Science & Technology REVIEW

November 2005

National Nuclear Security Administration's Lawrence Livermore National Laboratory

Unlocking the Secrets of Metal Hardening

Also in this issue:

- Digital Imaging of Deep Space
- New Applications for Graphics Processors
- Revised Calculations for Plasma Densities

About the Cover

As the article beginning on p. 4 describes, Livermore scientists are combining advances in supercomputing and materials experiments to shed light on dislocation dynamics and how materials deform and fail. Dislocation dynamics—the interaction among dislocation lines—is believed to be responsible for strain hardening, a property of metals in which a material's strength increases as deformation increases. The cover shows a dislocation dynamics simulation of strain hardening in body-centered-cubic molybdenum.

Cover design: Daniel Moore

About the Review

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

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National Nuclear Security Administration

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Science & Technology REVIEW

November 2005

Lawrence Livermore National Laboratory

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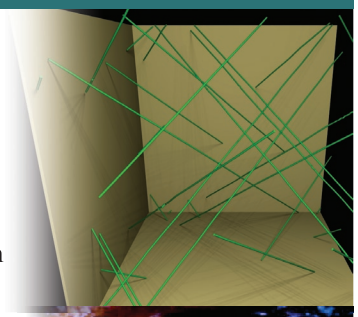

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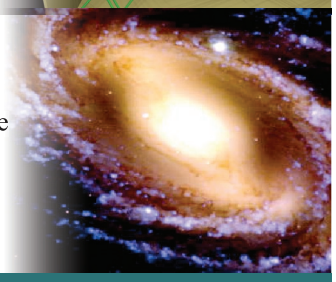

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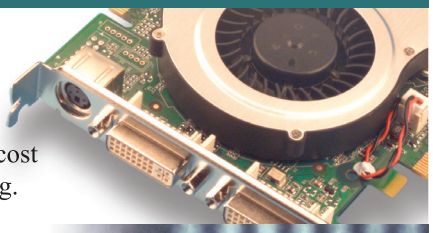

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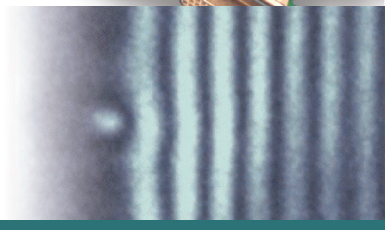

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Laser energy milestone is surpassed

In August 2005, the National Ignition Facility (NIF) fired shots that achieved energy output surpassing the highest levels ever reached on Livermore's now-deactivated Nova laser or on the 60-beam OMEGA laser at the University of Rochester's Laboratory for Laser Energetics.

NIF recently commissioned its second quad, which is a group of four beams. The combined output from the eight beams, known as a bundle, totaled 152 kilojoules, surpassing NIF's main laser operational bundle goal of 125 kilojoules. The energy, in the form of infrared light, was measured by an instrument called a calorimeter. This and other diagnostics showed that beam quality, as well as total energy, exceeded design specifications.

The program is now transitioning from its NIF Early Light phase and preparing for ignition experiments scheduled to begin in 2010. When complete, NIF will consist of 192 laser beams, with a total energy capability of 1.8 megajoules. Operating with its current eight beams, NIF is already the world's largest and most energetic laser system.

Contact: Ed Moses (925) 423-9624 (moses1@llnl.gov).

Tech transfer contributes to new portable fuel cell

Fuel-cell technology developed at the Laboratory and transferred to UltraCell Corporation of Livermore has led to the development of a portable fuel cell that could power a laptop computer for an entire day without recharging. The company's reformed methanol fuel cell is based in part on microreformer and micro-fuel-cell technology developed at Livermore and licensed to UltraCell in 2002.

According to UltraCell, its new fuel cell has twice the energy density of standard lithium batteries and can provide continuous power at remote locations. Users can swap out the methanol fuel canisters for fresh fuel while the computer is in use. The compact fuel reformer efficiently converts methanol fuel to hydrogen. Jim Kaschmitter, chief executive officer of UltraCell, credited key advances by the company, the Laboratory, and other partners for the breakthrough in fuel-reformer technology.

UltraCell has an exclusive licensing agreement with Livermore for using microelectromechanical systems (MEMS) microreformer and micro-fuel-cell technology developed by Jeff Morse and his team in the Engineering Directorate's Center for Micro and Nano Technology.

