January/February 2009

Science & Technology REVIEW

National Nuclear
Security Administration's
Lawrence Livermore
National Laboratory

A Nose for Danger

Also in this issue:

- Supercomputing Grand Challenge Tackles High-Energy-Density Physics
- Imaging Ultrafast Dynamics of Nanoscale Structures
- Safety and Environmental Stewardship in the Extreme

About the Cover

Livermore researchers have designed and built a new sensing device that selectively identifies chemicals of interest from a typical background "soup" of airborne compounds. This device, as described in the article beginning on p. 4, uses minuscule diving boards (artist's conception on the cover) called microcantilevers. The Livermore design is based on the differential bending of silicon microcantilevers coated with specialized polymers.

Cover design: Daniel Moore

About the Review

At Lawrence Livermore National Laboratory, 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 eight 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.

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Lawrence
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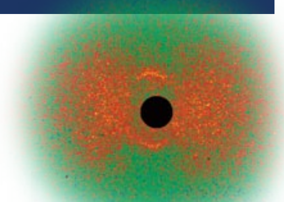
Features

Research Highlights



Departments

Squeezing Out Information about "Super Earth" Planets

A team of Laboratory researchers has developed a new technique to identify phase transitions that may one day reveal the interior structure of "super Earth" planets. Using one beam of Livermore's Janus laser, Raymond Smith of the Physical and Life Sciences Directorate and colleagues Jon Eggert, Michael Saculla, Marina Bastea, and Damien Hicks launched a ramp-compression wave lasting several nanoseconds against a bismuth sample and measured the telltale signature of a structural phase transformation. Phase transition kinetics are the time-dependent changes that materials undergo when transforming from one structure to another, whether it's a gas, liquid, solid, or plasma.

Experimental results showed that at the ultrafast timescales of laser-driven ramp-wave-loading, the pressures associated with phase transformations in bismuth increased dramatically compared with previous slower experiments. "We discovered that at a critical pressurization rate, the pressure where the phase transition takes place begins to deviate from its equilibrium value," says Smith. "The difference between this observed pressure and the equilibrium phase-transition pressure increased logarithmically with pressurization rate."

The laser ramp platform can be used at pressures relevant to the interiors of recently discovered super Earth planets, which are several times larger than our own. The technique could help map regions of the structural phase space of materials within these planets, providing critical information for understanding how planets formed and evolved. The research appeared as the cover article in the August 8, 2008, edition of *Physical Review Letters*.

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New Spin on Atoms at Earth's Core

Laboratory researchers William Evans and Heather Watson, along with colleagues at the University of Texas at Austin and other institutions, determined materials in the lowermost mantle of Earth display atomic properties that could lead to clues about what goes on deep inside the planet. "For the first time scientists have seen a broad region in the subsurface with partially paired electrons," says Evans, coauthor of the research with former Lawrence Fellow Jung-Fu Lin, who is now an assistant professor at the University of Texas at Austin. "This pairing doesn't normally occur in other geologic formations."

The scientists used Argonne National Laboratory's synchrotron light source to probe the material's electronic and atomic structure. A palm-size diamond anvil cell re-created pressures in the material similar to those in Earth's mantle, and the material was heated. The spin and valence of the electrons were then measured. The researchers unexpectedly found that at conditions present in the lowermost mantle, the electrons of iron are partially paired. High pressure caused some of the electrons, which typically repel each other, to pair up. These results indicate that changes in the radiative thermal conductivity of iron in the lowermost mantle are controlled by the structural transition of perovskite (the most common mineral found in Earth's mantle) rather than the electronic transition of iron.

The new findings about the properties of the lowermost mantle materials will help scientists decipher seismic observations and improve geochemical modeling and geodynamic simulations of the Earth's deep interior. The research appeared in the October 2008 issue of *Nature Geoscience*.

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Melting Ice under Pressure

A team of scientists from the Laboratory and the University of California at Davis performed first-principles molecular dynamics simulations using a two-phase approach to determine the melting temperature of ice VII (a high-pressure phase of ice) in pressures ranging from 100,000 to 500,000 atmospheres (1 atmosphere is the pressure at the Earth's surface). The team, led by Livermore's Eric Schwegler, found that for pressures between 100,000 and 400,000 atmospheres, ice melts as a molecular solid (similar to how ice melts in a cold drink). However, at higher pressures, the onset of molecular dissociation and proton diffusion under pressure occurs gradually and bears many similarities to a superionic solid phase.

The team's results pinpoint the melting curve at extremely high pressures (from 350,000 to 450,000 atmospheres), similar to those found in the interiors of Neptune, Uranus, and Earth. Determining the melting curve of water is important in many scientific fields, including physics, chemistry, and planetary science. Researchers have proposed that the cold subduction zones in Earth are likely to intersect with the high-pressure melting curve of water. If accurate, this hypothesis would have profound implications for the composition and transport of materials in the interior and the long-term evolution of the planet as it cools. The team's results appeared in the September 23, 2008, edition of *Proceedings of the National Academy of Science.*

Contact: Eric Schwegler (925) 424-3098 (schwegler1@llnl.gov).

Continued on p. 22

Protecting Our Military Forces

THE use of chemical weapons has a long history, stretching from ancient poisoned arrows aimed at a single person to modern nerve gases that can affect thousands and persist in the atmosphere for long periods. During the Iran–Iraq War, which began in 1980, Iraq directed chemical warfare agents not only at Iranian forces but also at several thousand of its own people. In 1995, the terrorist group Aum Shinrikyo released the nerve gas sarin in a Tokyo subway, killing a dozen civilians and injuring hundreds more. Today, anyone could be a target.

There can be no question, however, that those who are in most need of protection are the men and women who serve in the U.S. armed forces and put their lives on the line every day. As a former officer in the U.S. Army, I feel a special commitment to each and every soldier, especially those who are in harm's way at the frontiers of freedom. Fortunately, Lawrence Livermore has the scientific and technical capabilities to help keep these individuals as safe as possible.

The article beginning on p. 4 describes a new sensor that can detect deadly chemicals, including chemical weapons on the battlefield and toxic compounds that could be used in a terrorist attack. This project for the Departments of Defense and Homeland Security aims to provide an electronic early warning system that is small yet rugged, requires little power, accurately detects chemicals at low concentrations, and can be manufactured inexpensively. In this "electronic nose," microcantilevers coated with various polymers react with chemical molecules to detect and identify agents. Its development took advantage of the expertise at Livermore's Forensic Science Center, one of only two U.S. laboratories certified by the Organisation for the Prohibition of Chemical Weapons to analyze chemical samples collected under the Chemical Weapons Convention. The current prototype is a handheld device. One plan is to miniaturize the detector to the size of a lapel pin and replace the cumbersome and sometimes unreliable detectors now in the field. A tiny detector helps to keep soldiers as agile as possible.

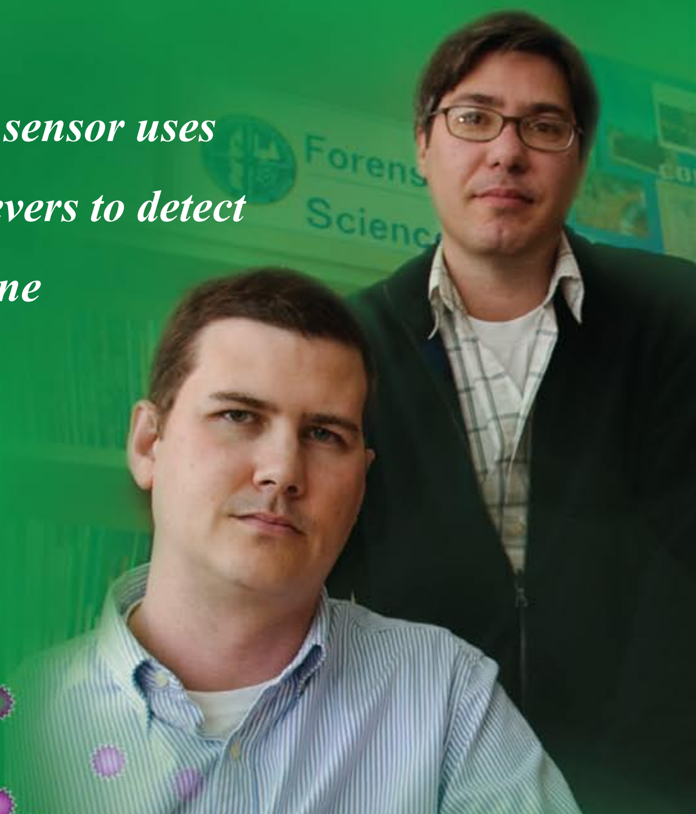
Our task in the Laboratory's Global Security Principal Directorate is twofold: to keep soldiers and civilians safe and secure from harm and to make it as difficult as possible for adversaries to act against the U.S. or national interests. We have developed an array of sensors for biohazards, radiation, and other toxins that have already been deployed in the U.S. and around the world. Our researchers continue to fine-tune these devices to make them smaller, more easily hidden, and more rugged for harsh environments. In addition, new technologies that build on previous successes will soon be available to provide even greater protection. The microcantilever electronic nose is a prime example of such technology.

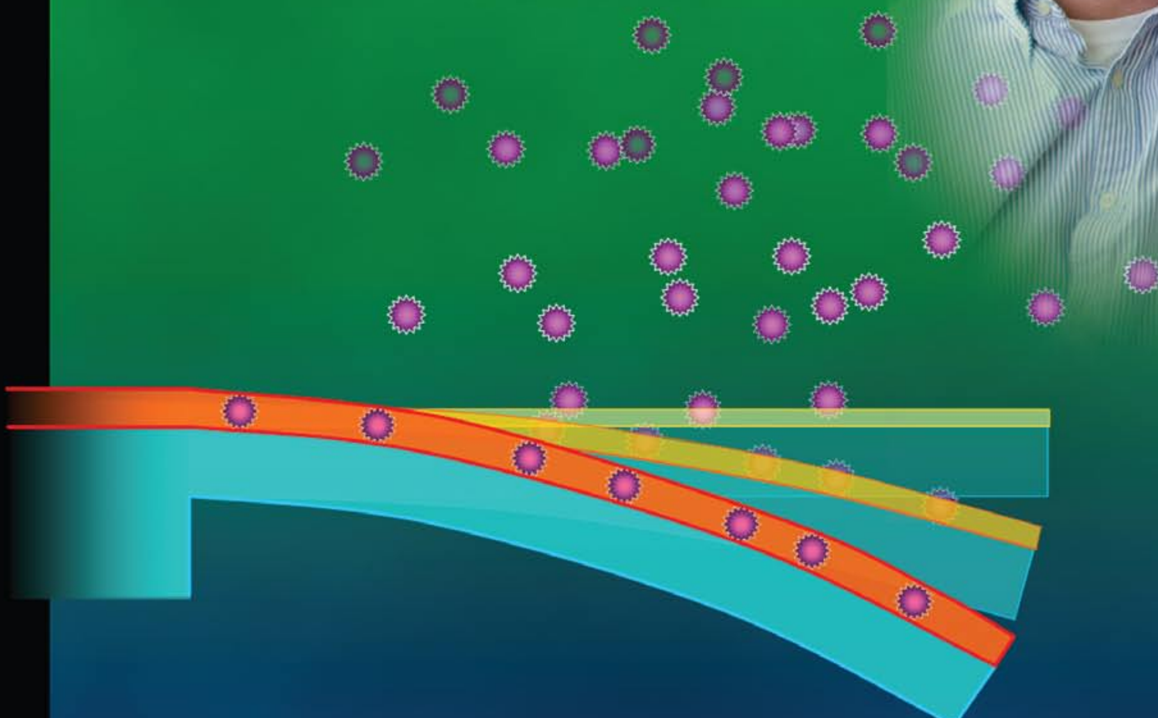
The microcantilever chemical sensor is one of many successes of which imaginative and innovative Laboratory scientists and engineers can be proud. I am confident that soon soldiers and first responders will be provided with this reliable device to strengthen the nation's chemical detection capabilities.

■ John C. Doesburg is principal associate director for Global Security.

Sniffing the Air

A new Livermore sensor uses minuscule cantilevers to detect dangerous airborne chemicals.





The Livermore sensor research was led by (from left) chemist Brad Hart, former Laboratory chemist Timothy Ratto, and physicist Albert Loui. The artist s rendering represents a side view of a polymer coated microcantilever responding to the presence of chemical vapors of interest. The chemical molecules (pink balls) are absorbed by the microcantilever s thin polymer coating. When this coating swells, a surface stress is applied to the cantilever, causing it to bend. The more the microcantilever bends, the more its electrical resistance changes.

with an Electronic Nose

THE human nose is a marvel at detecting more than 10,000 different airborne chemicals. For more than a decade, scientists have been attempting to emulate and even surpass the capabilities of the human nose with devices sometimes called "electronic noses." New sensor technologies have been invented to aid medical diagnosis, ensure quality control in the food and beverage industries, detect high explosives in airports, and search for toxic gases in factories.

