November/December 2008

Science & Technology Review

National Nuclear Security Administration's
Lawrence Livermore National Laboratory

Also in this issue:

- The Remarkable Properties of Nanolaminates
- Predicting the Behavior of Plutonium

About the Cover

Livermore researchers garnered three R&D 100 awards in *R&D Magazine*'s annual competition for the top 100 industrial innovations worldwide. This issue of *Science & Technology Review* highlights the award-winning technologies: DTEM, the dynamic transmission electron microscope (p. 4); AAPLF, an autonomous alignment process for laser fusion systems (p. 6); and SecureBox, a sensor for monitoring cargo containers (p. 8). All three technologies were developed by multidisciplinary research teams, a hallmark of the Laboratory's approach to innovative science and technology. Since 1978, Laboratory researchers have received 121 R&D 100 awards. (The R&D 100 plaque on the cover and the logo on p. 1 are reprinted courtesy of *R&D Magazine*.)

Cover design: Alexandria Ballard

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 six 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 Livermore National Laboratory

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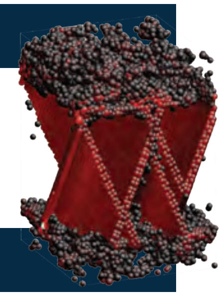

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Researchers peer into the nanoscale

Laboratory researchers have captured time-series snapshots of a solid as it evolves on the ultrafast timescale. Using the x-ray free-electron laser (FEL) at the Deutsches Elektronen-Synchrotron Research Centre in Hamburg, Germany, the team observed the condensed-phase dynamics of an object as it undergoes laser ablation. The team's research marks the first time that optical pulses have been used to image samples with nanometer-scale spatial resolution. Results from this research appeared in the July 2008 issue of *Nature Photonics*.

The FEL blasts a sample with femtosecond-long pulses, where a femtosecond is one-billionth of one-millionth of a second. Before the sample is destroyed, high-speed diagnostics record images that have a 50-nanometer spatial resolution and a 10-femtosecond shutter speed. This shutter speed, which is determined by the duration of the x-ray pulse, allows the team to observe events occurring at the atomic level before a sample is completely destroyed. "The ability to take images in a single shot is key to studying nonrepetitive behavior mechanisms in a sample," says project leader Anton Barty of Livermore's Physical and Life Sciences Directorate.

With the new technique, researchers can study the ultrafast dynamics occurring in noncrystalline materials under extreme conditions, such as fracture, shock, and plasma formation. The technique also allows researchers to image dynamic processes in the solid state such as nucleation and phase growth, phase fluctuations, and various forms of electronic or magnetic segregation.

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Bioterrorism instrument adapted to detect tuberculosis

An instrument originally designed for detecting the malicious use of biological pathogens has a potential application in the public health sector—to rapidly screen for tuberculosis. In experiments over the past year, a Livermore research team has used single-particle aerosol mass spectrometry (SPAMS) to detect a tuberculosis surrogate, even when surrounded by sputum and mucuslike substances. The team also differentiated two similar bacteria, distinguishing an avirulent strain of tuberculosis from *Mycobacterium smegmatis*. The team's research, which was funded by Livermore's Laboratory Directed Research and Development Program, is described in the July 15, 2008, issue of *Analytical Chemistry*.

"We used two similar mycobacteria because many bacterial infections cause tuberculosislike symptoms, not just tuberculosis," says lead author Kristl Adams, a postdoctoral biological physicist in Livermore's Physical and Life Sciences Directorate. The "gold standard" diagnostic tool is to culture samples, a process that can require days to weeks. Health-care providers and emergency response personnel need a method to differentiate the infections within minutes.

With current methods, diagnosing tuberculosis can be difficult and expensive. While waiting on cultures to grow, medical personnel may release patients, allowing them to infect the general public. In addition, valuable resources may be wasted when unneeded precautions, such as chest x rays or patient isolation, are taken for people who, in the end, do not have the disease.

According to Adams, SPAMS could potentially detect tuberculosis in concentrated samples within 5 minutes, although, she notes, the team's work is only a first step toward this application. "Having a rapid tuberculosis screening technique could improve patient care," she says, "and reduce the toll on health-care facility resources."

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Method distinguishes different kinds of seismic events

Using data from the Crandall Canyon Mine collapse that occurred on August 6, 2007, researchers from Lawrence Livermore and the University of California's (UC's) Berkeley Seismological Laboratory have successfully applied a full waveform-matching technique to determine the source of seismic events. The team's results, which were published in the July 11, 2008, issue of *Science*, indicate that seismic signatures can distinguish disturbances caused by nuclear explosions, earthquakes, and collapse events.

The tragic collapse of the Utah coal mine killed six miners and three rescue workers. The 3.9-magnitude event was recorded at seismic stations operated by the U.S. Geological Survey and the National Science Foundation Earthscope USArray. "We were already developing a full waveform-matching technique to distinguish events by seismic signals," says Livermore geophysicist Bill Walter of the Physical and Life Sciences Directorate. The research team, which included Sean Ford, a UC Berkeley graduate student and Lawrence Scholar, and Douglas Dreger, a professor at the UC Berkeley Seismological Laboratory, applied the technique to the Crandall Canyon data.

When the researchers compared recorded data to the modeling results, the Crandall Canyon seismograms clearly matched the source type for a collapse event. The team also detected Love waves, surface seismic waves that cause horizontal shifting of the earth. Love waves are typically small in large mine collapses or when a hole collapses after an underground nuclear test. In contrast, Love waves from the Crandall Canyon collapse were larger than expected for a purely vertical collapse caused by gravity. "One explanation consistent with the data is that the collapse was uneven," says Walter, "with one side closing more than the other."

Ford also notes that the mine collapse was relatively small in magnitude. "The fact that we could identify the Crandall Canyon event from its seismic signature gives us confidence that we can use the waveform-matching technique to identify even relatively small nuclear explosions."

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Innovation Is Key to Prosperity and Security

THIS year's R&D 100 Award winners exemplify the Laboratory's pursuit of excellence at the nexus of innovation and economic and national security. Highlights of the three winners—an autonomous alignment process for laser fusion systems, the dynamic transmission electron microscope, and a detector for protecting shipping containers from unauthorized access—begin on p. 4. With these three awards, Lawrence Livermore and its collaborators have received 121 of *R&D Magazine*'s "Oscars of Invention" since 1978.

In what *New York Times* columnist Thomas Friedman calls a "flat world," powerful companies can instantaneously move capital around the globe to access resources, means of production, and sources of innovation. In this increasingly global economy, where capital flows in ever greater quantities to countries of the developing world to manufacture and provide services, economic competitiveness depends more and more on the strength of U.S. innovation.

The congressionally mandated report, *Rising above the Gathering Storm: Energizing and Employing America for a Brighter Economic Future* (National Academies Press, 2007), proposes four ways in which the U.S. can maintain its economic competitiveness. Three of these recommendations relate to classroom education; commitment to basic research; and recruitment and retention of top students, scientists, and engineers. The fourth recommendation is to "ensure that the United States is the premier place in the world for innovation."

Innovation is also important to our national security. The Hart-Rudman Commission on National Security concluded that a failure to maintain our ascendancy in innovation poses a greater threat to U.S. national security over the next 25 years than any potential conventional war we might imagine. As the world flattens (and warms up), economic welfare and national security will depend increasingly on our ability as a nation to innovate.

The Laboratory specializes in scientific and technological research that is critical to the nation's continuing prosperity and security in a flat world. For example, the quest for virtually limitless energy from nuclear fusion at the National Ignition Facility (NIF) is vital for future economic security. In 2010, experiments will begin at NIF with the goal of achieving fusion ignition and burn in a laboratory setting. Meanwhile, the novel sensors, detectors, and low-error modes of gathering intelligence developed at the Laboratory are important for protecting our borders.

In 2008, Deborah Wince-Smith, the president of the Council on Competitiveness, spoke at the Laboratory as part of the Director's Distinguished Lecture Series. In her presentation, she noted that Lawrence Livermore is an "innovation hot spot" of the type needed to lead the next scientific revolution. Our success in *R&D Magazine*'s annual competition strongly supports her statement.

One award winner is the dynamic transmission electron microscope (DTEM) developed in collaboration with JEOL USA, Inc., a leading supplier of high-resolution instruments such as scanning and transmission electron microscopes. A new tool for basic research, DTEM is the first device that can capture nanometer-scale images in increments as short as 15 nanoseconds. With DTEM, scientists can "watch" changes occurring in materials under stress or observe a biological function in action.

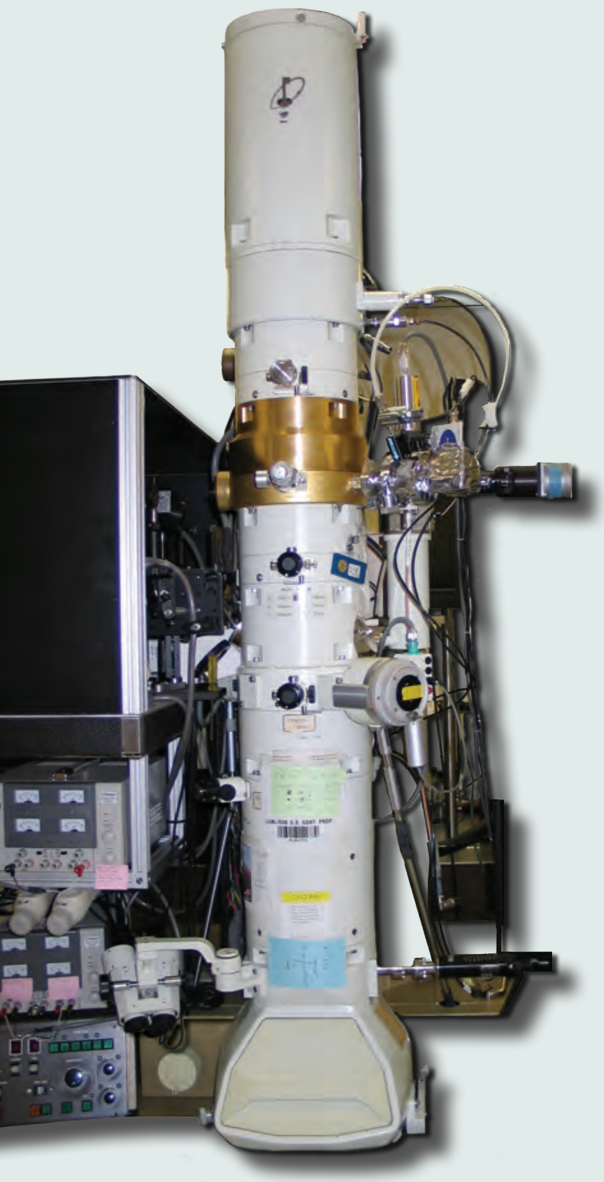
Our second R&D 100 Award went to the autonomous alignment process for laser fusion systems (AAPLF, pronounced apple-f), a key operating system at NIF. AAPLF operates 35,000 separate optical devices to precisely align NIF's 192 beams to within a tolerance of 10 micrometers.