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Modeled and observed climate data agree

Three papers published in the August 11, 2005, edition of *Science Express* provide new insight on the global warming debate. The first two studies revisit temperature data obtained from satellites and weather balloons and provide compelling evidence that the tropical troposphere has warmed since 1979. The third study, led by Benjamin Santer in the Laboratory's Program for Climate Model Diagnosis and Intercomparison, finds that these new observational estimates of temperature change are consistent with results from current climate models.

The computer models used in the Livermore-led study show that in the deep tropics, temperature changes in the troposphere are larger than at Earth's surface. This amplification effect is caused by the release of heat when moist tropical air rises and condenses into clouds. The size of the amplification effect is very similar in nearly 50 simulations performed with 19 different models. The newly revised observational data described in the first two *Science Express* papers have amplification behavior that is in agreement with the model results and with basic physical theory.

"This strongly suggests that a fundamental discrepancy no longer exists between modeled and observed temperature trends in the tropical atmosphere," says Santer. "The new observational data help remove a major stumbling block in our understanding of the nature and causes of climate change. Our work illustrates that progress toward an improved understanding of the climate system requires a combination of observations, theory, and models."

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A Major Advance in Understanding Metals

A principal element of Lawrence Livermore's national security mission is stockpile stewardship, the program to ensure that the nation's nuclear stockpile is safe and reliable. Many of the key components of nuclear warheads are crystalline metals. The fundamental defect governing the mechanical behavior of a crystalline metal is a dislocation line—that is, a displaced row of atoms. The interaction among thousands of dislocation lines, called dislocation dynamics, is the key to a metal's plasticity and strain hardening. Plastic deformations confer strength that is proportional to the number of deformation lines and their entanglements.

For the past decade, Livermore researchers have been developing increasingly realistic three-dimensional simulations of dislocation dynamics because this phenomenon is the missing link in multiscale modeling. Dislocation dynamics lies at the microscale, between atomistic descriptions of materials that incorporate atomic-scale physics and mesoscale and continuum scales that describe the engineering performance of a material component. By understanding how dislocations behave at all scales, we can predict how materials respond under many different conditions and why and how they fail.

As the article beginning on p. 4 describes, a team of Livermore researchers has developed a new code, called Parallel Dislocation Simulator (ParaDiS), that models the behavior of large ensembles of dislocations in unprecedented detail and under a wide range of conditions. The development of ParaDiS is significant because the code will help us to better predict the performance of materials in the stockpile as a function of age and under extreme conditions. In short, ParaDiS allows us, for the first time, to use a strong scientific basis to understand and predict dislocation dynamics performance of crystalline metals.

In developing ParaDiS, we built on two foundations. The first is an improved understanding of the physics of crystalline metals obtained using atomic-scale simulations and laboratory experiments. Our findings were the subject of several papers published in scientific journals over the past few years. This work provided the data about atomistic phenomena used in ParaDiS. The second foundation is the availability of massively parallel supercomputers, such as Livermore's Thunder and BlueGene/L, which use thousands of microprocessors working in tandem. Developing a code to work on these machines was an enormous challenge requiring the combined efforts of Livermore materials scientists, computational scientists, and physicists. Over a period of 4 years, the team, led by materials scientist Vasily Bulatov, worked to produce the world's highest performance dislocation dynamics code—a code based on the physics of dislocation lines that also takes advantage of the latest advances in supercomputers.

The capability of the code was demonstrated in its unexpected discovery of a new type of dislocation microstructure, called a multijunction. Multijunctions are thought to play an essential role in the strength evolution of crystalline metals as they deform. As the article describes, the existence of multijunctions was confirmed in images taken with a transmission electron microscope. We are currently exploring the full practical significance of multijunctions.

ParaDiS will allow us to examine other issues of materials phenomena, especially plasticity, that have been unexplained for decades. In particular, we now have a major new tool for predicting the performance of the aging components in our current nuclear stockpile and for possibly helping to guide the development of advanced materials for the National Nuclear Security Administration's Reliable Replacement Warhead Program. This program is evaluating the feasibility of providing replacements for existing stockpile weapons that are more reliable, less expensive to maintain, and more easily manufactured using readily available and environmentally benign materials.

In addition, we anticipate that ParaDiS will be useful in strengthening America's energy security. For example, it could predict the performance of materials for fission power plants and for magnetic fusion energy and inertial confinement fusion plants. We are confident that other applications will be found for ParaDiS as it becomes adopted throughout the materials science community.