For more than two decades, Lawrence Livermore scientists have been among the leaders in developing miniaturized electronic tools to detect chemical, seismic, magnetic, pressure, acoustic, and nuclear signals. For example, Livermore researchers have built highly accurate and extremely sensitive sensors that can detect trace amounts of airborne radioactive contaminants emanating from a suspected nuclear weapons facility.

The Laboratory is now working to meet the requests of Departments of Defense and Homeland Security planners for lightweight, accurate, and inexpensive handheld sensors to sniff out deadly chemicals, including chemical weapons on the battlefield and toxic compounds that could be used in a terrorist attack. The ambitious goal is to simultaneously fulfill the requirements of small size, low power consumption, rapid and reliable detection of chemicals at extremely low concentrations, ruggedness for potentially harsh environments, and low cost per unit for mass production and widespread use.

A team of physicists, chemists, and engineers is working toward this goal with a new sensing device that selectively identifies chemicals of interest from a typical background "soup" of airborne compounds, using minuscule diving boards called microcantilevers. The Livermore electronic nose can detect nearly any chemical vapor, including chemical warfare agents, once the sensor has been "trained" to recognize them. The device has reliably detected 11 different chemical vapors, plus the chemical warfare agents VX and sulfur mustard, representing a wide breadth of chemical classes.

Building an Early Warning System

"We want to provide national emergency responders and soldiers in the field with an electronic early warning system for detecting chemical agents, one that will be far more efficient and cost-effective than those currently available," says chemist Brad Hart. "Many sensors can readily detect chemical agents in the low parts per million concentration range with rapid response rates, but those devices are bulky, heavy, require power-hungry electronics, suffer from false-positive readings, and have price tags exceeding $10,000 per unit. We don't believe any commercial sensor system matches the small size, low power consumption, robustness, sensitivity, and other characteristics of our design." Hart leads the team of researchers whose pioneering sensor design was spotlighted on the May 2008 cover of the scientific journal *The Analyst*.

In studying different sensor designs and materials, the team focused on the potential of microcantilevers as transducers to communicate the presence of chemical vapors of interest. The Livermore design is based on the differential bending of a microcantilever made from silicon and wrapped in silicon nitride—a durable, chemically inert material. A final plastic coating that is relatively impervious to water vapor is then applied. The greater the amount of material absorbed by the microcantilever, the more it bends, until a maximum deflection of about 1 percent is achieved. “Microcantilevers have no intrinsic capability to sense chemicals,” says physicist Albert Loui. “The application of a swellable coating gives them this capability.”

The device is an example of a microelectromechanical systems– (MEMS-) based chemical sensor, which requires specific materials to imbue it with chemical sensitivity. These materials, usually specialized polymer (plastic) coatings, have an affinity for the chemical vapors of interest and undergo a change when interacting with them. In the Livermore design, gas absorption creates volumetric strain; thus, a chemical signal is rendered into a mechanical one.

The sensor technology takes advantage of a physics principle called piezoresistance, which is a change in the electrical conductivity (or resistivity) of a solid material as it is deformed. Piezoresistive microcantilevers are commercially manufactured by standard microfabrication techniques. In the current Livermore prototype, different plastic formulations are applied to each microcantilever, with uncoated microcantilevers acting as electrical references. (See the box at left.)

When a cantilever bends from the swelled coating, its resistance changes, which is measured by an electrical circuit. “We’re not measuring mass, as with a mass spectrometer, but rather the electrical resistance,” Hart notes. He also points out that a mass spectrometer gives a readout of everything in the atmosphere, but the Livermore sensor is designed for applications in which only one or two specific chemicals are detected.

The current research effort is funded by the Department of Defense’s National Consortium for Measurement and Signatures Intelligence Research. Hart works in Livermore’s Forensic Science Center, one of only two U.S. laboratories certified as an analytical laboratory for the Organisation for the Prohibition of Chemical Weapons. Much of the sensor research has been carried out at the Laboratory by Hart, Loui, and chemist

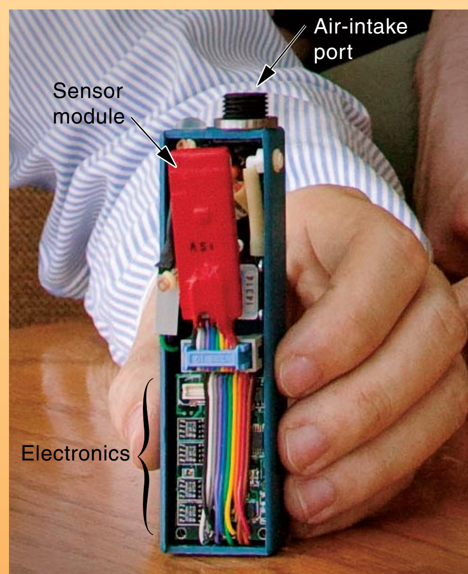
Livermore Sensing Microcantilevers in Action

Laboratory scientists have designed a new chemical detector that uses a pair of commercially manufactured sensor arrays packaged inside a flow cell, exposing both arrays to a common air stream. Each array integrates four rectangular piezoresistive microcantilevers. Six of these microcantilevers (three per side) are coated with six different polymer (plastic) formulations. When gas-phase molecules land on the cantilevers, they diffuse into the polymer, changing its physical and chemical properties.

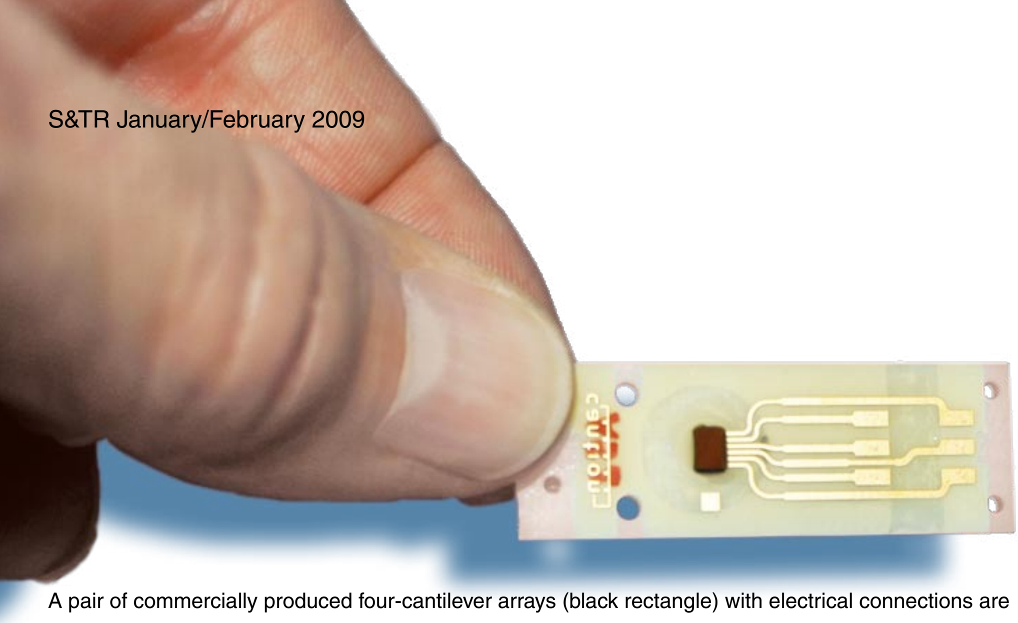
The polymer coating swells as its constituent molecular strands move past one another, changing the coating’s physical dimensions and exerting a stress on the underlying silicon substrate. The resulting deflection changes the microcantilevers’ electrical piezoresistance, which is readily measured. The amount of swelling is proportional to the amount of material absorbed, and the pattern of swelling among the six microcantilevers indicates which chemical vapor is present.

During operation, each of the six sensor channels continuously outputs a voltage that is proportional to the changes in the piezoresistance caused by the bending of the polymer-coated microcantilevers. These signals, along with the voltages from the two uncoated reference cantilevers, are sent to an electronics module. For each microcantilever, the deflection response is measured with respect to a single reference cantilever. This strategy permits rejection of electronic noise. The reference signal is subtracted from the signal of each cantilever, and the resulting deflection voltages are sent to a laptop computer for processing. On average, it takes 1 to 2 minutes for the software to identify the vaporous chemical.

Once the ambient vapor dissipates, the absorbed molecules will naturally diffuse, and the polymer coatings will dry out, much like wetted sponges. This process can be hastened with added air flow or gentle heating.



During operation, eight microcantilevers inside the sensor module are exposed to chemical vapors drawn in at the air-intake port by a miniature pump. The resulting bending response of the microcantilevers is detected and processed by the device’s electronics.



A pair of commercially produced four-cantilever arrays (black rectangle) with electrical connections are combined with Livermore-developed components to create the sensor airflow cell shown here.

Timothy Ratto (formerly of Livermore). Other researchers from Livermore include Tom Wilson, Scott McCall, Erik Mukerjee, Adam Love, Jim Zumstein, and John Chang. Researchers at Oak Ridge National Laboratory, University of Illinois, and Texas Tech University have also contributed to the sensor development effort.

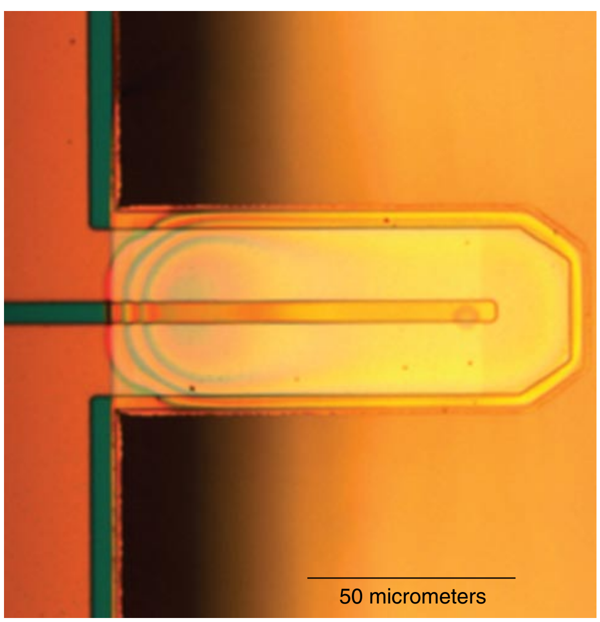
Sensor Requires No Consumables

The prototype sensor system consists of a pair of arrays, each with four silicon microcantilevers. Each cantilever measures 120 micrometers long by 50 micrometers wide by 0.5 micrometers thick. The arrays require no consumable materials (unlike many commercial detectors) and are resistant to common mechanical vibrations. Also, they are commercially available and relatively inexpensive, making the sensor system potentially cost-effective for widespread production and use.

Engineers Zumstein and Chang helped develop the sensor's electronic circuitry, which is based on novel embedded microprocessors. These microprocessors facilitate scalable, multichannel, low-noise, high-fidelity signal processing. The Livermore-designed circuits reduce the electronic noise to levels comparable to those attained with much larger and expensive benchtop systems. The result is greater differentiation of a wider variety of low-concentration chemicals. The sensor system operates on 9-volt, AA, or AAA batteries, using just 750 milliwatts of power, less than a typical cell phone.

Initially, the team found that despite the promise of microcantilevers, some of the materials used in early designs were vulnerable to not only humidity but also high temperatures and corrosive environments. Because of these vulnerabilities, the team chose to coat the microcantilevers with amorphous polyolefins, a common class of plastics. The stiffness of the coatings allows for greater stresses to be exerted on the microcantilevers during absorption of a chemical. The plastic coatings also make them more resistant to corrosive and moist environments. Millions of compositions of polyolefins are available, enabling a different coating formulation to be applied to each sensing microcantilever. Because the thickness of the plastic coating must be precise for the sensor to work, the team developed a method for applying a highly uniform film as thin as a few tens of nanometers. "We have a rich palette of chemical properties to play with when selecting interactions for the volatile chemicals of interest," says Hart.