The third award winner, SecureBox, is designed to protect ships, ports, and people from the possible use of a cargo container to transport a weapon of mass destruction. The device, about the size of a 12-ounce soda can, uses ultrawideband radar and communication technology to detect intrusions along any of the six sides of a sealed cargo container. If an intrusion is detected, SecureBox transmits an alarm to authorized individuals. The device was tested during transatlantic voyages and has been commercialized by Secure Box Corporation.

With these three awards, Lawrence Livermore has again demonstrated its ability and commitment to developing innovative solutions to address important national needs. It is this spirit that will continue to help the U.S. remain strong and secure.

■ Erik J. Stenehjem is director of the Industrial Partnerships Office.

Taking Ultrafast Snapshots of Material Changes



The dynamic transmission electron microscope (DTEM) captures nanoscale images a million times faster than conventional instruments.

SINCE the invention of the transmission electron microscope (TEM) in 1938, scientists have slowly improved its maximum spatial resolution to less than 0.1 nanometers (1 ten-billionth of a meter). However, they have had less success at improving the TEM's temporal resolution, the time interval required to capture a single microscopic image. As a result, researchers have had to scrutinize before-and-after images separated by tens of milliseconds and then infer the fleeting, irreversible processes that account for significant changes in a material's internal microstructure—and its physical properties.

To address the temporal inadequacy of modern TEMs, a team of Lawrence Livermore scientists and engineers, working with researchers from JEOL USA, Inc., has developed the dynamic transmission electron microscope (DTEM). The instrument captures images at less than 10-nanometer resolution in 15 nanoseconds, a million times faster than the typical 30-millisecond exposure time required by a conventional TEM. DTEM is the only technology available for generating direct nanometer-resolution images of irreversible events at time scales ranging from 15 nanoseconds to 10 milliseconds.

Using DTEM, scientists can see for the first time how materials behave under unusual conditions, such as an applied stress, extreme temperature change, and corrosive environment. In this way, the instrument will help them engineer materials that will exhibit new properties, be stronger, or be more resistant to corrosion.

Biological Processes in Action

DTEM may also provide a new tool for biological research. Conventional TEMs image biological samples in a fixed or frozen state. Life processes could only be viewed with a light microscope at low spatial resolution (about 200 nanometers). With DTEM, researchers will be able to observe a biological function in action, allowing them to analyze the changing structures of chromosomes, membrane proteins, and other biomolecules or the cell activities occurring in processes such as mitosis.

The DTEM development team includes researchers from the Laboratory's Physical and Life Sciences Directorate; Engineering Directorate; and National Ignition Facility and Photon Science Principal Directorate. The work was supported by Livermore's Laboratory Directed Research and Development Program and the Department of Energy's Office of Basic Energy Sciences. In addition to receiving an R&D 100 Award, the team earned a Nano 50 Award. Presented by *Nanotech Briefs*, Nano 50 awards annually recognize the top 50 technologies, products, and innovators in nanotechnology.

"Everything we can do with a conventional TEM, we can do with DTEM, but with improved temporal resolution," says Livermore materials scientist Nigel Browning, who co-leads the DTEM project. "With DTEM, we can see actual processes occurring, such as a metal transforming from one state to another." He explains that in experiments with current instruments, dynamic processes are often stopped to "freeze" microstructural features in place, or they are recorded at

DTEM development team (from left): Thomas LaGrange, Bryan Reed, Geoffrey Campbell, Wayne King, William DeHope, Nigel Browning, Richard Shuttlesworth, Judy Kim, Benjamin Pyke, and Michael Armstrong. Not pictured: Brent Stuart, Mitra Taheri, J. Bradley Pesavento, and Benjamin Torralva.

video rates (about 30 frames per second), which are much too slow. In contrast, DTEM captures never-before-seen details of material processes in 15-nanosecond exposures. With upgrades currently under development, DTEM will be able to take several consecutive images, creating a movielike record of microstructural features as they rapidly evolve.

Bursts of Electrons

The Livermore technology combines pulsed-laser technology with the electron optics of a standard TEM. It incorporates a laser system that allows users to control pulse shape and duration. A high-current lens system regulates the focus and current of the pulse for optimizing exposure times. A single-electron sensitive charge-coupled device camera records extremely fast, high-resolution images. Conventional TEMs produce a steady stream of electrons, but DTEM bunches them into pulses. These short bursts of electrons illuminate a specimen using only 10 electrons per square nanometer, well below the damage threshold even for biological samples.

DTEM also has a sample drive laser that enables in situ experiments. The laser intensity can be adjusted precisely to produce effects ranging from gentle, localized heating to nearly instantaneous vaporization as temperature is increased thousands of degrees in a few nanoseconds. This rapid heating is confined to an area less than 100 micrometers across, unlike conventional in situ TEM heating experiments in which the entire sample is heated at once. The sample drive laser can also be used to synthesize materials inside the microscope, for example, to fabricate silicon nanowires.

Applications for DTEM technology include imaging chemical reaction fronts; examining complex, rapid phase transformations in metals, semiconductors, and memory-storage materials; and exploring the nucleation and growth of semiconductor nanowires and other nanostructures. Livermore scientists are using the machine to track the evolution of a material's dislocations, impurity particles, grain boundaries, and phase boundaries. These transient features, which are critical to material performance, are invisible to techniques that record only the before-and-after states of material processes.

The DTEM team is working to improve the microscope's electron optics and lasers and the ease with which operators can change parameters. Browning anticipates that the instrument will approach about 1-nanometer spatial and 1-nanosecond temporal resolution in the next few years. Within a decade, DTEM could become one of the standard instruments helping scientists illuminate the inner worlds of metals and new materials or unravel the secrets of cell function.

—Arnie Heller

Key Words: dynamic transmission electron microscope (DTEM), materials science, Nano 50 Award, R&D 100 Award.

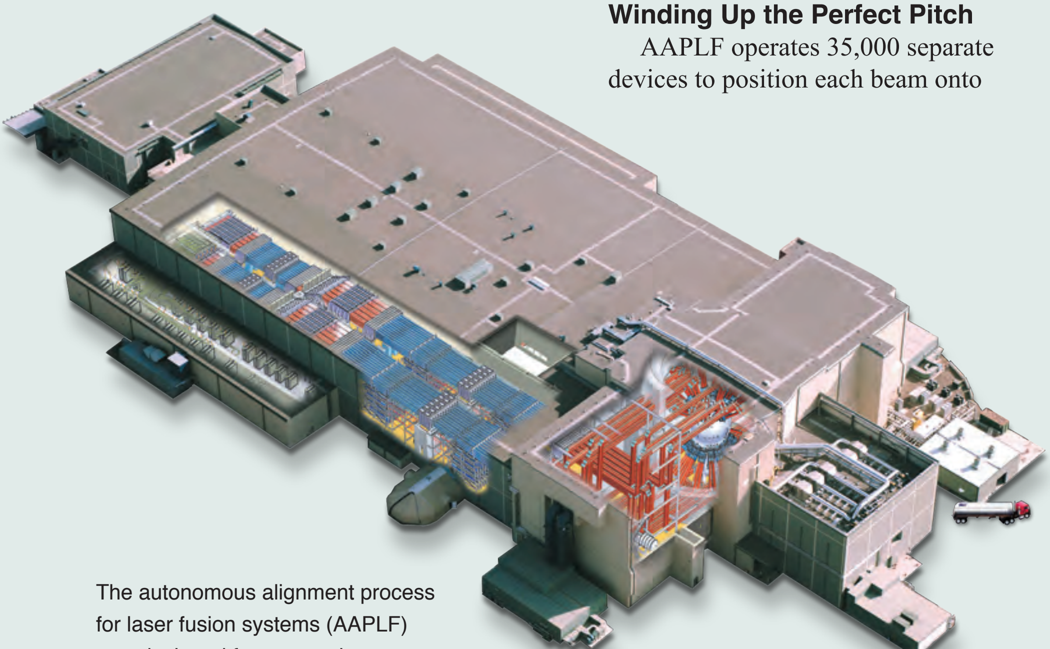
For further information contact Nigel Browning (925) 424-5563 (browning20@llnl.gov).

Automated Technology for Laser Fusion Systems

THE day is fast approaching when Lawrence Livermore's National Ignition Facility (NIF) will conduct experiments to achieve controlled fusion reactions in a laboratory setting. The success of these experiments relies on the precise alignment of NIF's 192 laser beams, which will direct light down a 300-meter optical path onto a cylindrical target a few millimeters in diameter—slightly larger than the head of a pushpin.

Laser systems typically use manual or semiautomated processes to adjust optics and configure beamlines. Manual operations can be unreliable or imprecise. Semiautomated methods work well only under optimal conditions, for example, when beam quality is unaffected by noise or other external influences.

A completely autonomous alignment process developed by a team of Livermore researchers eliminates human error while effectively aligning the beams with high accuracy in less than 15 minutes. In developing the autonomous alignment process for laser fusion systems (AAPLF, pronounced apple-f), the Livermore team received a 2008 R&D 100 Award. AAPLF not only performs the optical adjustments for each beamline, but it also directs the focused beams to the target, where they produce the extremely high temperatures and pressures needed for fusion experiments.



The autonomous alignment process for laser fusion systems (AAPLF) was designed for use on the National Ignition Facility.

Winding Up the Perfect Pitch

AAPLF operates 35,000 separate devices to position each beam onto the NIF target within a tolerance of 10 micrometers. Aligning the beams within such a small margin of error is analogous to hitting a baseball strike zone with a pitch thrown from approximately 560 kilometers away. To make this perfect pitch possible, AAPLF analyzes images of each beam and adjusts the optics as needed. It begins by retrieving the alignment plans for an experiment from a database. The beams, which are grouped into 24 bundles of eight, are sampled from within the NIF subsystems, such as the Preamplifier Modules (PAMs), in ways that do not interfere with normal beam operations.

