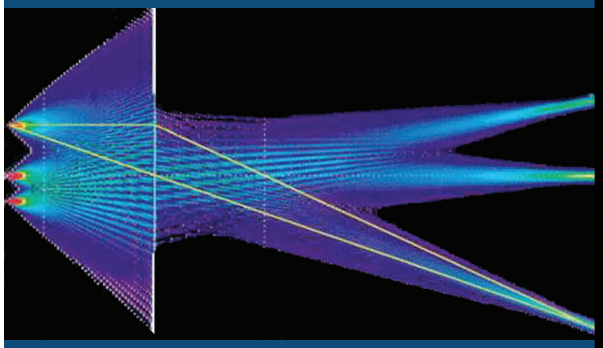
Since the Laboratory's founding in 1952, Livermore scientists have helped advance the science of plutonium and its closely related elements, called actinides. Livermore scientists used some of the most advanced and accurate instruments in the world to measure the microstructural, physical, and chemical properties of plutonium and its alloys. Advanced computational models of weapons physics and theoretical studies helped researchers design the experiments and provided data to complement the experimental results. In 1997, researchers at Lawrence Livermore and Los Alamos national laboratories began a multidisciplinary study examining the long-term effects of radioactive decay on the plutonium contained in the pits, or cores, of nuclear weapons. In 2006, the National Nuclear Security Administration announced the study's results, which indicate that the nuclear warheads in the nation's stockpile would remain reliable over the next several decades. The Livermore effort included dynamic and static experiments to examine how radioactive decay affects plutonium's structure, phase stability, and equation of state. Researchers also measured the element's density and volume with unprecedented accuracy and reviewed data from past nuclear tests. In addition, calculations of weapon design sensitivity determined the extent to which aging pits would affect performance decades from today. By combining experimental and computational resources, scientists working on the study derived the most accurate estimates ever obtained for pit lifetimes.

Contact:

Adam Schwartz (925) 423-3454 (schwartz6@llnl.gov).

U.S. Government Printing Office: 2007/670-074-10028

Stretching Time



A Livermore-developed "time microscope" slows very fast signals to magnify details that were previously undetectable.

Also in June

• Livermore engineers are demonstrating the extended driving range of a liquid-hydrogen-fueled hybrid car.

• Laboratory computer simulation expertise is helping determine the seismic safety of the nation's dams.

• An implanted retinal prosthesis restores partial sight to those blinded by retinal diseases.

Coming Next Month

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P.O. Box 808, L-664
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