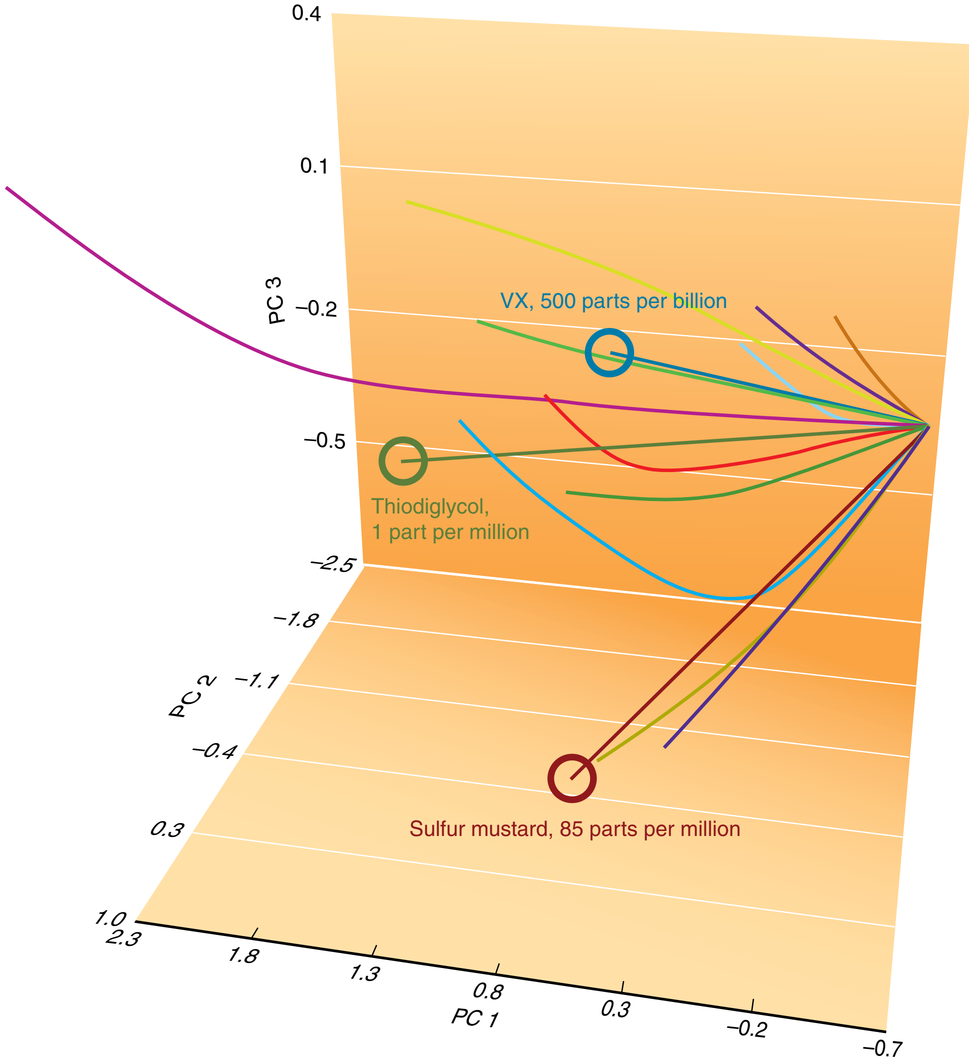
The set of six deflection voltages collectively represents a signature that uniquely identifies one vaporous chemical. However, the team must first perform calibrations, during which a sensor array is "trained" to identify certain chemical signatures; that is, it must associate the pattern of deflection across the microcantilevers with the presence of a certain volatile chemical.



This photomicrograph shows a rectangular-shaped cantilever (extending to the right) coated with a thin film of vapor-sensitive polymer.

Testing the Unit

In 2008, the prototype sensor was trained to recognize a small library of preexisting chemical signatures based on the collective response of the microcantilevers. Tests were then conducted to gauge performance, in particular with respect to the reproducibility of response and the sensor's ability to discriminate one chemical signature from another as well as from system electronic noise. The microcantilevers were exposed to the chemicals at concentrations corresponding with those to which they were trained, between about 200 parts per million (ppm) and 16 parts per thousand. Prepared vapors were pumped through the sensor at a rate of 10 to 220 cubic centimeters per minute until all six cantilevers achieved maximum deflection. The onset of bending was nearly instantaneous for all microcantilevers following initial exposure to each chemical.



In this three-dimensional graph, each colored line represents a distinct chemical signature detected by the Livermore sensor over a range of concentrations. All lines originate from a common point (right) representing the zero concentration state of pure air. The specific agent concentrations for the chemical warfare agents VX, sulfur mustard, and thiodiglycol (a sulfur mustard precursor) correspond to approximately 50 percent of the lethal concentration levels for human-skin exposure.

The sensor reliably detected 11 vapors, including hexane, 1,4-dioxane, benzene, toluene, ethyl acetate, acetone, acetonitrile, methylene, chloride, methanol, and isopropanol. The chemical species were selected as simple representatives of several classes: alkane, ether, aromatic, ester, ketone, nitrile, haloalkane, and alcohol.

The sensor also detected the chemical warfare agents VX and sulfur mustard, both of which were synthesized in trace quantities at Livermore's Forensic Science Center. Exposure to VX, a potent nerve gas, can lead to paralysis and respiratory failure. Sulfur mustard is a blister agent that was dispersed in aerosol form during World War I to incapacitate troops and contaminate areas to discourage entry. Few facilities can test chemical vapor detectors with actual chemical warfare agents. Typically, tests are performed using surrogates such as common cleaning products. The sensor was exposed to VX and sulfur mustard at concentrations of 520 parts per billion (ppb) and 90 ppm, respectively. These values can be compared to the median lethal concentrations of 450 ppb for VX and 25 ppm for sulfur mustard, which correspond to percutaneous (passing through the skin) vapor exposure for 30 minutes.

The results of the experiments can be rendered in a single, three-dimensional graph representing all 13 signatures. The data for each chemical align along a trajectory that originates at the zero concentration state and ultimately terminates at the saturation state. "Clearly, the sensor can identify the different chemicals it was trained to detect throughout the concentration ranges we looked at," says Hart. "Although discriminating from among many different compounds may be challenging, we are confident that the signals for chemicals of interest will predominate." *The Analyst* article represented the first published report of detecting a chemical warfare agent using a sensor array of polymer-coated microcantilevers.

Transitioning from the Laboratory

Any new sensor design must successfully transition from the laboratory with its carefully controlled environment to applications in the real world where users will have little or no control over the operating environment. "If a sensor is used in an enclosed environment where the humidity and temperature are constant, then compensation for these effects is straightforward," says Loui. Because temperature, humidity, and other meteorological conditions can vary widely outdoors, the Livermore sensor was also tested for 24-hour periods in an external environment.

In addition, a viable sensor for use in a real-world application must balance advanced capabilities with the requirements for a particular assignment. "If reliable trace detection at the parts-per-trillion level is absolutely required or we need to analyze gas samples with dozens or more constituents, then a traditional mass spectrometer is needed," says Loui. "MEMS-based sensors will likely never achieve these capabilities. However, sensors such as our cantilever array are suitable for applications in which a detector's size, power economy, and unit cost are of paramount importance. For these applications, the mass spectrometer would be less than ideal because of its bulky size and hefty price tag of $10,000 and more."

Loui is developing a mathematical model that explains how environmental factors contribute to the sensor's response. The goal is for the sensor to "smell" past these interfering phenomena and still respond to the chemical vapor of interest. The model incorporates various physical, chemical, and mechanical properties to determine how the device, in particular the microcantilever coatings, is affected by environmental changes.

Many Possible Applications

The Livermore sensor could potentially be used in a variety of applications because it is small, robust, and sensitive; needs only commercial support electronics; and can be mass-produced. The device is ideal for autonomous operation for long periods. Example applications include environmental and industrial monitoring, such as for chemical leaks in manufacturing plants or storage facilities. Of particular interest to homeland security and defense experts is the speedy detection of gases that could indicate the onset of a chemical warfare attack. Soldiers could carry handheld sensors, or even miniaturized lapel pins, that warn of a chemical agent in the environment. "The sensors could also be scattered around a military base and run autonomously, sensing for incoming plumes of chemicals," says Hart. In addition, the sensors could prove useful as explosives "sniffers" in airports and as spoilage indicators for the food industry.

A novel application for the sensor is as a disease diagnostic. Hart notes that the presence of specific chemicals is associated with certain disease states. A microcantilever-based device could become an important diagnostic tool in analyzing the breath of a patient and searching for a telltale molecule indicative of a particular disease. In 2008, a team of University of California at Davis students captured top awards in two business plan competitions with a plan based on the Livermore microcantilever technology. Their business plan featured a device that would allow people with diabetes to test their blood-sugar levels by blowing into a small handheld device. This technology could offer an alternative to glucose monitoring, which requires that people prick their fingers to draw a blood sample, in some cases several times a day.

The current Livermore prototype cannot be used to detect biological agents, which typically do not exist in the vapor phase. However, a sensor designed to detect biowarfare agents in water would be possible if the microcantilevers' plastic coatings were replaced with nucleotides or antibodies. Previously, Livermore researchers have demonstrated

The Livermore sensor easily fits in one hand. Researchers are working to shrink the electronics even more, so the sensor can be incorporated into a cell phone or even a lapel pin.

biological applications for sensors using microcantilevers covered with biomolecules.

Looking to the Future

The team is exploring additional features for the chemical sensor such as onboard data storage and wireless transmission capabilities. Hart has discussed with government agencies the feasibility of designing a wireless sensor that would permit units to "talk" to one another as well as to a control server. Such a network could aid in mapping the presence of a chemical vapor of interest. Another feature being explored incorporates a resistive heater into each microcantilever to hasten desorption when the microcantilevers are purged, which would lessen the approximate 2-minute interval between readings in the current design. A transition to coatings of cross-linked polymers for greater mechanical stability is also planned. In addition, Hart is reviewing the feasibility of using nanocantilevers measuring only a few hundred nanometers wide because of their potential sensitivity to tiny amounts of material. Finally, Hart is investigating how the Livermore sensor might be incorporated into a cell phone that would also have sensors for detecting radiation and biological warfare agents. A network of these advanced cell phones could quickly warn, identify, and determine the extent of a contamination.

A prototype offshoot of the device is part of a Livermore effort to develop tiny, rugged sensors that could be embedded in every U.S. nuclear warhead and last for decades. The sensors could potentially be used to detect and measure gas molecules, such as volatile organic compounds and water vapor, which might impede the performance of critical warhead components. Embedded sensors could provide information currently obtainable only through disassembly. Such devices might make possible for the first time "persistent surveillance"—continuous monitoring of every weapon and practically instantaneous detection of anomalies. (See *S&TR,* July/August 2008, pp. 12–19.) "Our goal is a sensor that can 'smell' the outgassing of tiny amounts of chemicals," says Loui, who is the lead investigator on adapting the sensor to stockpile surveillance. "If successful, we could have warheads capable of indicating when an internal problem exists."

"We want to move the new sensor technology out in the field as rapidly as possible," says Hart. The Laboratory has received several inquiries from industrial firms interested in licensing the technology. With mass production of the device in sight, Hart is hopeful Livermore's sensor will become ubiquitous throughout industry as well as a dependable element of chemical warfare detection and defense—in essence a trusty network of "smoke detectors" for toxic chemicals.

—Arnie Heller

Key Words: chemical weapon, detector, Forensic Science Center, microcantilever, microelectromechanical systems (MEMS), National Consortium for Measurement and Signatures Intelligence Research, polyolefin, sensor, sulfur mustard, VX.