The software "brain" of AAPLF, called the Segment Manager, coordinates other parts of the control system, including the Components Manager and Image-Processing Cluster, to configure the beamlines, capture the necessary images, and execute image-processing algorithms. The Components Manager processes requests from the Segment Manager to use devices, such as actuators and cameras, that are shared between beams within the system. It places requests in a queue and blocks access to devices already in use. Once a device becomes available, the Segment Manager can use it to adjust mirrors and beam optics. Adjustments are executed by 26 control loops that center and point each beam down its respective path. The Segment Manager then acquires another set of images to determine if further changes are necessary.

AAPLF uses masks as passive references to locate a beam's position within a PAM. Masks are made from transparent glass plates that contain two types of markings, called fiducials. An initial mask adds fiducials to the beam, while downstream masks with different fiducials define desired beam positions. Mirrors reflect the laser beams onto these reference fiducials, and a video-camera sensor records images of a beam passing through each downstream mask. Image-processing algorithms then determine how far the laser beam is from the reference position. If the reference and laser beam locations do not match, AAPLF adjusts the optics and repeats the process until the beam is properly aligned.

During the alignment process, sensors acquire images from different areas, such as NIF's target chamber or PAMs. A suite of 22 image-processing algorithms analyzes the images to determine the beam positions. The algorithms also process complex images that would be difficult or impossible for an operator to accurately interpret. Conditions within the laser system can cause artifacts such as diffraction and noise to appear in the images. AAPLF algorithms mitigate these effects and determine if a system problem exists that needs attention.

AAPLF development team: (back row, from left) Wilbert McClay, James Candy, Christopher Estes, Lawrence Lagin, David McGuigan, Erlan Bliss, Sean Lehman, Abdul Awwal, Haiyan Zhang, and Suzanna Townsend; (middle row) Paul Van Arsdall, Charles Orth, Thad Salmon, Scott Burkhart, Allan Casey, and Charles Reynolds; (front row) Roger Lowe-Webb, Robert Carey, Ben Horowitz, Mark Bowers, Michael Flegel, Mark Miller, Walter Ferguson, Eric Stout, Karl Wilhelmsen, Victoria Miller Kamm, and Richard R. Leach, Jr. Not pictured: Stephanie Daveler, Holger Jones, and Karl Pletcher.

Endless Possibilities

AAPLF is an accurate, reliable, and effective method for precisely aligning NIF's complex laser system. "The AAPLF computer controls and parallel image-processing systems are teamed with sophisticated yet highly multiplexed sources and references to create a powerful, autonomous process," says Scott Burkhart, a laser engineer who monitors AAPLF from the control room. "Without this system, we could not achieve the precision needed for laser fusion." AAPLF has performed successfully in more than 1,200 system and 30,000 preamplifier beam shots. In addition, the system can be scaled to any number of laser beams and thus can be adapted for the laser fusion systems of the future.

With the AAPLF beam-alignment system, NIF will soon begin experiments to achieve fusion ignition and burn in a laboratory setting. "NIF will provide critical support for Livermore's national security missions," says Ed Moses, principal associate director for NIF and Photon Science. "It also opens up exciting opportunities to explore the high-energy-density physics of the cosmos and to develop an essentially inexhaustible supply of clean energy. Innovations like AAPLF are the hallmark of what makes our Laboratory great."

—Caryn Meissner

Key Words: autonomous alignment process for laser fusion systems (AAPLF), fusion, image-processing algorithm, laser beam path, National Ignition Facility (NIF), photon science, R&D 100 Award.

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Protecting the Nation through Secure Cargo

EVERY year, more than 200 million cargo-container shipments transport 90 percent of the world's cargo. Over 11 million of these shipments arrive in the U.S., carried on ships, trains, planes, and trucks. National security officials view cargo containers as a potential means for terrorists to import a weapon of mass destruction into the U.S.

Several security mechanisms, such as special door locks and electronic seals, have been implemented to protect the integrity of containers during transit. None, however, is as cost-efficient or reliable as SecureBox, a new device developed by Lawrence Livermore in collaboration with Secure Box Corporation of Santa Clara, California, and the National Infrastructure Institute.

SecureBox is a wireless device that can be installed within the metal corrugation of a cargo container to detect intrusions.

The development team, led by systems engineer Kique Romero, received initial funding from Livermore's Laboratory Directed Research and Development Program and, in 2008, won an R&D 100 Award for the technology. SecureBox uses Livermore-developed ultrawideband (UWB) radar and communication technology to accurately detect intrusions along any of a container's six walls. The compact device, about the size of a 12-ounce soda can, fits within the metal corrugation of common cargo containers. If an intrusion is detected, SecureBox transmits alarm reports to authorized individuals. In transatlantic field tests using containers shipped by different transportation modes, SecureBox achieved a 100-percent probability of intrusion detection and a zero false-alarm rate.

Electromagnetic Security Bubble

UWB technologies use extremely short electromagnetic pulses (from 50 to 100 picoseconds, where 1 picosecond is 10^{-12} seconds) to transmit and acquire data across a broad range of radio frequencies. UWB systems offer considerable advantages for tracking and monitoring cargo containers when compared with conventional narrowband technologies, which transmit higher average-power, continuous-wave signals over specific frequencies. The short pulses and broad spectrum of UWB systems make the signals difficult to detect and allow them to function in harsh radio environments, such as the hold of a ship. In addition, low power requirements permit operation for a much longer time than narrowband technologies using a battery with equivalent capacity.

SecureBox incorporates the Livermore-developed technology used in GUARDIAN, the general-purpose undetectable autonomous radar detection imaging and notification system. This UWB motion detection system transmits millions of subnanosecond radar pulses and detects changes in echo signals reflected back to the sensor. The GUARDIAN sensor uses precision timing techniques to selectively evaluate echo signals arriving at the sensor from a specific distance.

GUARDIAN turns this invisible ping-pong of electromagnetic pulses into a protective semispherical bubble around the container walls. A bubble-shaped electromagnetic field might seem to be ineffective at protecting a rectangular container. However, an innovative folded-bubble method developed by the Livermore team takes advantage of reflections from the container's metal walls to precisely time the received echo signals while maintaining sufficient signal energy to trigger the alarm.

Once a container is sealed for transport, any breach of its walls disrupts the radar's echo pattern and activates an alarm. SecureBox systems also include sensors, such as accelerometers, to help differentiate movement by an intruder from the normal vibrations that occur during shipping.

Sending an Alarm

If an intrusion is detected, SecureBox transmits encrypted data through various communication modes to alert authorized individuals of the breach. The device's communication system can transmit data up to 122 meters and works effectively even when a container is buried in a stack of other containers or located deep within the hold of a ship.

Commercial UWB communications systems designed for high data rates typically correlate the data pulse with a preset template. This technique does not work well inside ships because they are primarily made of metal. Metal surfaces create a massive number of reflections that distort or stretch the radio-frequency signals emitted by the sensor. Distorted signals are difficult to detect because they do not resemble the template of the transmitted energy.

To counter this issue, the Livermore team used the Laboratory's transmitted reference modulation technique in designing the communications radio for SecureBox. The radio transmits a pair of pulses, a modulated data pulse closely followed by an unmodulated reference pulse. Each pair has a designated binary value based on the relative polarity of the two pulses. During transmission, both pulses are stretched and distorted identically by the same environment. A reference receiver then correlates the pulses to detect the transmitted data stream. This technique enables the UWB communication system to function in highly metallic environments where traditional communication systems often fail.

A More Secure Future

Finding a reliable, cost-effective way to secure cargo containers has been a challenge for national security officials. SecureBox remains the only tamper-proof device that can protect all six walls of a cargo container, whether the container is stationary or in transit. The device is also economical. Its UWB sensor components are made from commercially available products and are powered by small lithium batteries that can work for years without being recharged. The low power requirements also make SecureBox an appealing application for the transportation industry because the device's sensors do not interfere with normal radio operations.

SecureBox devices are available from Secure Box Corporation, which licensed the Livermore technology in 2007. Thanks to the efforts of the development team, the nation has a more effective way of securing cargo and improving national security.

—Caryn Meissner

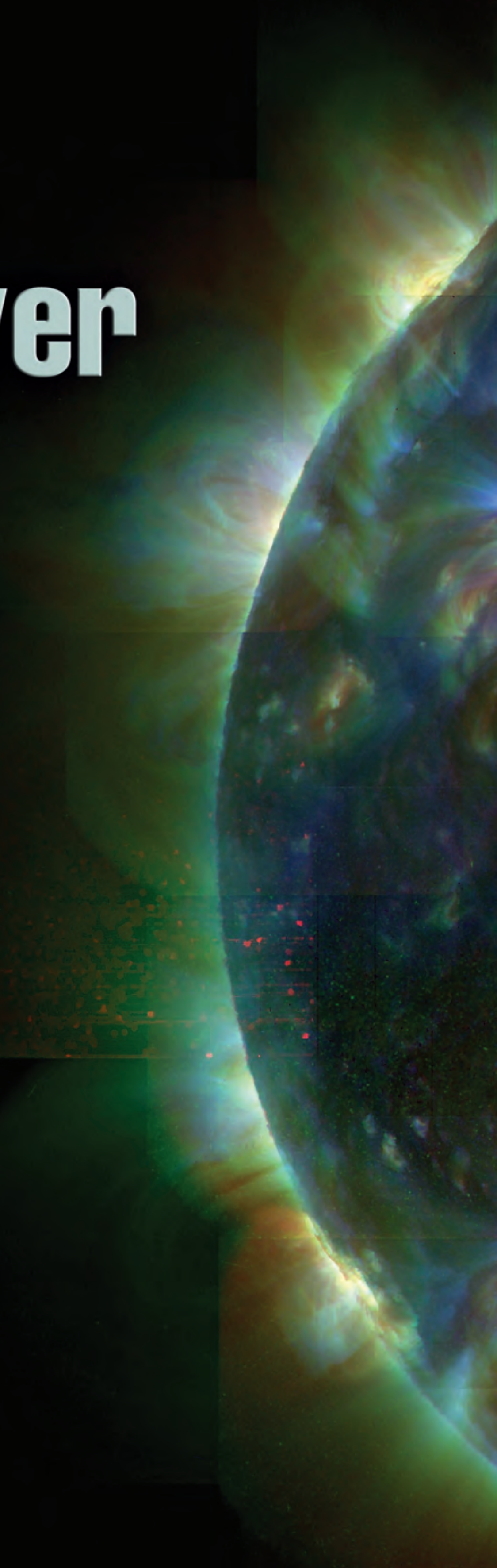
The SecureBox development team (from left): John Chang, Howard Lowdermilk, Bruce Henderer, Gregory Dallum, Richard R. Leach, Jr., Faranak Nekoogar, Garth Pratt, Vickie Abreu, Patrick Welsh, Kique Romero, Mark Vigars, James Zumstein, Peter Haugen, William Dunlop, Philip Top, and Christine Paulson. Not pictured: Stephen Azevedo, David Benzel, Kristian Chubb, Arden Dougan, Farid Dowla, Michael Newman, Ronald Shaw, and Kenneth Waltjen.