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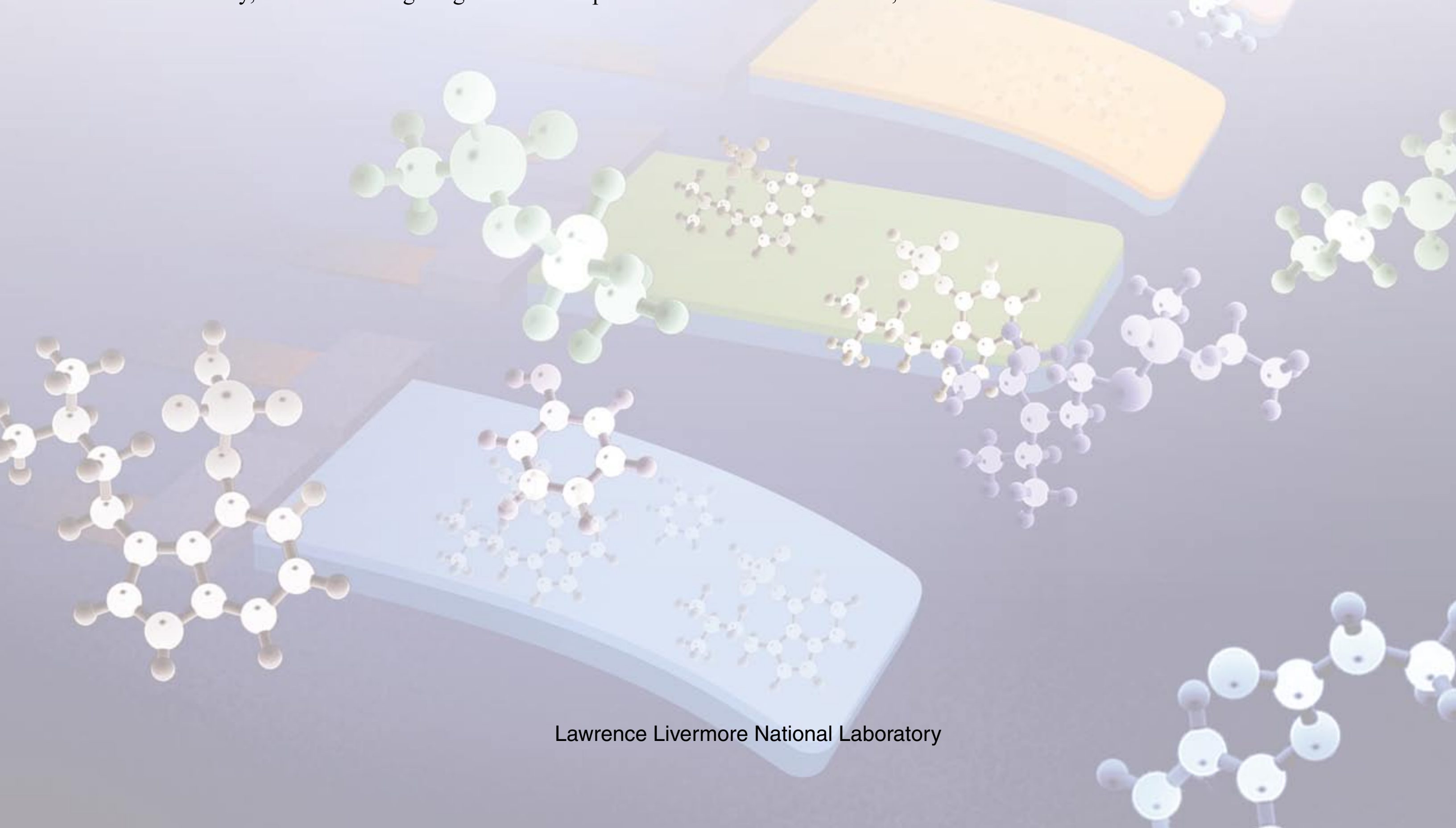


Simulations Explain High-Energy-Density Experiments

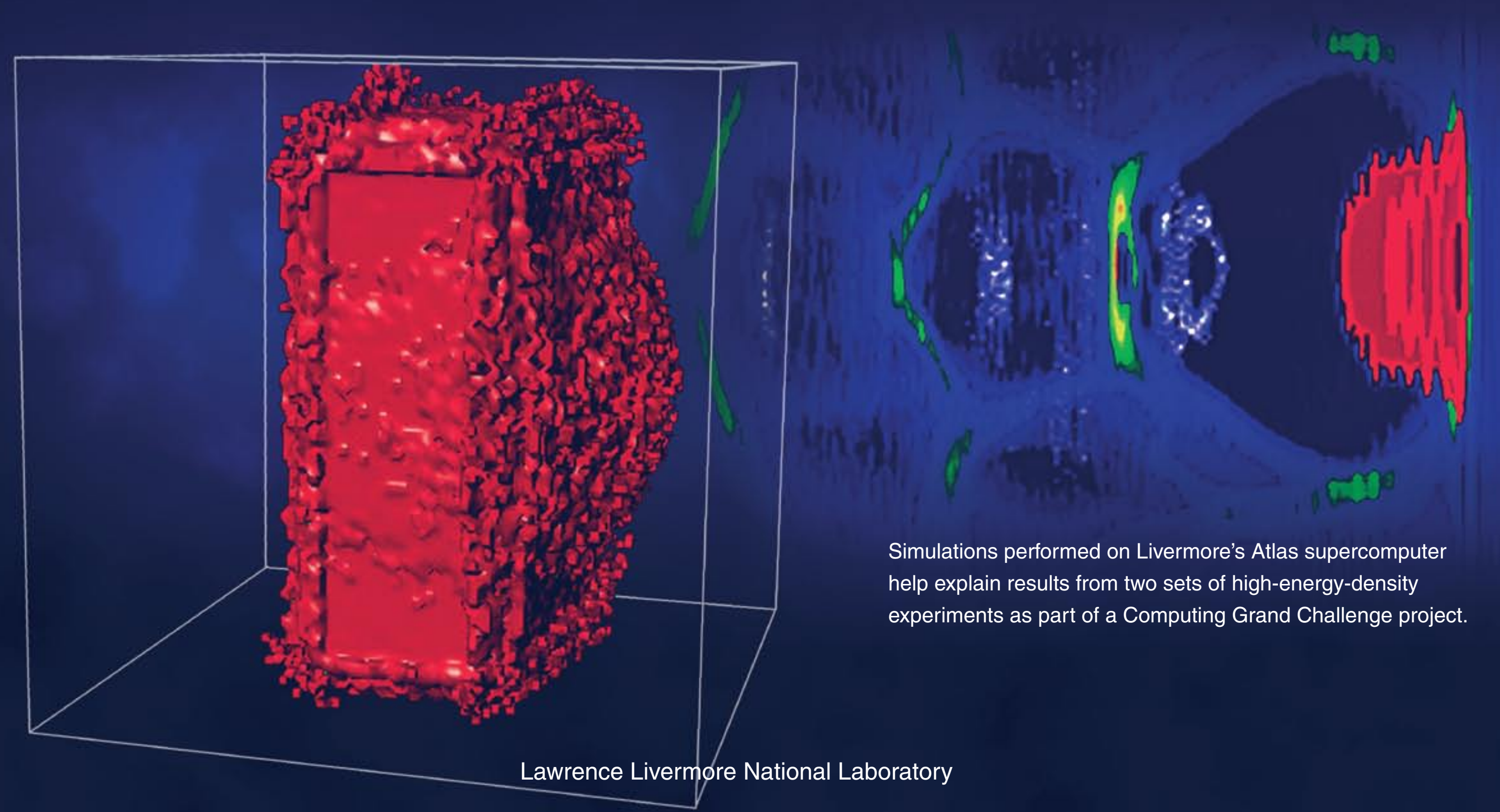
Simulation and experiment work in tandem to advance high-energy-density science.

MAXIMIZING energy density—the amount of energy stored in a given volume—is a common research theme at Lawrence Livermore. Energy density can take many forms. Aeronautical engineers want a fuel with maximum energy density for rocket liftoff. High-energy-density foods are vital to endurance athletes, such as cyclists in the Tour de France. The object with the highest energy density ever created by humankind is an exploding thermonuclear weapon.

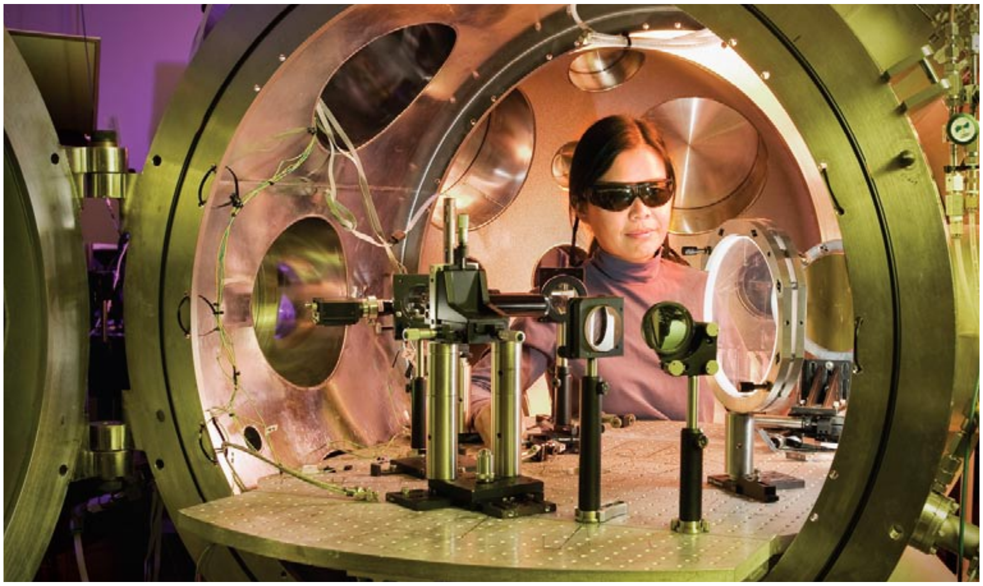
Recently, a Computing Grand Challenge project on Livermore's Atlas supercomputer simulated the results from two sets of laser-driven high-energy density (HED) experiments. These simulations have helped explain the physics behind what was seen and measured in the experiments.

In one set of experiments, researchers zapped very small reduced-mass targets with ultrahigh-intensity lasers to get the dense targets as hot as possible. (See the box on p. 14.) Such targets, which produce high-energy electrons, protons, and x rays, are being considered as backlighters for radiography diagnostics on the 192-beam laser system at the National Ignition Facility (NIF).

In a second set of experiments, researchers used intense laser light to create a laser wakefield accelerator to speed up electrons in a low-density plasma. Such accelerators are anticipated to reach energies of 10 gigaelectronvolts (GeV,



Simulations performed on Livermore's Atlas supercomputer help explain results from two sets of high-energy-density experiments as part of a Computing Grand Challenge project.



Physicist Hui Chen adjusts the optics in the target chamber of Livermore's Callisto laser during a proton acceleration experiment using a reduced-mass target.

1 billion electronvolts) over a meter, which is much shorter than the multikilometer length of most particle accelerators.

"In the laboratory, tightly focused, intense laser light in ultrashort pulses is one of the most efficient ways to quickly transfer large amounts of energy into a small volume of material," says physicist Scott Wilks, who led the Grand Challenge project. "In fact, it is the basis for the fast-ignitor fusion concept." In 2007, the Laboratory's annual Computing Grand Challenge Program allocated 83.7 million hours of machine time on the Atlas and Thunder supercomputers to just 17 research projects, one of which was Wilks's.

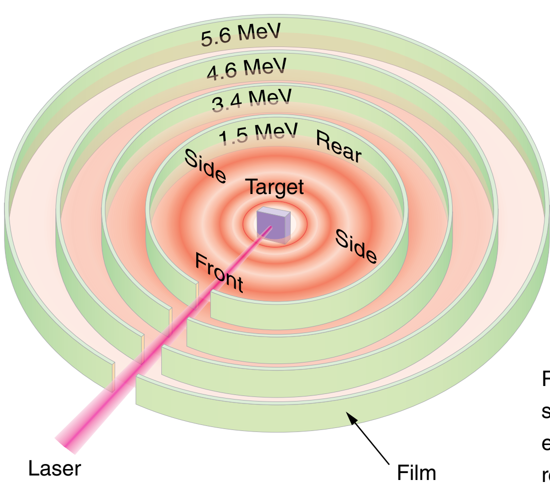
"Intense" laser light means more than a quintillion watts of energy per square centimeter (10^{18} W cm^2). During HED experiments, laser light slams into a tiny target and then interacts with the plasma that is created. This interaction generates electrons that move in targeted materials at almost the speed of light. Diagnostic devices abound, but understanding the results can be difficult because laser energy and plasma interact in complex, highly nonlinear ways.

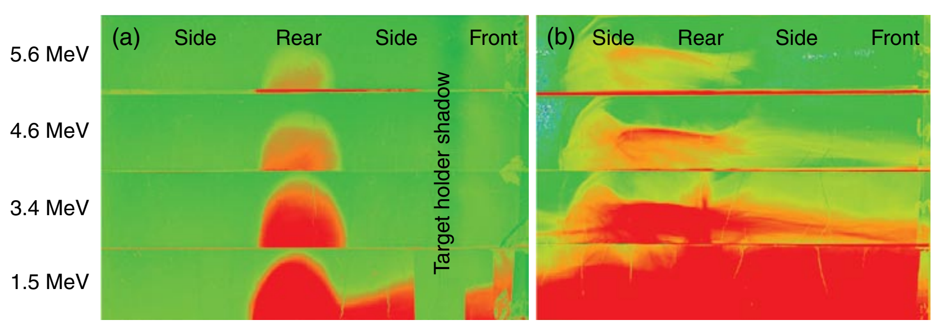
Simulating the physics of the experiments on powerful supercomputers is often the only way to both understand the results in detail and develop physical insight into these complex processes. Simulations can parse the physical constituents that affect the whole and examine microscopic details not easily detected during an experiment. In addition, computer simulations can explore regimes of temperature, density, and pressure that experiments cannot yet achieve, serving as a guide for future experiments. Ultimately, scientists must depend on both experiments and simulations working in tandem to advance HED physics research.

Explaining the Unexpected

In one set of HED experiments, researchers used ultrahigh-intensity lasers with ultrashort pulses to zap one side of a reduced-mass target. "These very small, square targets [100 micrometers across and 7 micrometers thick] were initially designed for studying certain aspects of neutron stars," says physicist Hui Chen. "Our goal was to get a dense target as hot as possible in the presence of a large magnetic field."

The 2007 experiments performed on the Callisto laser in Livermore's Jupiter





Results from the Callisto laser experiments (captured on strips of film placed around the target, shown schematically at far left) indicate that laser-driven proton acceleration at various megaelectronvolt (MeV) energies from (a) a large, multimillimeter-size target is unexpectedly very different than it is from (b) a reduced-mass target. In the large target, protons are accelerated off the rear of the target. In the smaller target, they accelerate from all sides.

Laser Facility showed that the target did get hot, but an unexpectedly large number of protons were ejected from the entire surface of the target. In contrast, when a laser zaps a larger (millimeter size) target, a beamlike pattern of protons blows off the back of the target.

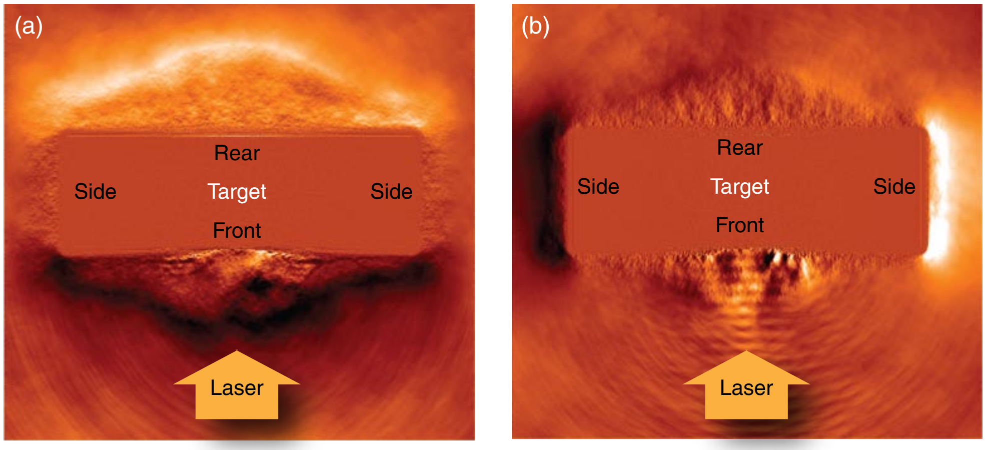
To simulate Chen's experimental results, physicist Andreas Kemp used the Particle Simulation Code (PSC), a particle-in-cell code specifically designed for studying electrons in a high-energy plasma. The computational capabilities of Atlas allowed Kemp to simulate laser–plasma interactions in reduced-mass targets at full scale from first principles.

In a two-dimensional (2D) simulation of a large target, electrons accelerated by the laser generated an electric field on both the top and bottom of the target. In a simulation of a smaller, "finite" reduced-mass target, large electric fields developed on the sides of the target as well, which explained the signal detected all around the target in experiments. This simulation showed that shrinking a target to a smaller size does not increase target temperature but instead increases the total number of ions accelerated from all of its surfaces. In fact, it was precisely the pattern seen in Chen's puzzling data. A 3D simulation also predicted maximum proton energies out the back of the target to be about 5 megaelectronvolts, which agreed with experimental results. Results from the Atlas simulations indicate that smaller targets may be more efficient ion accelerators than larger targets, which could make fast ignition using proton beams competitive with hot electron–based fast ignition.

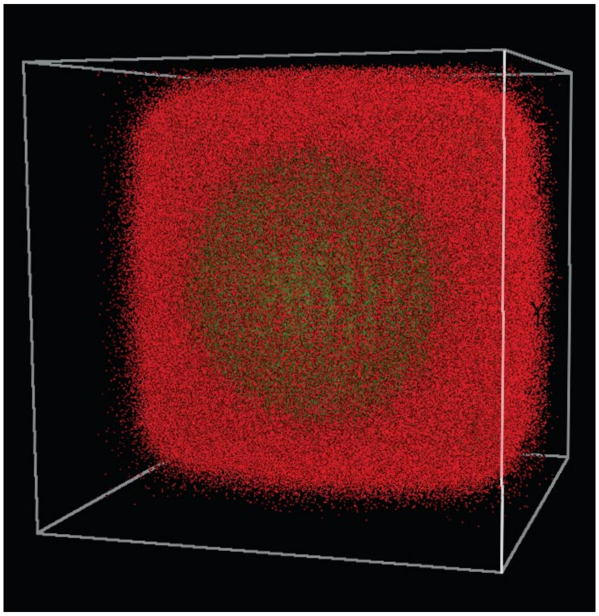
Kemp notes that a full-physics code such as PSC is expensive to run. As a consequence, he performed just a few 3D simulations. In addition, Kemp developed a number of 1D simulations that were derived from 2D results. He found that the interface where the laser interacts with the plasma recedes significantly. A series of in-depth, 1D simulations helped researchers understand the hydrodynamics at the interface.

Kemp was delighted to have so much dedicated computer time. Laser–plasma interaction simulations are highly complex and computationally intensive. "Although the events we simulate occur on a subpicosecond timescale [less than a trillionth of a second], hundreds of CPUs [central processing units] running in parallel for a long time are needed to examine the many interactions in that brief moment of activity," says Kemp.

In the past, PSC has been run for limited periods on machines at the National Energy Research Scientific Computing Center in Berkeley, California, and on the Earth Simulator in Japan. "The access we had to Atlas made quite a difference," says Kemp. "We could do a run, make some changes, and do another run. The time on Atlas allowed us to make a lot of progress."



Two-dimensional simulations on Atlas incorporate full physics and help explain the Callisto laser experimental results. Electrons accelerated by the laser generate an electric field (a) on both the front and rear of the reduced-mass target and (b) on the target sides as well.



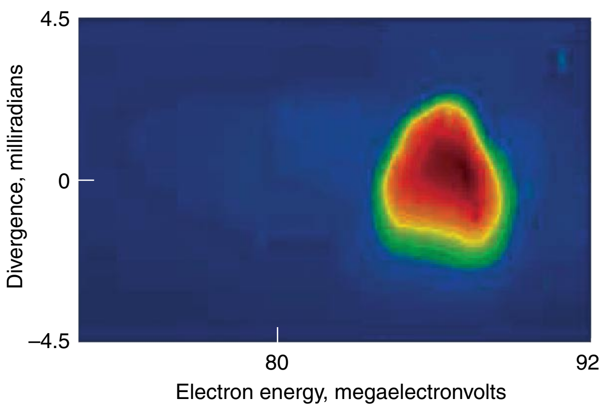
A three-dimensional simulation of a reduced-mass target shows vertical striations in electron density due to a laser polarization effect—a phenomenon that can only be observed in three dimensions.

Simulations Ride the Wave

In the second set of HED experiments simulated on Atlas, a short-pulse, high-intensity laser system accelerated electrons within a plasma. The 2004–2006 experiments were run by the Laser Optics and Accelerator Systems Integrated Studies (LOASIS) Program on the LOASIS laser at Lawrence Berkeley National Laboratory under the leadership of Wim Leemans and in collaboration with Simon Hooker's group from Oxford University. They demonstrated that gigaelectronvolt beams can be produced by a channel-guided laser plasma accelerator.

In these experiments, a laser pulse propagates through a low-density plasma channel, leaving behind a plasma density oscillation, or wakefield. The electric field of this wakefield pulls electrons forward, accelerating them thousands of times faster, and hence requiring much shorter distances, than a conventional particle accelerator. (See the box on p. 15.)

Experiments and simulations to date have demonstrated production of 1-GeV energies over a distance of 3 centimeters and indicate that a laser wakefield accelerator (LWFA) could reach energies of 10 GeV in a mere meter. The availability of an accelerator this small could put experiments with high-energy electron beams in many laboratories.



The spectrum of electrons accelerated in a laser wakefield showed for the first time the formation of a high-quality bunch of electrons with a narrow energy spread. Experiments were run on Lawrence Berkeley National Laboratory's LOASIS laser.

Simulations on Atlas probed the dynamics of how electrons are trapped by the wake to better understand the LOASIS experiments and to plan future experiments. The LWFA simulations were conducted by physicists Cameron Geddes and Estelle Cormier-Michel of LOASIS and by David Bruhwiler and John Cary of Tech-X Corporation in Boulder, Colorado. The team performed the simulations using the particle-in-cell capabilities of VORPAL, a parallel computational framework. Tech-X scientists, who have collaborated for several years with the LOASIS group, developed VORPAL.

Although simulations in the past have shown how the particles are trapped and concentrated as they outrun the wake, a crucial challenge has been to accurately model the particle beam's divergence and energy spread. Particle-in-cell simulations of plasma incorporate particles moving in space with an electromagnetic field on a grid. "The particles are discrete objects," says Bruhwiler, "while the electromagnetic field is continuous." The discrete particles and interpolation from the grid create noise in the simulations.

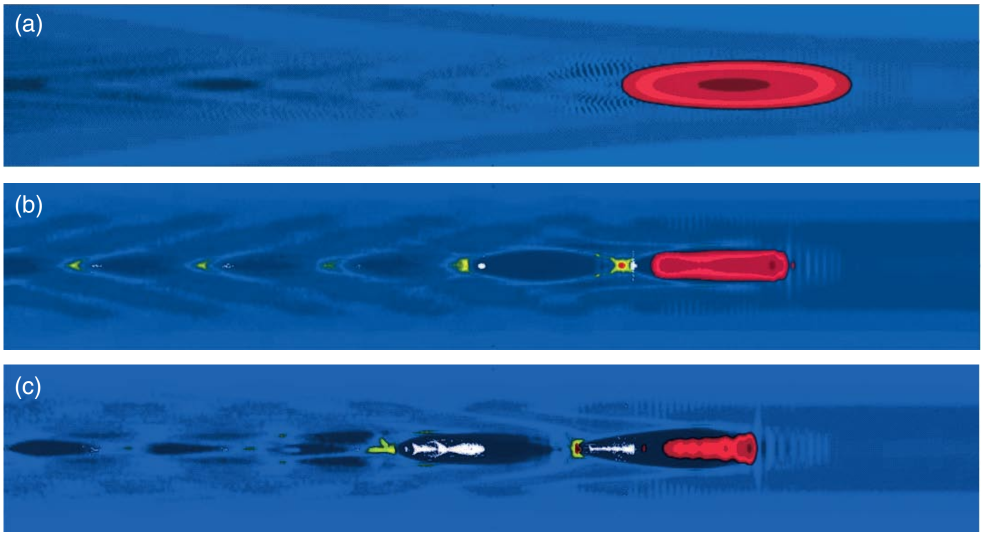
The time on Atlas gave the team the opportunity to improve VORPAL's algorithms and reduce this noise by weighting both forces and particle currents more smoothly across the grid. Two-dimensional simulations showed that these new algorithms more accurately model the electron-beam divergence and energy spread measured in earlier experiments. Three-dimensional modeling verified that the algorithms reduce noise and also incorporate more realistic physics. This new accuracy allows design of next-generation experiments to further improve beam quality.

Short-Pulse Laser Slams Tiny Targets

Driving high-energy-density (HED) phenomena requires quickly coupling the energy contained in a laser pulse with the target material. An extremely short laser pulse is ideal. It couples a large fraction of the laser energy with the target nearly instantaneously, ionizing the entire target while it is still solid and before it has a chance to expand. This quick coupling of energy and matter, which does not substantially change the volume of the target, is called isochoric heating.

The first experiments with a high-energy, ultrashort-pulse laser were performed at Lawrence Livermore in 1996 on the Petawatt laser, which delivered a record-setting 1.25 petawatts (quadrillion watts) of power. The Petawatt laser was developed to test the fast-ignition concept for inertial confinement fusion. Achieving the fast-ignition route to nuclear fusion requires a detailed understanding of electron generation and transport, some of which has come from experiments using reduced-mass targets (RMTs).