Key Words: cargo container, GUARDIAN, R&D 100 Award, SecureBox, security, sensor, transmitted reference modulation, transportation, ultrawideband (UWB) communications.

For further information contact Kique Romero (925) 423-2830 (romero29@llnl.gov).

Atom by Atom, Layer by Layer

Thousands of atomically engineered layers add up to strong, wear-resistant, and even energetic materials.



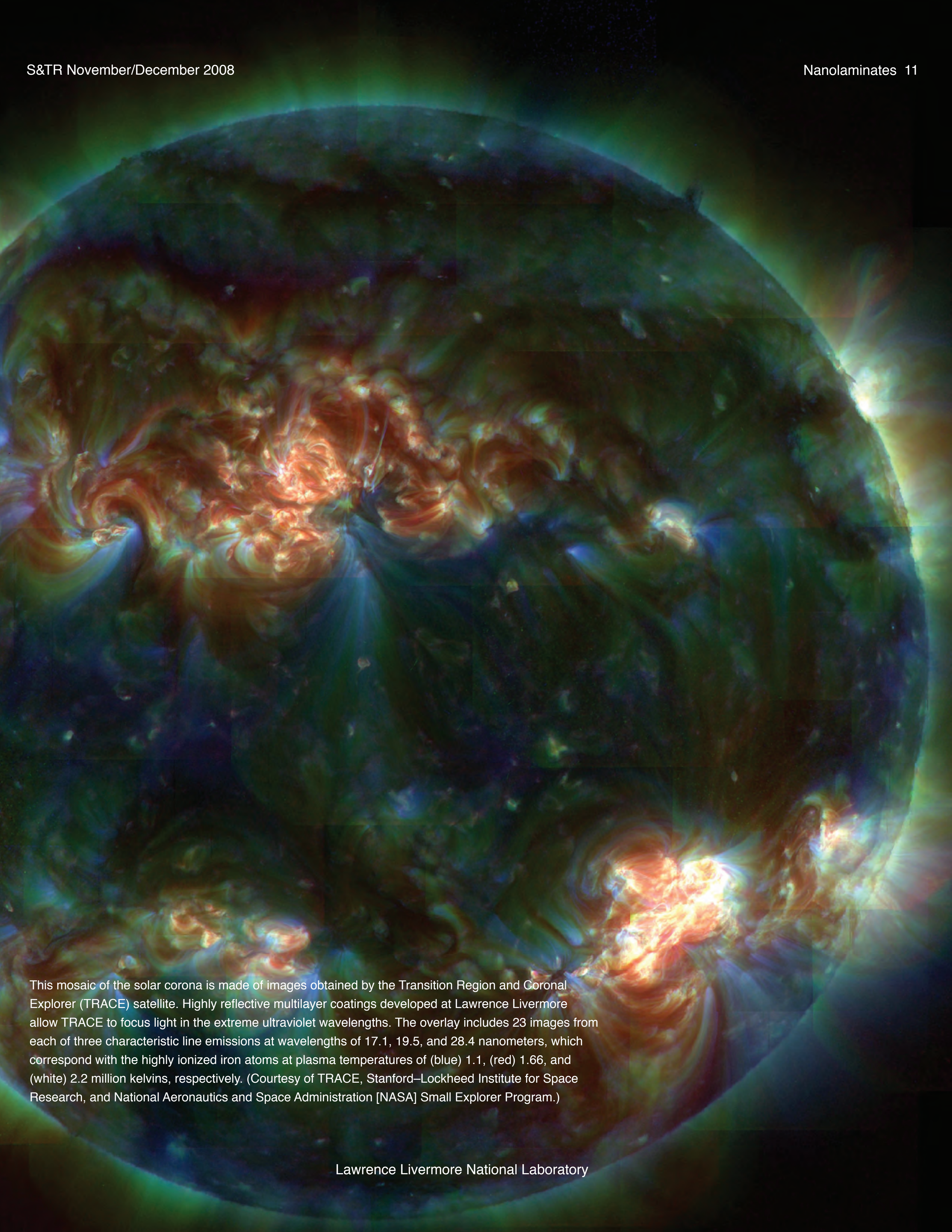
CALL them nanolaminates, or call them multilayers. In either case, they are atomic-scale sandwiches, composites made from dozens of alternating layers of materials, with each layer just 0.2 to 200 nanometers thick. The thickest layer may be only a few thousand atoms across, 1 one-hundredth the width of a human hair.

By carefully combining various elements and layer thicknesses, researchers can fabricate multilayers to almost any specification. These "designer" materials may be extremely strong; highly reflective; unusually ductile; or exceptionally resistant to heat, wear, and corrosion. Or they may incorporate several of those properties at the same time.

Many space-based solar astrophysics mirrors incorporate highly reflective multilayer coatings, allowing researchers to view the Sun's corona in the x-ray and extreme ultraviolet wavelengths. Another early use of multilayer synthesis technology was to manufacture magnetic hard-disk drives for computers. In this application, various metallic alloys are layered together with a magnetic layer on top for storing data. A more recent nanolaminate development—a layered foil that releases heat energy in a controlled manner—can be used to bond dissimilar materials without damaging them.

Most of these innovations are the brainchild of materials scientist Troy Barbee, who has been leading the Laboratory's multilayer effort since he arrived in 1985. Many of his successes received funding in the incubation stage from Livermore's Laboratory Directed Research and Development Program. Now 71, Barbee shows no sign of slowing and remains as creative as ever.

After receiving a Ph.D. in materials science engineering from Stanford University, Barbee was named Laboratory Director of the Stanford Center for Materials Research, where he performed



This mosaic of the solar corona is made of images obtained by the Transition Region and Coronal Explorer (TRACE) satellite. Highly reflective multilayer coatings developed at Lawrence Livermore allow TRACE to focus light in the extreme ultraviolet wavelengths. The overlay includes 23 images from each of three characteristic line emissions at wavelengths of 17.1, 19.5, and 28.4 nanometers, which correspond with the highly ionized iron atoms at plasma temperatures of (blue) 1.1, (red) 1.66, and (white) 2.2 million kelvins, respectively. (Courtesy of TRACE, Stanford–Lockheed Institute for Space Research, and National Aeronautics and Space Administration [NASA] Small Explorer Program.)

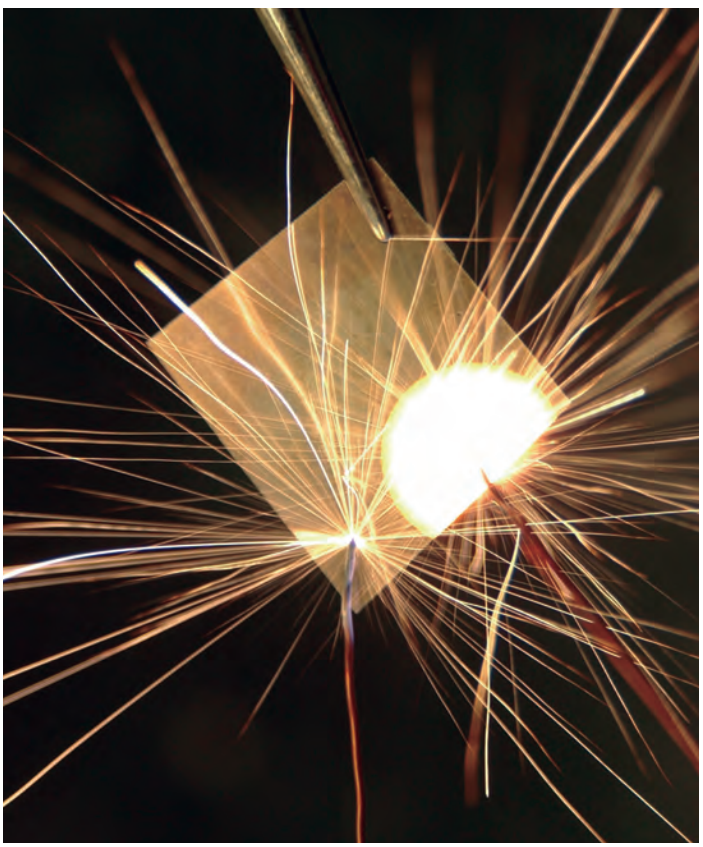
some of the earliest work with atomically engineered multilayers. Barbee notes that multilayer technology proved so successful in magnetic memory hard drives, technologists put it to use before anyone thought to patent it.

Atomic engineering does not rely on thermodynamics and kinetics to create new or advanced materials. Fabricating nanolaminates using atom-by-atom sputter deposition transcends the limits of standard manufacturing methods, resulting in materials with surprising properties, always different from those of the component substances in bulk form. These properties are due to the nanometer-scale environment of the atoms in each layer. Layers range from several atoms to a few thousand atoms thick, and the atoms within a layer are strongly influenced by the interfaces between the component layers.

Finding applications for these unusual materials is one part of the fun for Barbee, who works in Livermore's Physical and Life Sciences Directorate. "I get great enjoyment from seeing these creations put to work," he says. "So I have always emphasized working with collaborators and finding uses for our new multilayers."

Collaborations with the National Aeronautics and Space Administration (NASA) and various branches of the U.S. government put multilayered telescope mirrors and other optical devices into space. Working with Pratt & Whitney, researchers developed refractory oxide nanolaminates to enhance the performance of aircraft turbine blades. That cooperative effort produced the technology now used to fabricate high-energy-density electrical capacitors. Livermore nanolaminates also make possible extreme ultraviolet lithography (EUVL), a new lithographic method for cramming more devices onto a silicon chip.

Companies have worked with the Laboratory to determine whether the reactive nanolaminates can deploy automobile air bags or deliver inhaled medications. Government agencies have discussed using a reactive nanolaminate as an anti-tamper device on a weapon or other high-value item. And the list goes on.



The reactive nanolaminate commercialized by Reactive NanoTechnologies, Inc., is a new tool for soldering. In the reaction area (white), the temperature has jumped to 1,500°C, while the remainder of the foil is still at room temperature. (Courtesy of Reactive NanoTechnologies, Inc.)

The Shortest Wavelengths

While at the Stanford Center for Materials Research, Barbee developed the process for fabricating fully dense thin films using the then-new magnetron sputter sources. With these materials, he could study the mechanical properties at the size limits of microstructure control. In fact, the results opened the scientific door to a new world of atomic engineering and designer materials. (See the box on p. 13.)