Physicist Hui Chen performed the most recent RMT experiments in 2007 on the ultrashort-pulse Callisto laser in Livermore's Jupiter Laser Facility. She was also at Rutherford Appleton Laboratory in the United Kingdom when the first-ever RMT experiments were performed in 2003. Earlier experiments examined x-ray production from RMTs and confirmed important characteristics such as high temperatures and heating uniformity. Tiny RMT targets may be useful as highly efficient ion accelerators, with accelerated protons providing the energy required to ignite a larger target.



An Atlas simulation of a laser wakefield accelerator experiment shows the plasma density (blue-green) driven by the laser (red) during the evolution of a laser wakefield. (a) As the laser propogates in a very low-density plasma and is modulated, (b) the wake amplitude increases and particles (white) are trapped (c) and accelerated.

Channeling through Plasma

In 2006, during the highest-energy laser wakefield acceleration experiments to date, scientists at Lawrence Berkeley National Laboratory accelerated electrons to energies exceeding 1 gigaelectronvolt (GeV) over a distance of just 3.3 centimeters. The high electron energies achieved with moderate input laser energy demonstrated just how effective a laser wakefield can be for accelerating electrons.

Two parameters must work together precisely to achieve efficient electron acceleration. One parameter is the plasma's density profile. A plasma density channel—a structure with lower plasma density along the axis of the laser beam—is essential to extend and control the laser's focus over longer distances than would otherwise be possible. This focusing must be done at low plasma densities to allow for the acceleration of electrons to high energies before outrunning the wake. The second parameter is the shape of the laser pulse, including its power and length, which drives the wake's oscillations. If the amplitude of the oscillations is too low, no particles are trapped. Too high of an amplitude results in uncontrolled trapping, which degrades beam quality.

Just as a surfer can ride the wake of a powerboat, so can electrons ride a "wakefield" behind a laser beam channeling through plasma.

Atlas simulations have been used to design experiments planned for 2012 at LOASIS. These experiments are expected to generate 10-GeV energies in a channel half a millimeter wide and a meter long. The plasma's density will need to be lower than in past experiments to maintain the necessary conditions over the longer distance. Because a 3D simulation of a single centimeter of beam propagation requires a million CPU hours, modeling a meter-long stage with traditional particle-in-cell codes is prohibitive. However, Bruhwiler successfully used 1D simulations to verify 10-GeV energy gain and evaluate the evolution of the laser beam over a 1-meter length. By comparing these results with those from much faster, reduced-physics algorithms, he was able to simulate 10-GeV LWFAs in 2D and 3D.

The Power of Atlas

All of these HED experiments and simulations help bring the Laboratory closer to its goal of achieving inertial confinement fusion on NIF and to applying HED science to new particle accelerators. "This grand challenge project not only gave us the computer time needed to quickly make a lot of progress toward understanding the underlying physics by doing many smaller runs," says Wilks, "but also allowed us to simulate full-scale laser–target experiments in 3D for the first time. We learned a great deal about the complex ways that intense, short-pulse lasers transfer their energy to electrons."

—*Katie Walter*

Key Words: Atlas computer, Computing Grand Challenge Program, high-energy-density (HED) physics, Jupiter Facility, laser wakefield accelerator (LWFA), National Ignition Facility (NIF), reduced-mass target (RMT).

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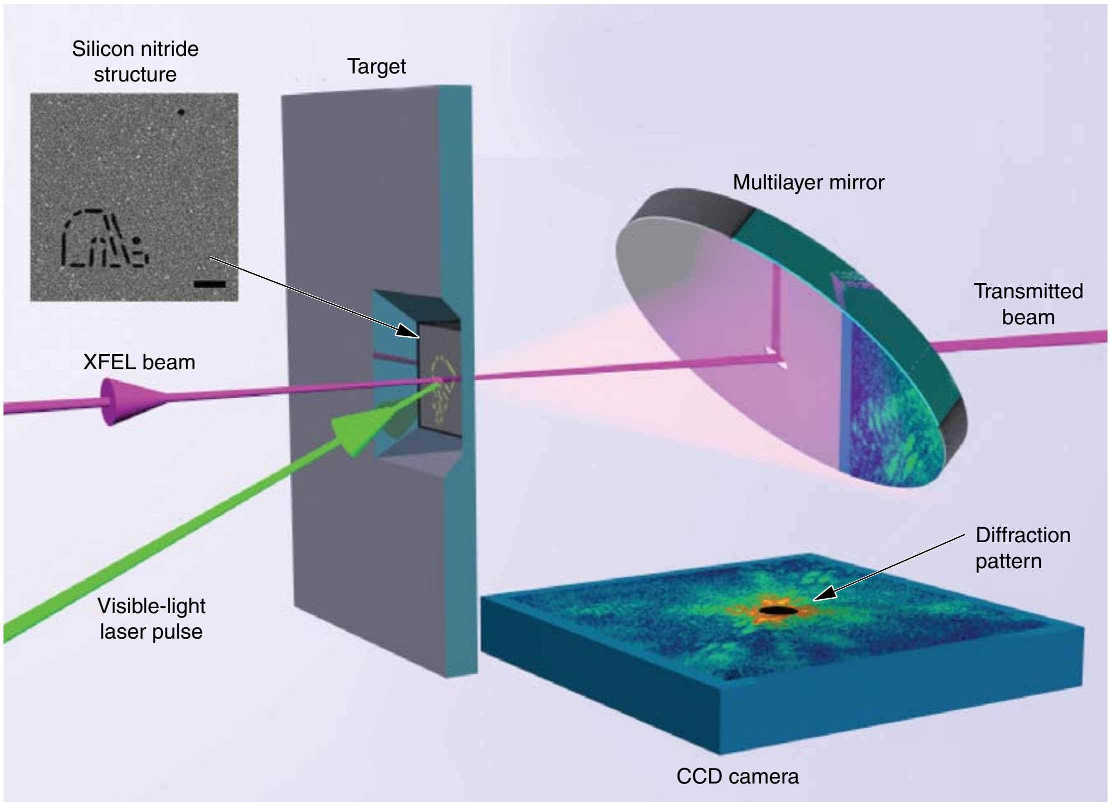
Seeing Condensed Matter in a New Light

RESEARCHERS have long been interested in unraveling the secrets of molecular dynamics. Watching a molecule as it evolves over time when exposed to external influences helps reveal how complex biological systems, such as those in the human body, function and change under varying conditions. X-ray crystallography is useful for examining the detailed atomic structure and motion of macromolecules in their crystalline forms. This process has been used for many materials science applications. However, some macromolecules and materials cannot be crystallized. Studying the dynamics of these structures requires a different x-ray diffraction technique that uses faster, shorter, and stronger x rays.



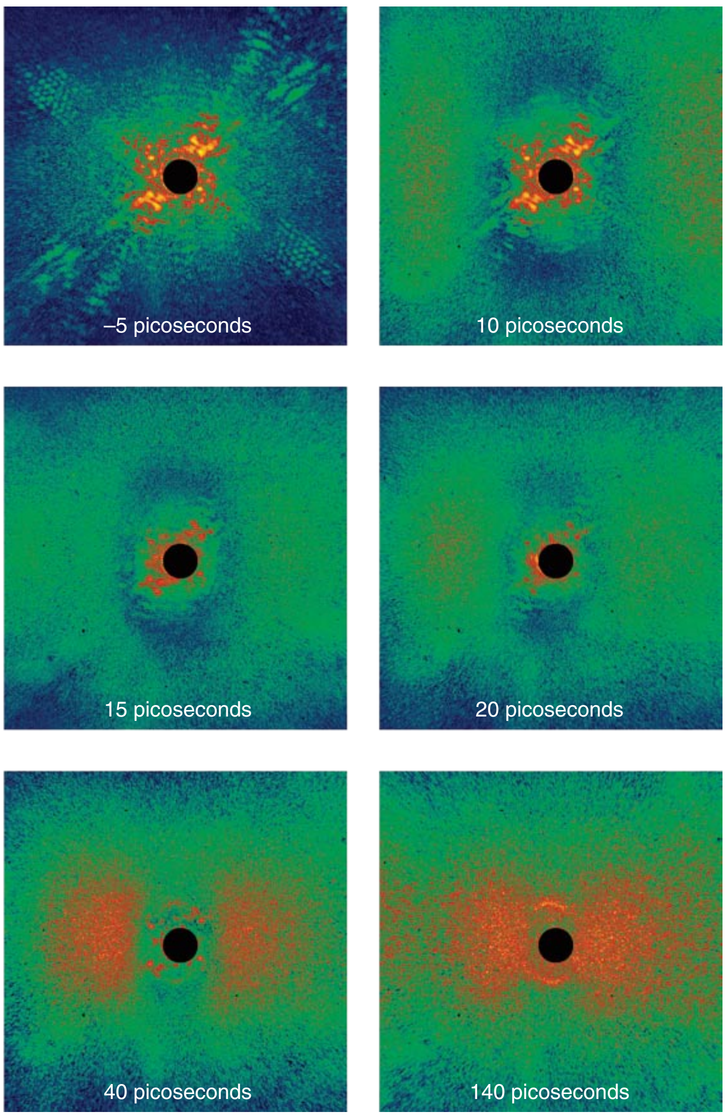
In dynamic imaging experiments, a visible-light laser pulse excites a silicon nitride structure before an x-ray free-electron laser (XFEL) is fired on the structure. A multilayer mirror reflects the diffraction pattern from the scattered light onto a charge-coupled device (CCD) camera, while the main light beam travels through the hole in the center of the mirror.

The soft x-ray free-electron laser at Deutsches Elektronen-Synchrotron (DESY) in Hamburg, Germany, known as FLASH, is currently the only laser that can generate the pulses needed for these experiments. An x-ray free-electron laser (XFEL) is a source of intense coherent electromagnetic radiation. It produces femtosecond pulses of 1- to 0.1-nanometer-wavelength light containing trillions of photons. With these fast, short, and powerful beams of light, researchers can obtain high-resolution diffraction patterns and images of noncrystalline structures with nanometer-size features.

In collaboration with the University of California at Davis, Stanford Synchrotron Radiation Laboratory, Uppsala University in Sweden, University of Duisburg-Essen in Germany, and DESY, Livermore researchers demonstrated how XFELs can be used to image the transient, ultrafast dynamics of nanoscale materials and biological structures. The team used FLASH to image the vaporization of a nanometer-size structure etched into a silicon nitride target. With FLASH, the team achieved highly detailed, time-resolved images of the structure as it was destroyed by the laser. This new imaging technique allows researchers to study the noncyclic, or nonrepetitive, phenomena of structures as they undergo violent processes. In addition, researchers can use the technique to better understand the dynamics of condensed matter. The Livermore researchers were funded by the Laboratory Directed Research and Development Program.

Faster than a Disintegrating Material

When an electromagnetic pulse hits a noncrystalline structure, light from the pulse scatters, creating a diffraction pattern that characterizes the structure at that specific point in time. The wavelength of light used to create the diffraction pattern determines the size and quality of the features that can be resolved. Prior to FLASH, short-pulse x-ray sources used for imaging either contained an insufficient number of photons to create strong diffraction patterns or produced light at wavelengths that were too long—hundreds of nanometers—to resolve noncrystalline structures measuring only tens of nanometers. Because weak diffraction patterns produce low-resolution images, minute features were blurred and unidentifiable. Non-XFEL pulses also last longer, transferring too much energy to the structure and destroying it before researchers can capture an image.



With the x-ray free-electron laser FLASH, researchers produce diffraction patterns of a structure as it undergoes laser vaporization. The patterns show the structure 5 picoseconds before the excitation laser pulse and then as it evolves 10, 15, 20, 40, and 140 picoseconds after the pulse.

FLASH produces light at 6- to 60-nanometer wavelengths, making it possible to image features smaller than 100 nanometers. FLASH pulses also contain 10^{12} photons. Enough of these trillions of tiny light particles are scattered to create clear diffraction patterns of nanometer-size noncrystalline structures. And, because FLASH pulses are only 10 femtoseconds long, researchers can capture an image of a structure before the laser destroys it. According to Livermore physicist Anton Barty, who led the project at DESY, "With these femtosecond pulses, we can break through the radiation damage limit."

Picoseconds in Time

In previous experiments on FLASH in 2006, the team, then led by former Livermore physicist Henry Chapman, who now works at DESY, showed for the first time how femtosecond XFEL pulses could be used to capture static images of a nanometer-size noncrystalline structure. (See *S&TR,* May 2007, pp. 21–23.) These experiments proved that high-resolution images of a noncrystalline material could be acquired before the XFEL pulse destroyed the structure. Because one XFEL pulse contains enough energy to destroy the structure in a single shot, the current team had to develop a method for hitting the structure with a pulse only after it had already begun to disintegrate. The team used a visible-light laser to induce excitation of the structure and then timed the XFEL pulse to fire after the excitation pulse.

For each target, a nanometer-size structure was etched onto a 20-nanometer-thick silicon nitride membrane using a focused-ion beam. The membrane was embedded into and held in place by a silicon wafer. The targets, fabricated at Livermore and shipped to DESY, were produced with low variability.

During the experiments, the XFEL and a visible-light laser were focused onto a micrometer-size spot on the target. First, the system fired the visible-light laser, hitting the target with a 543-nanometer-wavelength pulse lasting 12.5 picoseconds. Shortly after this excitation pulse—at a predetermined time delay—the XFEL fired a 13.5-nanometer-wavelength, 10-femosecond-long pulse. A photodiode connected to the lasers regulated the pulse timing. This process was repeated for multiple targets, with each XFEL pulse firing at a continuously variable delay after the excitation pulse. Thus, each diffraction pattern represents a different point in time during a structure's breakdown.

A highly reflective multilayer mirror, positioned just behind the structure at a 45-degree angle from the target, separated the diffracted photons from the main XFEL beam. The main

Computer algorithms transform the structure's diffraction pattern into an actual image. These images are produced from diffraction patterns corresponding to 5 picoseconds before the excitation laser pulse and 10 and 15 picoseconds after the excitation laser pulse.

beam traveled through a hole in the center of the mirror, while the coherent diffraction pattern was reflected onto a charge-coupled-device camera, which recorded it. An iterative computer algorithm transformed the recorded pattern into an actual image of the structure. With FLASH, the team acquired images with 50-nanometer spatial resolution and 5-picosecond temporal resolution.

Because the team can image a single structure at any point in its evolution over time, they can study nonrepetitive phenomena in violent processes, such as the destruction of a molecule or material. Prior to these experiments, the only way to study a noncrystalline structure's reaction to external conditions was to take a single shot of multiple samples at the same interval, then average the images together—a technique that blurs any shot-to-shot sample variation. With this new process, the team's individual snapshots can be sequenced together to create a "movie" of the structure's evolution over picosecond timescales.

An Even Brighter Beam

Soon the team will be able to image noncrystalline structures with even smaller features. When the Linac Coherent Light Source (LCLS) comes online this year at Stanford Linear Accelerator Center in Menlo Park, California, it will produce hard x-ray laser pulses with light wavelengths of 1 to 0.15 nanometers, billions of times brighter than existing x-ray synchrotron sources. LCLS will allow researchers to study materials with finer details at atomic-scale resolutions.

Barty looks forward to the team's new imaging technique being used in other research applications as well. "These experiments are useful for bioimaging and other Laboratory mission-related areas such as understanding how lasers interact with materials," says Barty. "They are also important in determining phase transition, crack formation, nucleation, and other material transformations." With LCLS, just imagine the secrets that will be revealed when the team can study never-before-seen noncrystalline structures on an atomic scale.

—Caryn Meissner

Key Words: condensed matter, Deutsches Elektronen-Synchrotron (DESY), FLASH, Linac Coherent Light Source (LCLS), ultrafast dynamics, x-ray diffraction, x-ray free-electron laser (XFEL).

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Environment, Safety, and Health in the Extreme

The McMurdo Research Station is located at the southern tip of Antarctica's Ross Island on the shore of McMurdo Sound, about 3,500 kilometers south of New Zealand. To reach this isolated place, personnel must take an hours-long flight onboard a C-130 aircraft from New Zealand. (Courtesy of the National Science Foundation; photographer Elaine Hood.)

ANTARCTICA is not a place for the faint of heart. The below-freezing temperatures, unpredictable weather, and desolate landscape make it one of the most extreme environments in the world. Except for the few brave souls who visit Antarctica to work at research stations and conduct scientific investigations, the continent remains a virtual island of solitude. The director of Livermore's Environment, Safety, Health, and Quality (ESH&Q) Directorate, Allen Macenski, is one of those brave souls.

During his two-and-a-half years on and off "the ice" in the 1990s, Macenski managed environment, safety, and health (ES&H) activities that supported the McMurdo Research Station, an American facility located on Antarctica and operated by the National Science Foundation. He oversaw contracts for science and engineering operations, managed training and worker assurance programs, and implemented plans for waste cleanup and removal. For Macenski and his team, effective execution of industrial hygiene requirements, waste management, and environmental stewardship was paramount to the safety and success of scientific expeditions and to minimizing humanity's footprint in one of the most pristine and scientifically valuable places on Earth.

Today, Macenski applies these same concepts at Livermore. Drawing on his experience, Macenski leads the ESH&Q Directorate in developing solutions and maintaining standards that enable the Laboratory to conduct safe and environmentally compliant operations in support of its missions.

A Delicate Balance

Safe operations begin with verifying that personnel are qualified and able to perform the planned work activities. While in Antarctica, Macenski was responsible for ensuring that personnel were screened and trained to live and work in an extreme

Expecting the Unexpected

One of Allen Macenski's most memorable moments on the ice occurred when he and four other people were sent to remove asbestos from a biology station near a penguin rookery. What was supposed to be a one-day project turned into a 72-hour ordeal.

The plan was to get dropped off in the morning, work until about 1:00 p.m., and then return to the station via air transportation. But the afternoon came and went, and no one arrived to pick them up. Macenski says, "The temperature began to drop, and the wind started to pick up. We looked up at the summit, and saw the snow being blown off the top ridge. We knew there was a storm coming." The winds reached approximately 170 kilometers per hour and visibility was less than 1 meter.

Team members had to anchor themselves to one another and then to the building. The building was located on a peninsula, a few hundred feet from a 240-meter cliff. Macenski says, "If the building had become detached, we would have gone over." Three days later, when the weather cleared, they were rescued. Antarctica's unpredictable weather is just one reason why survival training is so important for living and working safely in the extreme.

Inside the "cozy" biology station near the penguin rookery, Allen Macenski finds shelter from an unexpected storm.

environment. On the ice, individuals must live for extended periods of time in confined spaces, almost completely isolated from the outside world. As a result, all personnel undergo extensive medical evaluations for physical and psychological conditions that could become dangerous or deadly. "The phrase 'cabin fever' is colorful terminology, but it doesn't accurately describe the seriousness of the condition," says Macenski. Additionally, all personnel must complete a survival-training program when they arrive. Proper training helps reduce the risk of accidents and prepares people for life-threatening situations. (See the box at left.)

Worker assurance programs and training are just as essential at the Laboratory as they are in Antarctica. For example, training is needed for using specialized equipment, working with hazardous materials, or conducting experiments. Also, personnel must be trained and qualified for maintenance operations that include electrical-, hydro-, or gas-powered mechanisms or that require entering a confined space. Whether at the Laboratory or in Antarctica, personnel must be both physically able and competent to perform the work.

Another step in conducting safe operations is to evaluate the processes that will be used for completing the work. "In Antarctica, the main mission is science, specifically scientific exploration of the environment," says Macenski. "Performing risk assessments of the proposed work was a large part of my job." He would review research proposals, help plan work activities, evaluate whether those activities fit within the confines of the project, and develop work controls. These processes helped evaluate the efficacy of the work tasks, protect the participants, and predict and minimize any negative effects of research on the environment.

During his time in Antarctica, Allen Macenski managed the cleanup of a 5-acre legacy waste dump at McMurdo Research Station. (Inset) The waste was excavated, segregated, containerized, and shipped off the continent, revealing a more pristine landscape.

Achieving this delicate balance between safety, scientific necessity, and environmental viability is also important at the Laboratory. Using an integrated safety management (ISM) approach, Livermore organizations define the work, analyze the hazards, develop controls, and perform the work. The final step is to gather feedback and improve processes. The ISM approach encompasses all the people and processes needed to conduct work safely and in accordance with environmental regulations.

Cleaning Up a Legacy

Pollution prevention and waste management are necessary components of safe operations to protect the environment. According to Macenski, before a proposed research project begins, every part of the project must be evaluated. These evaluations help define environmental aspects such as the disposal of potential by-products and waste, including leftover supplies and equipment. Macenski has seen firsthand what happens when this step is left out of the process.

During his time at the McMurdo Research Station, he oversaw the cleanup of a waste dump that had existed for decades. "We found items dating back to the 1930s," says Macenski. "We had to develop an environmental stewardship program to reexcavate the waste, segregate it, containerize it, and then ship it off the continent." He and his team also had to develop an environmental project plan on how to dispose of waste in the future to prevent the situation from recurring.

The Laboratory also understands the importance of cleaning up legacy issues and reducing its environmental footprint. Prior to the Laboratory being established in 1952, the land it now occupies was the site of a U.S. naval air station. At that time, products used to clean jets at the base contained chemicals that eventually seeped into the ground and contaminated the groundwater. Through effective groundwater contamination treatment procedures, the Laboratory provided remedial solutions to the problem. Groundwater monitoring continues to be an important aspect of safe operations at the Laboratory.

Two Places, One Goal

Living and working in the extreme environment of Antarctica presents challenges that require resourcefulness and flexibility. Surviving the below-freezing temperatures and erratic weather patterns is part of everyday life. The experiences Macenski gained during his time on the ice serve him well in his role at the Laboratory. "I can find a path to success based on the challenges I faced in that environment," says Macenski.

"In Antarctica and at the Laboratory, the people are driven and hard working, they want to succeed, and they want to go home as healthy as when they arrived," he says. Through effective application of ES&H policies and procedures, Macenski and the ESH&Q team help ensure safe operations that protect employees and the surrounding community and reduce the Laboratory's environmental footprint on the future.

—Caryn Meissner

Key Words: environment, safety, and health (ES&H); environmental stewardship; industrial hygiene; integrated safety management (ISM); waste management.

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Continued from p. 2

Lab Radiation Technology Hits the Road

A radiation detection device developed by Livermore scientists and engineers is being used by state and local governments to monitor for nuclear materials that could be part of a "dirty bomb" or nuclear device. The technology was licensed to Textron Defense Systems Corporation in Wilmington, Massachusetts.

One U.S. state has deployed more than 20 of the radiation detectors, called the adaptable radiation area monitor (ARAM), and placed them at state vehicular entrances to monitor for nuclear materials. The ARAM system can detect concealed radioactive material about the size of a grain of sand moving at 72 kilometers per hour, nearly freeway speed. A second state, New Jersey, has acquired from Textron Defense Systems a fleet of sport utility vehicles (SUVs) outfitted with the ARAM detection technology to patrol its highways and streets for nuclear materials. The New Jersey SUVs, known as RadTrucks, have been in operation for more than a year, when the state joined multiple agencies in the New York City region in a federal pilot program that aims to detect terrorist nuclear material before it can be detonated.

One advantage of the technology, according to Brian Adlawan, program director for detection systems for Textron Defense Systems, is that it can be rapidly redeployed based on intelligence and new developments. Another advantage is that the technology allows state agencies to continue their normal law-enforcement functions, even as they are monitoring for nuclear materials. The Department of Homeland Security provides grants through its Securing the Cities initiative to enhance regional capabilities for detecting and interdicting illicit radioactive materials.

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Technology License Royalties Top $9 Million

In its best year ever for securing royalty income from technology licenses, the Laboratory garnered more than $9 million in the recently completed 2008 fiscal year. The $9.4 million total represents one of the highest amounts of royalty income ever achieved in a fiscal year by a Department of Energy national laboratory.

"Clearly, our royalty income this year is a tribute to the quality of the intellectual property that is coming out of the Laboratory," says Erik Stenehjem, the director of Livermore's Industrial Partnerships Office (IPO). "The products being developed from Livermore technology help both in combating disease and in protecting national security. This success is directly attributable to the creativity of our employees."

The efforts of Livermore's scientists, engineers, technicians and IPO not only benefit the U.S. economy, but also make important contributions to homeland security. Currently, more than 20 companies are manufacturing homeland security products based on Livermore technology to protect the nation. Some of the Laboratory's royalty income is plowed back into groundbreaking research. For example, $1 million research efforts have been undertaken both for proton therapy as a cancer treatment and for an inertial confinement fusion energy project. In addition, last year 38 percent of the total revenue income, or approximately $1.7 million after direct expenses, was distributed to Livermore inventors.

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New Tools Model Amorphous Materials

A team of researchers from Lawrence Livermore and Lawrence Berkeley national laboratories and Rutherford Appleton Laboratory in the United Kingdom has identified tools that model the atomic and void structures of a network-forming elemental material. These tools could revolutionize the process of creating new solar panels, flat-panel displays, optical storage media, and myriad other technological devices.