"A combination of tungsten and carbon layers turned out to demonstrate the optical quality needed for x-ray optics," says Barbee. That finding led to the NASA collaboration to design multilayer coatings for telescope mirrors. Eventually, the coatings enabled the mirrors to focus light from space not only in the x-ray wavelengths but also in the extreme ultraviolet wavelengths. Livermore multilayer coatings are on the mirrors of NASA's Transition Region and Coronal Explorer (TRACE) satellite, which orbits Earth, pointing constantly at the Sun. Launched in 1998, TRACE records images and other data about the Sun's fluctuating magnetic fields, which cause sunspots, the corona, and other plasma structures. TRACE has vastly increased knowledge of the physics of sunspots and the Sun's corona.

A seemingly unrelated payoff to the successful use of multilayers in solar astrophysics was for computer chip manufacturing. Multilayer mirror coatings of molybdenum and silicon are a key technology for EUVL, a manufacturing technique that uses extremely short wavelengths of light to "write" on computer chips. EUVL will increase computer performance by shrinking the features printed on chips, thus allowing manufacturers to develop even smaller chips. Livermore is collaborating with other national laboratories and industrial partners to develop EUVL for commercial applications. (See *S&TR*, September/October 2008, pp. 21–23.)

Unusual Ductility

Barbee discovered an unusually ductile, high-strength nanolaminate by layering copper (Cu) with an alloy of copper and zirconium (CuZr). The Cu layer is nanocrystalline, with carefully ordered atoms in fine grains only a few atoms across. The atoms in the alloy layer have no order, resulting in an amorphous solid, similar to common window glass. Zirconium, often used in alloys, is soft, malleable, and highly resistant to corrosion. The Cu–CuZr laminate possesses significantly higher tensile strength than nanocrystalline copper. The thin, amorphous, atomically engineered metallic glass layers are highly ductile and plastic, deforming in conformity with the thicker copper layers and stretching considerably without fracturing.

Bulk metallic glasses such as window glass are brittle at room temperature. Likewise, most nanoscale microstructural materials easily crack under stress. Since the discovery of the highly ductile nanolaminate, various team members have explored the mechanical properties of this unusual material.

Using transmission electron microscopy (TEM) and subjecting a sample to various tensile strains, scientists can "watch" the microstructures change and see where dislocations and voids between grains of materials appear in the Cu–CuZr. Today, materials scientist Morris Wang, also of the Physical and Life Sciences Directorate, is collaborating with Barbee to determine why Cu–CuZr is so ductile. This past summer, *Nanotech Briefs* honored Wang with a 2008 Nano 50 Award for his work, part of which is with nanolaminates. The annual competition, held for the first time in 2005, recognizes the top 50 technologies, products, and innovators that have significantly advanced nanotechnology.

In the Cu–CuZr research, Wang tested amorphous layers ranging from 3 to 15 nanometers thick, with crystalline layers from 5 to 100 nanometers thick. Wang and Barbee's results, combined with molecular dynamics simulations by Ju Li of Ohio State University, indicate that the interfaces between the many layers are the key to the material's unusual ductility. Dislocations start at one interface, travel across a crystalline copper layer, and are absorbed at the next interface. TEM experiments also revealed that the tensile elongation occurs earlier in the amorphous CuZr at lower stress levels than in crystalline–crystalline multilayers. The interfaces are again critical for absorbing the dislocations, with all amorphous layers remaining intact during stress and strain tests.

A New Way to Join

A different collection of nanolaminate materials is helping things to explode in small ways—to fuse materials together—and in large ways—to detonate nonnuclear, conventional weapons. These nanolaminates, called energetic

Building a Better Nanolaminate

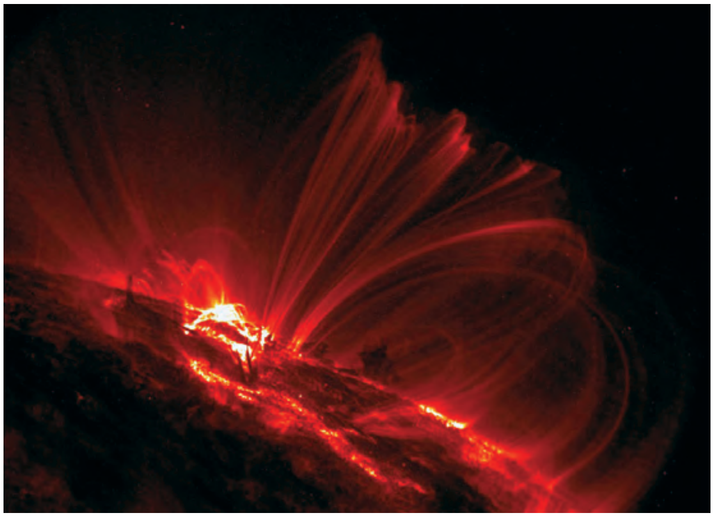
A multilayer, or nanolaminate, is a dense, ultrafine-grained solid composed of thousands of nanometer-scale layers. Each layer's thickness, composition, and structure are carefully controlled. On a substrate, such as silicon dioxide, the layers are laid down in a vacuum, leaving no opportunity for surface oxidation.

A multilayer product is typically synthesized using atom-by-atom processes such as molecular beam epitaxy, thermal physical evaporation, sputter deposition, chemical vapor deposition, and electrochemical technologies. The overall scale of the finished nanolaminate is determined during synthesis by controlling the thickness of the individual layers.

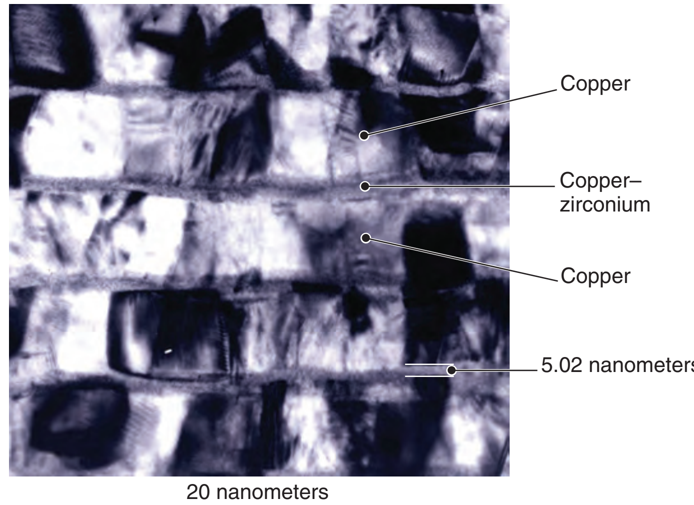
Livermore's primary method of building a nanolaminate is magnetron sputtering, a process developed by Laboratory materials scientist Troy Barbee for nanolaminate synthesis. In magnetron sputtering, a material is bombarded with electrically charged particles. Some of the material's atoms are knocked loose and travel to the item being coated, where atomic bonding forms a stable coating. Nanolaminates may have only 2 layers or as many as 200,000. Barbee, who leads the Laboratory's multilayer effort, says his team has synthesized nanolaminates from 80 of the 92 naturally occurring elements in elemental form, as alloys, or as compounds.

According to Livermore physicist Chris Walton, magnetron sputtering works extremely well, but it is slow and expensive. At the industrial level, large-scale roll coaters can be used for some nanolaminate applications, such as antireflective coatings and metallization. The high cost of most nanolaminates limits their use to critical, high-end applications or to small parts.

Walton leads a team that is modeling magnetron sputter deposition in support of Livermore's programmatic research. "We need to get on top of the physics," he says. The goal is to develop more precise models about crucial physical processes, which could be used to optimize the sputtering process. Faster deposition and lower costs would benefit all thin-film development efforts.



TRACE is acquiring data for research on the Sun's corona and other plasma formations. (Courtesy of TRACE, Stanford–Lockheed Institute for Space Research, and NASA Small Explorer Program.)



An unusually ductile nanolaminate is made by layering crystalline copper and the amorphous, unordered material copper–zirconium.

materials, store chemical energy in the same manner as rocket fuel, explosives of all kinds, and pyrotechnic products. Two or more nonexplosive solid materials are combined in layered form, remaining inert until activated by a mechanical thump, an electrical zap, or a scratch of friction.

Barbee and his postdoctoral researcher Timothy Weihs addressed the question of how or why energetic nanolaminates have such unique properties. As a result of their broad-ranging, systematic experiments, they developed a substantial advance in understanding the relationship between nanolayering and energetic response. Their research showed that materials in nanometer form, layered or not, would have this energetic property. Inherent in this understanding is the ability to relate the amount of stored potential energy, the scale of the material, and the rate of reaction and energy release in a quantitative, though parametric manner.

Weihs has since joined the faculty of Johns Hopkins University. In 2001, he and another Johns Hopkins faculty member founded Reactive NanoTechnologies, Inc., (RNT) in Hunts Valley, Maryland. Barbee and RNT won an R&D 100 Award in 2005 for NanoFoil®, the patented reactive nanolaminate developed in the Livermore–RNT collaboration. The same year, RNT received a Nano 50 Award for the material.

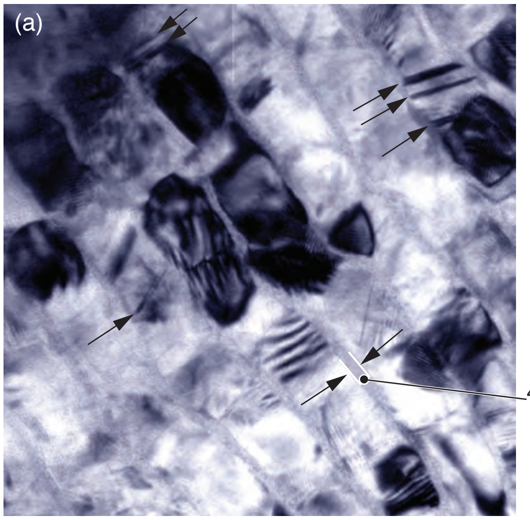
NanoFoil can be used to bond metals, ceramics, semiconductors, and polymers. It can replace lead-based soldering, which causes collateral damage to parts and is potentially toxic, and epoxies, which tend to degrade over time. With NanoFoil, a heat sink can easily be attached directly to a computer chip to conduct heat away from the chip.