The team, led by Livermore physical chemist Joe Zaug, created three-dimensional (3D) models of pressure-dependent structures of amorphous red phosphorus (a-rP) that for the first time are accurately portrayed by neutron and x-ray diffraction studies. The researchers also developed a new method to accurately characterize void structures within network-forming materials. In the 1970s and 1980s, amorphous or disordered materials were found to exhibit technologically viable properties for use in photovoltaic cells and portable optoelectronic storage media such as CDs, DVDs, and more recently Blu-ray disks. However, attempts by scientists to accurately characterize seemingly simple elemental materials such as a-rP were hindered because the appropriate analysis tools simply did not exist.

The diffuse scattering analysis tools developed by these scientists will enable more systematic engineering routes for designing and characterizing amorphous materials. The mechanical, optical, magnetic, and electronic plasticity of amorphous materials hold great promise toward enhancing current and emerging technologies. The research appeared in the November 2008 edition of *Nature Materials*.

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In this section, we list recent patents issued to and 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

Production of Hydrogen from Underground Coal Gasification
Ravindra S. Upadhye
U.S. Patent 7,431,084 B1
October 7, 2008
In this system, a coal gasification production well is extended into a coal seam to provide hydrogen. A conduit is positioned in the production well, leaving an annulus between the conduit wall and the well. The annulus is closed at the lower end to seal it from the coal gasification cavity and the syngas, providing at least a portion of the wall with a bifunctional membrane. This membrane serves the dual purpose of providing a catalyzing reaction and selectively allowing hydrogen to pass through the wall and into the annulus. Hydrogen is produced through the annulus.

Carbon Fuel Particles Used in Direct Carbon Conversion Fuel Cells
John F. Cooper, Nerine Cherepy
U.S. Patent 7,438,987 B2
October 21, 2008
This system prepares particulate carbon fuel for use in a fuel cell. Carbon particles are finely divided and placed in the fuel cell. A gas containing oxygen is also placed in the fuel cell. The carbon particles are exposed to carbonate salts; or molten sodium hydroxide, potassium hydroxide, or lithium hydroxide; or mixed hydroxides; or alkali and alkaline Earth nitrates.

Optically Measuring Interior Cavities
Gary Franklin Stone
U.S. Patent 7,440,121 B2
October 21, 2008
This method measures the three-dimensional volume or perimeter shape of an interior cavity. First, an optical slice of data that represents a partial volume or perimeter shape of the interior cavity is collected. Then additional optical slices of data that represent a partial volume or perimeter shape of the interior cavity are collected. Finally, the first optical slice and the additional optical slices are combined to calculate the three-dimensional volume or perimeter shape of the interior cavity.

Bipolar Pulse Forming Line
Mark A. Rhodes
U.S. Patent 7,440,568 B2
October 21, 2008
This bipolar pulse-forming transmission line module for linear induction accelerators has first, second, third, fourth, and fifth planar conductors. The conductors form an interleaved stack with dielectric layers between the conductors. Each conductor has a first end and a second end adjacent to an acceleration axis. The first and second planar conductors are connected to each other at the second ends. The fourth and fifth planar conductors are also connected to each other at the second ends. The first and fifth planar conductors are connected to each other at the first ends via a shorting plate adjacent the first ends. The third planar conductor is electrically connectable to a high-voltage source. An internal switch is used to short a high voltage from the first end of the third planar conductor to the first end of the fourth planar conductor, producing a bipolar pulse at the acceleration axis with a zero net time integral. An aperture through the shorting plate and its proximity to the switch allow for improved access.

Poynting-Vector Based Method for Determining the Bearing and Location of Electromagnetic Sources
David J. Simons, Charles R. Carrigan, Philip E. Harben, Barry A. Kirkendall, Craig A. Schultz
U.S. Patent 7,440,858 B2
October 21, 2008
This method and apparatus are used to determine the bearing and location of sources emitting electromagnetic-wave energy for which a Poynting vector can be defined. Such sources include alternating current generators and loads, power lines, transformers, and radio-frequency transmitters. When both a source and field sensors (electric and magnetic) are static, a bearing to the electromagnetic source can be obtained. If a single set of electric and magnetic sensors is in motion, multiple measurements permit location of the source. The method can be extended to networks of sensors to determine the location of both stationary and nonstationary sources.

Awards

Stan Howell, manager of the Laboratory's Small Business Program, received a **Recognition Award** for his support to the **Northern California Small Business and 8(a) Association**, a nonprofit organization dedicated to helping its members with resources, education, promotion, support, and networking.

Howell and 16 other representatives from local companies were honored for their work to educate association members and promote small business opportunities. Congressman Jerry McNerney, who presented the award, said, "As manager of the Lab's Small Business Program Office, Stan has worked to aid small businesses in marketing themselves to the Lab and has been integral in awarding $1 billion in small business contracts over the last four years." The Laboratory's goal is to award 45 percent of its contracts to small and minority or disadvantaged businesses, preferably located in but not limited to California.

Glenn Meyer and **Barry Olsen** of the Engineering Technologies Division and retirees **Michael Pocha** and **Chuck McConaghy** received a **Certificate of Recognition** from the **National Aeronautics and Space Administration** (NASA) for their contributions to the creative development of a microfiber coupled broadband light source. The unique filament and package design enables efficient light coupling into optical fiber without the use of coupling optics, resulting in a smaller, lighter device than is currently commercially available. Development of the device was a joint effort between the Laboratory and NASA, in conjunction with the Lighting Innovations Institute and the Aerospace Corporation. The team's paper "Miniature Incandescent Lamps as Fiber-Optic Light Sources" was published in the July 2008 *NASA Tech Briefs.*

The Laboratory's work in environmental stewardship and environmental restoration was honored with two **Pollution Prevention Awards**. The awards, from the **Department of Energy** (DOE), were presented to **Fleet Management's E85 Fueling Station Team** and to **Environmental Restoration Division's Space Action Team**.

The Space Action Team manages the demolition of Laboratory facilities that are no longer cost-effective to maintain because of age, condition, changing missions, or obsolescence. The team received its award in the Waste–Pollution Prevention category for the team's efforts in reducing the generation of waste and in recycling or reusing materials during the demolition of Building 431 in 2007. The Space Action Team Building 431 members included **William Collins**, **Matt Robison**, **Michael Auble**, **Kenneth Lane**, **Lisa Crawford**, **Paul Corrado**, **Joseph Albert**, and **Douglas Murray**.

Fleet Management received its award in the category of Alternative Fuels and Fuel Conservation in recognition of the Laboratory's E85 Fueling Station. E85 fuel is a blend of 85-percent ethanol and 15-percent unleaded gasoline. The Laboratory has 267 E85 alternative-fuel vehicles. The use of alternative fuels such as E85 helps reduce both greenhouse-gas emissions and the nation's dependence on petroleum-based gasoline. The E85 Fueling Station began operation in May 2007 and dispenses approximately 63,000 gallons of E85 annually. The Laboratory's fleet of E85-compatible vehicles is the largest alternative-fuel vehicle fleet in the DOE complex. The E85 Team members included **Jose Pineda**, **Dean Yoshida**, **Tim Kemper**, and **Mishell Pendleton**.

Randy Pico of the National Security Engineering Division (NSED) was recently honored as one of five **DeVry University Most Distinguished Alumni** in the university's 25-year history in California. During that time, DeVry has graduated about 70,000 students from its 14 California campuses. Pico received his electronic technician diploma from DeVry in 1981 and returned to receive a bachelor's degree in technical management in 2004.

Pico has served for many years as a DeVry advisory board member and is the primary architect of the relationship between the Laboratory and the university. The ceremony honoring Pico was attended by Joe Galkowski, NSED division leader, and Dennis O'Brien, chief electronics engineer. "We have had a wonderful relationship with DeVry over the years, in large part because of Randy's efforts," said O'Brien. "Engineering has hired some excellent technical people out of the DeVry program."

Retired Laboratory physicist and computational pioneer **Berni Alder** was inducted as a **fellow** of the **American Academy of Arts and Sciences** at a ceremony in Boston, Massachusetts, on October 11, 2008. The academy's 228th class of fellows was celebrated for their cutting-edge research, artistic accomplishment, and exemplary service to society. Laboratory physicist Claire Max joined the ranks of fellows in 2002, and Livermore cofounder Edward Teller became a fellow in 1954. Livermore's Science and Technology Principal Associate Director Cherry Murray also is a member of the academy.

Founded in 1780, the academy honors excellence each year by electing to membership the finest minds and most influential leaders of the day. The academy draws on its distinguished membership to address critical social and intellectual issues through studies, publications, meetings, and symposia.

Abstracts

Sniffing the Air with an Electronic Nose

A team of Livermore researchers has designed and built a device that selectively identifies a chemical vapor from a typical background "soup" of airborne compounds by using minuscule diving boards called microcantilevers. The Livermore electronic nose can detect nearly any chemical vapor, including chemical warfare agents, once it has been "trained" to recognize them. The device has reliably detected 11 different chemical vapors plus the chemical warfare agents VX and sulfur mustard, representing a wide breadth of chemicals. The research effort is in response to requests from planners of the Departments of Defense and Homeland Security for lightweight, accurate, and inexpensive handheld sensors to sniff out deadly chemicals, including chemical weapons on the battlefield and toxic compounds that could be used in a terrorist attack. The Livermore design is based on the differential bending of silicon microcantilevers coated with specialized polymers. When a chemical of interest reacts with the coating, the coating swells, the microcantilever bends, and the deflection of the microcantilever is measured by external electronics.

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Simulations Explain High-Energy-Density Experiments

A Computing Grand Challenge project on Livermore's Atlas supercomputer simulated results from two sets of laser-driven high-energy-density (HED) experiments. In one set of experiments, researchers zapped very small reduced-mass targets with ultrahigh-intensity lasers to get the dense targets as hot as possible. Such targets, which produce high-energy electrons, protons, and x rays, are being considered as backlighters for radiography diagnostics at the National Ignition Facility. In another set of experiments, researchers used intense laser light to create a laser wakefield accelerator and accelerate electrons in a low-density plasma. Such accelerators are anticipated to reach energies of 10 gigaelectronvolts over a distance of 1 meter, which is much shorter than the multikilometer length of most particle accelerators. Atlas simulations of these HED experiments revealed detailed insight into physical phenomena not measurable with test diagnostics, explained unexpected results, and gave experimentalists essential information for planning future tests. The power of the Atlas supercomputer made possible the simulation of full-scale experiments in three dimensions.

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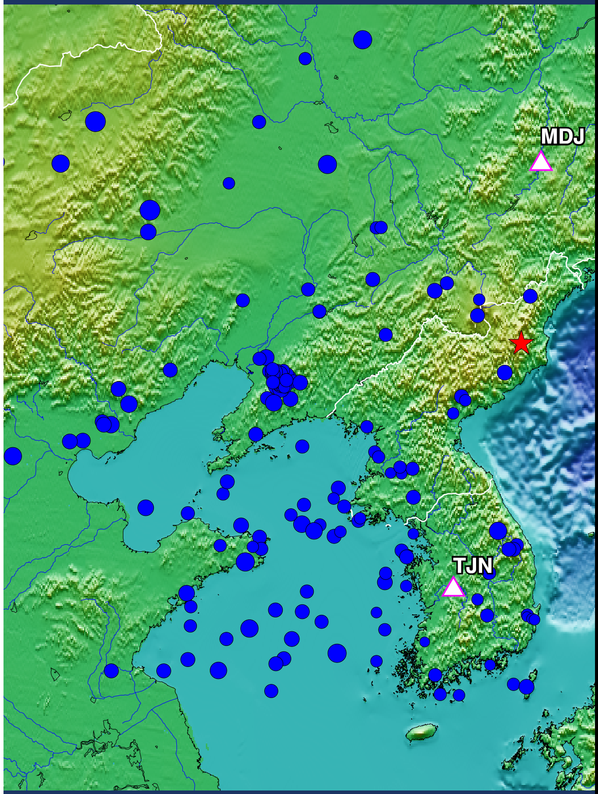
Deciphering Seismic Data



New supercomputing tools help seismic researchers calibrate data from earthquakes and clandestine nuclear tests.

Also in March

• Powerful amplifiers strengthen researchers' ability to detect for the first time axions, hypothesized particles that may constitute "dark matter."

• A Livermore-designed decontamination kit will provide an effective self-treatment for exposure to toxic chemicals.

• The Laboratory is working with government agencies and industry to more effectively integrate wind energy into the nation's electrical infrastructure.

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