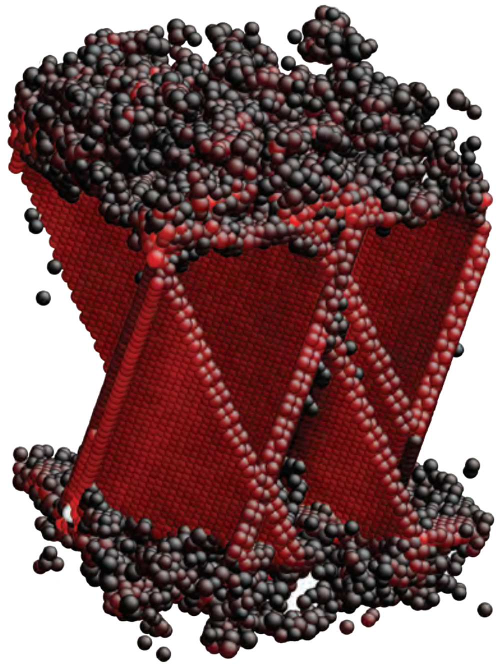
Today, RNT is bonding sputtering targets for companies that manufacture integrated circuitry, data storage devices, photovoltaic cells, and flat-panel displays. Says Weihs, "Since we make the bonding foil by sputtering, it's an interesting twist."

Packing Heat

Reactive nanolaminates are also being used in new warfare technologies. For example, RNT and Livermore worked with the U.S. military to develop materials that burn with the same heat signature as helicopters, which fly close to the ground and are often in harm's way. A nanolaminate decoy could distract a heat-seeking missile and save the helicopter and its occupants. The lightweight decoy would flutter in the air, staying aloft for a time rather than immediately plummeting to Earth.

In a detonator project, a Livermore team proposed using nanolaminate materials for the U.S. Strategic Environmental Research and Development Program, which is managed jointly by the Departments of Energy and Defense and the Environmental Protection Agency. "The project was part of the government's goal to 'green' the arsenal," says Laboratory chemist Alex Gash. In addition to Barbee and Gash, the Livermore team included solgel expert Joe Satcher from the Physical and Life Sciences Directorate and Randy Simpson, who along with Gash works in the Laboratory's Energetic Materials Center. The center conducts research on the performance of high explosives not only for the nuclear weapons program but also for advanced conventional weapons, rocket and gun propellants, homeland security,





(a) Under increasing strains, the Cu–CuZr nanolaminate shows streaks where deformation has occurred in the nanocrystalline copper layers. Despite the strain, the overall structure demonstrates its ductility by remaining intact. (b) Modeling reveals the sliding that occurs across the amorphous layers, which keeps the structure intact under strain.

demilitarization, and industrial uses of energetic materials.

The team's objective was to develop an environmentally safe stab detonator for medium-caliber (20- to 60-millimeter) munitions. Stab detonators, which are activated by a mechanical stimulus, ignite to detonate the main charge. The primer mix in conventional stab detonators contains two forms of lead and other highly toxic substances that pose a danger during manufacture and after detonation. In addition, some primer constituents are no longer made, so substitutes are needed.

The Livermore team developed an energetic nickel–aluminum nanolaminate that serves as the mechanically sensitive igniter for the energetic explosives in conventional munitions. Sensitivity can be enhanced with an energetic nanolaminate, which is environmentally safe yet fully functional as an igniter.

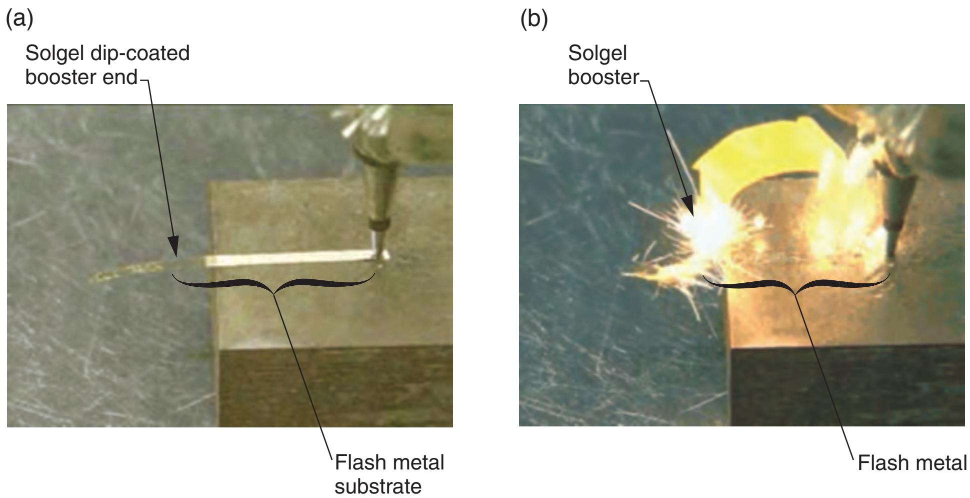
"By varying the layer thickness, we can modify the ignition sensitivity and the reaction speed," says Gash. A slower reaction could be used in a delay mechanism, similar to the device that keeps a parachute closed until a pilot is ejected from a plane. Specialized reactive nanolaminates with a delay mechanism may someday be used in commercial technologies, but at this time, the materials are too expensive for widespread application.

"Most energetic nanocomposites are powders whose combustion is difficult to control," says Gash, who also received a 2008 Nano 50 Award. In addition, most energetic nanocomposites do not age well because they are made of materials that readily oxidize in air. "With nanolaminates, the layers are self-contained, so they aren't as exposed to oxygen in the air," says Gash. "These materials also allow us to control the total energy output as well as the ignition conditions." Controlling the reaction is easily achieved by manufacturing the multilayer with specific layer thicknesses.

Barbee and others have explored many combinations of common elements for various weapons-related projects. For example, hafnium or zirconium layered with carbon may produce reaction temperatures well above 3,000 kelvins, perhaps even reaching 4,100 kelvins. "For all we know about nanolaminates, there is still a lot we don't understand," says Barbee. "Our experience in nanolaminate research has taught us to expect the unexpected."

Storing Energy

Livermore's Industrial Partnerships Office is marketing a commercial license for a nanolaminate fabrication process that can be used to create high-performance dielectric layers. With the Laboratory's Gary Johnson and Andrew Wagner, who is now at PPG Industries' Glass Technology Center, Barbee maximized the energy storage of the capacitor's dielectric layer while minimizing the capacitor's size. The team received initial funding from the U.S. government-sponsored Partnership for a New Generation of Vehicles. "The idea then was to use the capacitor in electric cars," says Barbee. Later, the Departments



In one Livermore project, researchers replaced the toxic materials typically found in the primers of munitions igniters with an environmentally friendly solgel material. (a) A nickel–aluminum reactive nanolaminate is dip-coated with the solgel booster. (b) A light spring-loaded punch activates the nickel–aluminum reaction, which in turn ignites the solgel booster.

of Energy and Defense funded research to adapt the capacitors for added reliability to nuclear weapons in the stockpile.

The prototype capacitor is 4 centimeters square and 1 millimeter thick and packs 50 joules per cubic centimeter of dielectric energy density. The goal is to develop a device no more than 1 centimeter on a side and half as thick as the prototype. These miniature capacitors could be used in power electronics control circuitry, automotive control systems, telecommunications, computers, radar systems, and other pulsed radio-frequency applications.

"Thirty years ago, the first nanolaminate pair I fabricated, niobium–copper, was designed for studying physical properties," says Barbee. "Today, that same material is being tested at Los Alamos [National Laboratory] as a radiation-damage-resistant material for use in future nuclear and fusion energy systems."

Who knows where a Livermore nanolaminate might turn up next. "Troy is amazing," says Weihs. "He just keeps going and going with lots of great ideas. In fact, I'd say he has more ideas than he can handle."

—Katie Walter

Key Words: energetic materials, extreme ultraviolet lithography (EUVL), magnetron sputter deposition, multilayers, nanolaminates, reactive materials.

For further information contact Troy Barbee (925) 423-7796 (barbee2@llnl.gov).

Predicting the Bizarre Properties of Plutonium

PLUTONIUM is arguably the most complex element known, and it is one of the least well understood. Before it liquefies, plutonium exhibits six solid material phases that vary considerably in density. Plus, a seventh phase may appear when the radioactive metal is under pressure.

To understand material phases, think of carbon and its most common solid phases: soft graphite and hard diamond. Both are made of carbon atoms, but the bonds that form between the atoms create two very different materials. Many elements have two or more solid phases, but most have no more than four. With six phases, solid plutonium is highly unusual.

The material's peculiarities do not stop there. Experiments over the years have demonstrated other anomalous properties, including an almost complete absence of magnetism and highly unusual resistivity.

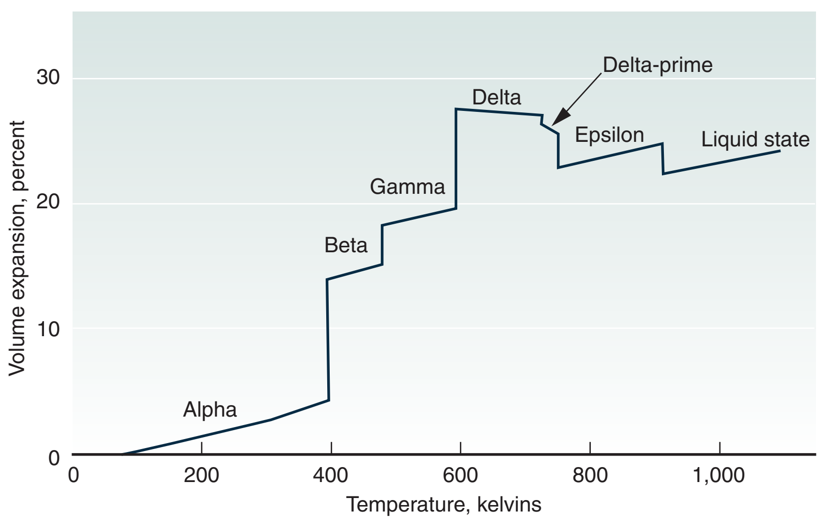
Solid plutonium is most malleable in the delta phase. People who work with plutonium—fabricating pits for nuclear weapons, for instance—use it in this phase. However, the delta phase of pure plutonium is stable only between 500 and 700 kelvins, well above the 300 kelvins of room temperature. Decades ago, weapons researchers discovered that plutonium would remain in a stable delta phase at room temperature when it is mixed with a small amount of gallium or certain other elements.

The Power of Atlas

In an effort to explain some of plutonium's strange behavior and better understand results from past experiments, a team of Lawrence Livermore scientists and international collaborators used the Laboratory's Atlas supercomputer to perform some of the most precise predictions yet of delta-phase plutonium. For these simulations, the team combined density functional theory (DFT) and dynamical mean field theory (DMFT) to calculate plutonium's delta-phase electronic structure, specifically its lack of magnetic "susceptibility."

All atoms have one or more electrons spinning around a nucleus in orbits called shells. Plutonium is one of several materials with electrons in a very narrow shell called 5*f*. The shell is so narrow and the influence of each electron on the others in the shell is so strong that no single electron can be treated independently. As a result, electron behavior in the 5*f* shell is "strongly correlated." Other strongly correlated substances include iron, nickel, many oxides, and high-temperature superconducting materials. Small changes in their control parameters often result in disproportionately large responses.

While DFT is useful for explaining the energy and interactions of many electronic systems, it may break down for certain properties of strongly correlated systems. Previous research combining the

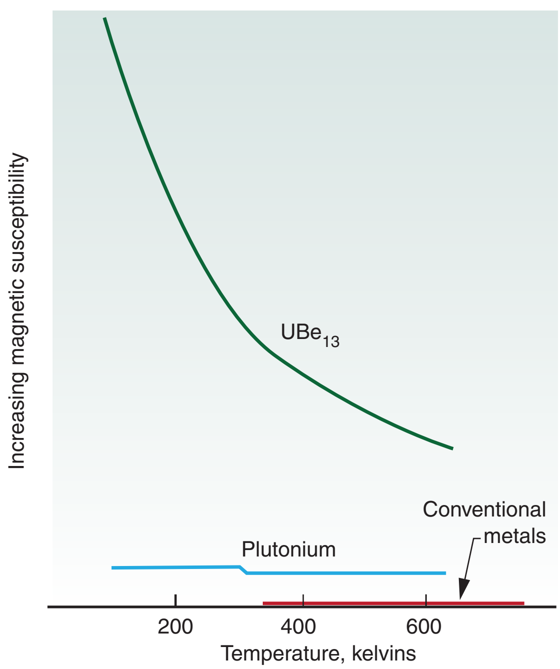


As temperature increases, plutonium's volume changes dramatically before it becomes a liquid. The radioactive metal is unique among elements in exhibiting six solid phases at ambient pressure.

two theories to simulate delta-phase plutonium could obtain only approximate solutions to the DMFT equations. Recent advances in the continuous-time quantum Monte Carlo method—and the Atlas computer—allowed exact solutions for the first time.

"This work would have been impossible without Atlas," says physicist Chris Marianetti, who led the computational effort. Atlas can process 44-trillion floating-point operations per second and is one of the Laboratory's workhorses for high-end, unclassified computing. This project was one of 17 Computing Grand Challenge initiatives selected in 2007 and was funded by Livermore's Laboratory Directed Research and Development (LDRD) Program.

"We used DMFT to treat plutonium's 5*f* electrons and DFT for electrons in the other shells," says Marianetti. He worked with the same combination of theories in his Ph.D. research at the Massachusetts Institute of Technology, where he studied the electronic correlations in cobalt oxide, one of the materials inside rechargeable batteries for cell phones, MP3 players, and other electronic devices.



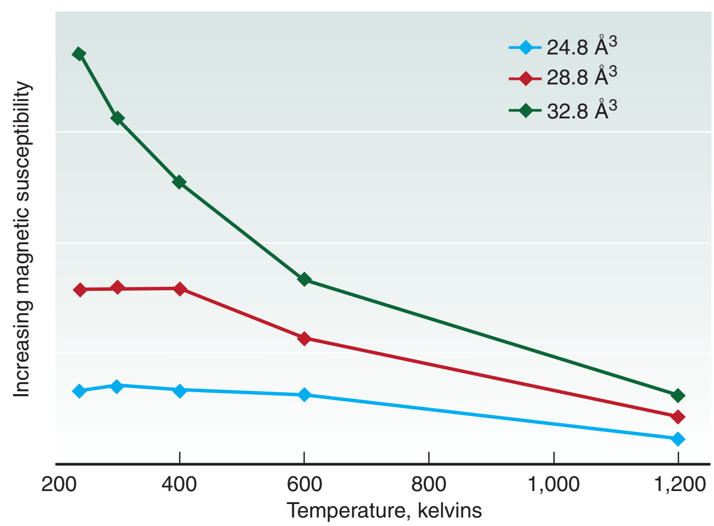
The magnetic susceptibility of plutonium is unusual. For conventional metals such as molybdenum, titanium, and platinum, magnetism does not change with temperature (red curve). Strongly correlated materials, however, are more magnetic at low temperatures than they are at higher temperatures. The green curve shown for uranium–beryllium-13 (UBe_{13}) is typical. Plutonium's magnetic susceptibility (blue curve) lies between these cases.

Unusual Magnetic Attraction

In DMFT simulations, one atom is ripped from a lattice of atoms and put in a "bath" of fictitious electrons whose properties duplicate the average properties of the lattice. With a large lattice reduced to an averaged, single-site problem, DMFT can calculate the electronic structure for the entire strongly correlated lattice.

The grand-challenge team's simulations predicted that at room temperature with delta-phase plutonium at its equilibrium volume, the *f* electrons are delocalized. That is, they easily move about the lattice and are not associated with one particular atom. Under these conditions, the material's magnetic susceptibility is very low above 600 kelvins and only slightly higher at lower temperatures.

A change in temperature does not affect the magnetism of conventional metals such as platinum or molybdenum. In contrast, most strongly correlated materials other than plutonium exhibit a distinct relationship between temperature and magnetic susceptibility. Their magnetic susceptibility is high at low temperatures and lower at high temperatures. Experiments demonstrate, however, that plutonium's magnetic susceptibility is unlike that of other strongly correlated materials. In fact, it behaves more like a conventional metal, although it exhibits slight temperature dependence.



In the Livermore simulations, the volume of plutonium was increased, pulling the plutonium atoms farther apart. Only under these circumstances and at the largest volume does plutonium's magnetic susceptibility begin to mimic the temperature dependence of other strongly correlated materials such as UBe_{13}. (Å^3 = cubic angstroms, where 1 Å^3 equals 1×10^{-30} cubic meters.)

If the plutonium volume is expanded—if the lattice is stretched so that the *f* electrons are farther apart—the magnetic susceptibility of plutonium changes. The Livermore simulations showed that as the lattice expands, the *f* electrons become heavier, or localized. That is, they are more associated with one particular atom and thus cannot easily hop through the lattice. The plutonium is then a more strongly correlated material. The transition from delocalized to localized behavior occurs at increasingly lower temperatures as the lattice volume continues to expand. With greater distance between the electrons, delta-phase plutonium begins to behave more like other strongly correlated materials. As temperature drops, the metal's magnetic susceptibility increases.

Future Phases

The team intends to tackle plutonium's alpha phase next. Marianetti will continue to lead this simulation effort, but he will do so from afar. He was a postdoctoral researcher at the Laboratory until August 2008, when he joined the faculty of Columbia University. Livermore physicist Mike Fluss, who leads a larger LDRD project that includes the plutonium DMFT simulations, notes that Marianetti's expertise with DMFT is unique. "I look forward to a strong collaboration with Chris well into the future," says Fluss.

Predicting the behavior of alpha-phase plutonium will be more challenging than the delta-phase simulations. The smallest individual crystal in delta-phase plutonium contains one atom. In the alpha phase, 16 atoms make up the smallest crystal. Another challenge will be to explain the role that other materials play in stabilizing delta-phase plutonium. Only with the aid of powerful supercomputers can researchers answer plutonium's many riddles.

—Katie Walter

Key Words: Atlas supercomputer, Computing Grand Challenge Program, delta phase, density functional theory (DFT), dynamical mean field theory (DMFT), plutonium.

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The plutonium grand challenge research was conducted on Livermore's Atlas supercomputer, which has a peak operating speed of 44-trillion floating-point operations per second.

Each issue 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

Compact X-Ray Source and Panel
Stephen E. Sampayan
U.S. Patent 7,330,533 B2
February 12, 2008
For this compact, self-contained x-ray source and panel, multiple x-ray sources are arranged in a broad-area pixelized array. Each x-ray source includes an electron source for producing an electron beam, an x-ray conversion target, and a multilayer insulator separating the electron source and conversion target. The cylindrical multilayer insulator has alternating insulator and conductor layers surrounding an acceleration channel that leads from the electron source to the x-ray conversion target. A power source connected to each x-ray source produces an accelerating gradient between the electron source and x-ray conversion target in one or more of the x-ray sources to accelerate an electron beam toward the x-ray conversion target. The multilayer insulator enables relatively short separation distances between the electron source and the conversion target so that a thin panel is possible for compactness. The alternating insulator and conductor layers resist surface flashover when the high acceleration energies needed for x-ray generation are supplied to the x-ray sources.

Nonlinear Optical Crystal Optimized for Ytterbium Laser Host Wavelengths
Christopher A. Ebbers, Kathleen I. Schaffers
U.S. Patent 7,378,042 B2
May 27, 2008
A material for harmonic generation has been made by substitutional changes to the crystal $LaCa_4(BO_3)_3$, also known as LaCOB, in the form $Re1_xRe2_yRe3_zCa_4(BO_3)_3O$. Re1 and Re2, rare-earth ions 1 and 2, are selected from the group consisting of strontium, yttrium, lanthanum, cerium, praseodymium, neodymium, samarium, europium, gadolinium, thorium, dysprosium, holmium, erbium, thulium, ytterbium, and lutetium; Re3 is lanthanum; and $x + y + z = 1$.

Miniature Modified Faraday Cup for Micro Electron Beams
Alan T. Teruya, John W. Elmer, Todd A. Palmer, Chris C. Walton
U.S. Patent 7,378,830 B2
May 27, 2008
A microbeam Faraday cup assembly includes a refractory metal layer with an odd number of thin, radially positioned traces. Traces are located at the edge and center of the modified Faraday cup body. Each set of traces is connected to a separate data-acquisition channel to form multiple independent diagnostic networks. The data obtained from the networks are combined and input into a computed tomography algorithm to reconstruct the beam shape, size, and power-density distribution.

Digital Intermediate Frequency QAM Modulator Using Parallel Processing
Hsueh-Yuan Pao, Binh-Nien Tran
U.S. Patent 7,379,509 B2
May 27, 2008
This digital intermediate-frequency (IF) modulator applies to various modulation types and offers a simple, low-cost method to implement a high-speed digital IF modulator using field-programmable gate arrays. The architecture eliminates multipliers and sequential processing by storing the precomputed modulated cosine and sine carriers in read-only-memory look-up tables. The high-speed input data stream is parallel processed using the corresponding tables. This approach reduces the main processing speed, allowing the use of low-cost gate arrays.

Position Estimation of Transceivers in Communication Networks
Claudia A. Kent, Farid Dowla
U.S. Patent 7,383,053 B2
June 3, 2008
This system uses wireless communication interfaces and statistical processing of time-of-flight data to locate unknown wireless receivers using position estimation. The system can be applied in sensor network applications, such as monitoring water in the soil or chemicals in the air, where the position of the network nodes is deemed critical. Moreover, it can operate in areas where a global positioning system is unavailable, such as inside buildings, caves, and tunnels.

Solid Materials for Removing Arsenic and Method Thereof
Paul R. Coronado, Sabre J. Coleman, Robert D. Sanner, Victoria L. Dias, John G. Reynolds
U.S. Patent 7,393,810 B2
July 1, 2008
Solid materials have been developed to remove arsenic compounds from aqueous media. The arsenic is removed by passing the aqueous phase through the solids, which can be in molded, granular, or powder form. The solid materials adsorb the arsenic, leaving a purified aqueous stream. The materials are aerogels, xerogels and aerogels, or xerogels and solid support structures such as granulated activated-carbon mixtures. The species-specific adsorption occurs through specific chemical modifications of the solids tailored toward arsenic.

Energy Harvesting Using a Thermoelectric Material
Nersesse Nersessian, Gregory P. Carman, Harry B. Radousky
U.S. Patent 7,397,169 B2
July 8, 2008
This energy harvesting system uses a thermoelectric made of a material exhibiting a large thermally induced strain from a phase transformation and a material exhibiting a stress-induced electric field. A material with such a phase transformation will have a large increase in the coefficient of thermal expansion over an incremental temperature range (typically several kelvins). When the material is arranged in a geometric configuration—for example, a laminate with a material that exhibits a stress-induced electric field, such as a piezoelectric material—the thermally induced strain is converted to an electric field.

Aerogel and Xerogel Composites for Use as Carbon Anodes
John F. Cooper, Thomas M. Tillotson, Lawrence W. Hrubesh
U.S. Patent 7,410,718 B2
August 12, 2008
These aerogel and xerogel composite materials are suitable as anodes in fuel cells and batteries. Precursors to the aerogel and xerogel compounds are infused with inorganic polymeric materials or carbon particles and then gelled. The gels are then pyrolyzed to form composites with internal structural support.

3D Wavelet-Based Filter and Method
William C. Moss, Sebastian Haase, John W. Sedat
U.S. Patent 7,412,103 B2
August 12, 2008
This three-dimensional (3D), wavelet-based filter visualizes and locates structural features of a user-specified linear size in two- and three-dimensional image data. The only input parameter is the characteristic linear size of the feature, and the filter output contains only those regions that are correlated with the characteristic size, thus reducing noise in the image.

Detection and Quantification System for Monitoring Instruments
John M. Dzenitis, Claudia K. Hertzog, Anthony J. Makarewicz, Bruce D. Henderer, Vincent J. Riot
U.S. Patent 7,412,356 B1
August 12, 2008
This event detection method obtains a set of recent signal results and calculates the noise or variation and an expected baseline value. Next, it determines sample deviation, calculates an allowable deviation by multiplying the sample deviation by a threshold factor, and sets an alarm threshold from the baseline value plus or minus the allowable deviation. It then determines whether signal results exceed the alarm threshold.

System for Dispensing a Precise Amount of Fluid
William J. Benett, Peter A. Krulevitch, Steven R. Visuri, John M. Dzenitis, Kevin D. Ness
U.S. Patent 7,413,711 B2
August 19, 2008
This dispensing system delivers a precise amount of fluid for biological or chemical processing and analysis. A dispensing device operated by a pneumatic force moves the liquid, and a connection device delivers the fluid to the desired location. An actuator provides the pneumatic force to the dispensing device. A valving device transmits the pneumatic force from the actuator to the dispensing device.

Synthesis of Peptide α-Thioesters
Julio A. Camarero, Alexander R. Mitchell, James J. De Yoreo
U.S. Patent 7,414,106 B2
August 19, 2008
This method for solid-phase peptide synthesis of C-terminal peptide α-thioesters uses Fmoc/t-Bu chemistry and an aryl hydrazine linker that is stable under the required conditions. When peptide synthesis is complete, mild oxidation activates the linker. The oxidation step converts the acyl-hydrazine group into a highly reactive acyl-diazene intermediate that reacts with an α-amino acid alkylthioester (H-AA-SR) to produce the corresponding peptide α-thioester in good yield. Various peptide thioesters and cyclic peptides and a fully functional Src homology 3 (SH3) protein domain were prepared using this method.

Imaging Spectrometer Wide Field Catadioptric Design
Michael P. Chrisp
U.S. Patent 7,414,719 B2
August 19, 2008
This wide-field catadioptric imaging spectrometer with an immersive diffraction grating compensates optical distortions. The catadioptric design has zero Petzval field curvature. The imaging spectrometer comprises an entrance slit for transmitting light, a system with a catadioptric lens and a dioptric lens for receiving and directing the light, an immersion grating, and a detector array. The entrance slit transmits light to a light-receiving system that directs the light to the immersion grating. The immersion grating receives the light and directs it back through the light-receiving system to the detector array.

Method of Fabrication of High Power Density Solid Oxide Fuel Cells
Ai Quoc Pham, Robert S. Glass
U.S. Patent 7,422,766 B2
September 9, 2008
This method produces ultrahigh-power-density solid-oxide fuel cells (SOFCs). A colloidal spray-deposition technique is used to form multilayer structure cells wherein a buffer layer of doped ceria is deposited between a zirconia electrolyte and a cobalt iron–based electrode. For example, a cobalt iron–based cathode composed of (lanthanum, strontium) (cobalt, iron)oxygen may be deposited on a zirconia electrolyte via a buffer layer of doped ceria. The thus-formed SOFCs have a power density of 1,400 milliwatts per square centimeter at 6,000°C and 900 milliwatts per square centimeter at 7,000°C, which is a power density two to three times greater than that in conventionally produced SOFCs.

Acoustic System for Communication in Pipelines
Louis Peter Martin II, John F. Cooper
U.S. Patent 7,423,931 B2
September 9, 2008
In this system for communicating in a pipe, pipeline, or network of pipes containing a fluid, an encoding and transmitting subsystem transmits a signal in the frequency range of 3 to 100 kilohertz. A receiver and processor subsystem receives the signal and uses it for a desired application.

Spectroscopic Feedback for High Density Data Storage and Micromachining
Christopher W. Carr, Stavros Demos, Michael D. Feit, Alexander M. Rubenchik
U.S. Patent 7,426,028 B2
September 16, 2008
Optical breakdown by laser pulses in transparent dielectrics produces an ionized region of dense plasma confined within the bulk of the material. Such an ionized region is responsible for broadband radiation that accompanies a desired breakdown process. Spectroscopic monitoring of the accompanying light is used to determine the morphology of the radiated interaction volume. This method provides a commercial approach for rapid prototyping of optoelectronic devices, optical three-dimensional data storage devices, and waveguide writing.

Awards

Computer scientist **Steve Suppe** was awarded a **Fulbright Student Grant** to study at the University of Haifa in Israel. Sponsored by the **State Department**, the Fulbright Program provides students, scholars, and career professionals access to graduate study, advanced research, and teaching opportunities at institutions around the world. Suppe, who works in Global Security's Computing Application Division, will work in conjunction with IBM Research Labs, also in Haifa.

Livermore retiree **Charlie Westbrook** of the Physical and Life Sciences Directorate received the **Bernard Lewis Gold Medal** from the **Combustion Institute**. Westbrook was honored "For brilliant research in the field of combustion, particularly on the pioneering development of detailed chemical kinetic mechanisms for use in practical applications." Founded in 1954 by Lewis, the Combustion Institute promotes and disseminates research on combustion science.

The **Department of Energy's Office of Science Office of Advanced Scientific Computing Research** (OASCR) gave an **OASCR** (pronounced Oscar) award to **Dave Eder** and the **Facility Modeling Group** of the National Ignition Facility (NIF) and Photon Science Principal Directorate. OASCR awards are presented for research visualizations either directly funded by the Office of Science or created on tools provided by that office.

Eder's group is working on issues related to electromagnetic pulses that result from extremely short but very high-energy laser bursts, such as those that will be created inside the NIF target chamber. The group's visualization, made with the Laboratory's VisIt software, shows a burst of electrons coming off a laser target after it is hit by a short-pulse laser. The experiment was designed to determine the best placement and shielding of diagnostic instruments located inside or near laser chambers.

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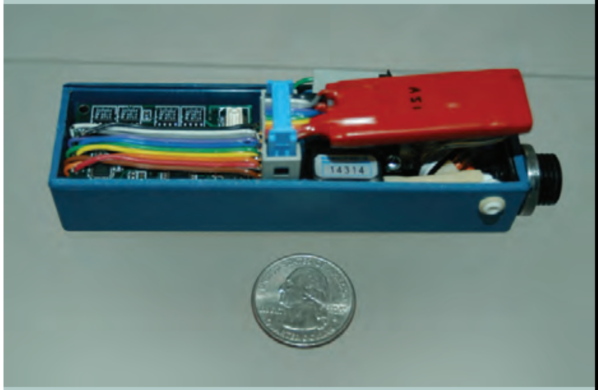
Atom by Atom, Layer by Layer

By carefully combining various elements and layer thicknesses, researchers can atomically engineer multilayers, or nanolaminates, to almost any specification. These "designer" materials may be extremely strong; highly reflective; unusually ductile; or exceptionally resistant to heat, wear, and corrosion. They may even incorporate all of those properties at the same time. For example, many space-based solar astrophysics mirrors incorporate highly reflective multilayer coatings for viewing the Sun's corona in the x-ray and extreme ultraviolet wavelengths. In addition, a layered foil that releases heat energy in a controlled manner can be used to bond dissimilar materials without damaging them. Igniters and detonators for new weapon technologies are also being developed with reactive nanolaminates. In fact, Livermore researchers found that, by varying the thickness of the nanolaminate layers, they can modify the ignition sensitivity and speed of the reaction. Today, a nanolaminate miniature capacitor is adding reliability to nuclear weapons in the stockpile.

Contact: Troy Barbee (925) 423-7796 (barbee2@llnl.gov).

U.S. Government Printing Office: 2008/570-075-71008

"Smoke Detectors" for Chemicals



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

Also in January/February

• A Computing Grand Challenge project performed on Livermore's Atlas supercomputer explains results of earlier high-energy-density experiments.

• Livermore x-ray diffraction experiments reveal the ultrafast dynamics of a nanoscale solid structure as it evolves over picosecond timescales.

• Working in the extreme conditions at an Antarctica base camp provides one Laboratory manager with important lessons in safety and environmental stewardship.

Coming Next Issue

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