■ Tomás Díaz de la Rubia is associate director of Chemistry and Materials Science.

Materials Scientists Discover the Power of ParaDiS

Livermore researchers have developed a code to better understand dislocation lines and how materials gain strength.

SCIENTISTS know that the strength of most crystalline materials, including metals, derives from the motion, multiplication, and interaction of defects called dislocation lines. Dislocation dynamics—the interaction among dislocation lines—is believed to be responsible for strain hardening, a property of metals in which a material's strength increases as deformation increases. For example, the more one twists and bends a paper clip, the stronger it becomes due to the formation and interaction of dislocation lines.

However, scientists lack a detailed understanding of the mechanisms that confer strength, based on changes to a metal's crystalline microstructure. This knowledge is vital to predicting a metal's performance under extreme conditions, such as in the detonation of a nuclear weapon system. Achieving this knowledge requires obtaining a quantitative understanding of how plastic deformation arises from the dynamics of dislocations. This understanding will help in constructing a comprehensive numerical model that will provide accurate predictions of how materials respond under extreme conditions.

Livermore scientists are providing new insight on dislocation dynamics and how materials deform and fail by combining advances in supercomputing and materials experiments and characterization. The research, funded by the National Nuclear Security Administration's Advanced Simulation and Computing (ASC) Program and Livermore's Laboratory Directed Research and Development (LDRD) Program, involves materials scientists, chemists, physicists, computer scientists, and engineers. Their focus is on body-centered-cubic (bcc) metals, such as molybdenum and tantalum, because these metals are similar to some materials in the nuclear stockpile. In bcc crystals, an atom at the center of a hypothetical cube is surrounded by identical atoms at each corner of the cube. Other types of metals have different repeating arrangements of atoms.

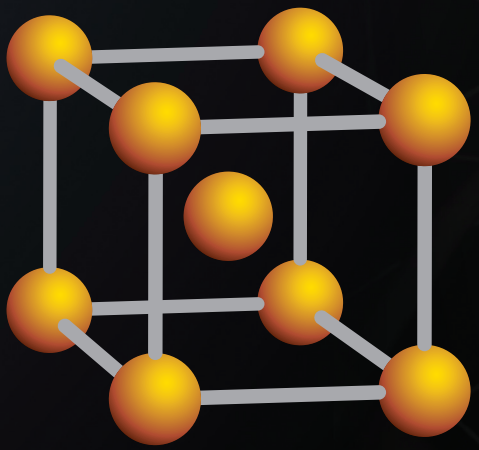
Materials scientist Vasily Bulatov of the Chemistry and Materials Science (C&MS) Directorate has been leading the effort to develop a code, called Parallel Dislocation Simulator (ParaDiS), that models in unprecedented detail the mechanisms of dislocation motion. Bulatov's team includes Gregg Hommes from the Computation Directorate, Moon Rhee from the Engineering Directorate, Meijie Tang from the Physics and Advanced Technologies Directorate, and Masato Hiratani and Tom Arsenlis from C&MS. Wei Cai, an assistant professor from Stanford University, is also on the team. Cai received a 2004 Presidential Early Career Award for Scientists and Engineers for work on ParaDiS while serving as an Ernest O. Lawrence Fellow at Livermore.

The team works closely with engineer Jeff Florando, who is the principal investigator on an LDRD project that conducts complementary experiments on well-characterized, high-purity crystals. Slices from the experimental samples are examined for dislocation microstructures with transmission electron microscopes and are further analyzed at the Advanced Light Source at Lawrence Berkeley National Laboratory. The results form a more complete model of the way crystalline materials behave on the microscale. Together with the ParaDiS simulations, the experiments contribute to multiscale modeling, a process that links data from codes operating on different time and length scales. (See the box on p. 6.)

Modeling Dislocation Evolution

ParaDiS models the evolution of dislocation lines into highly complex microstructures in response to an applied stress. Designed to run on massively parallel supercomputers, ParaDiS allows researchers to follow tens of thousands of simulated dislocations in a 10-micrometer-long cube over several seconds. "Before ParaDiS, the extreme computational cost of dislocation dynamics simulations made it unfeasible to simulate the motion and interactions of many dislocation lines over an adequate amount of time," says Bulatov. ParaDiS can simulate hundreds of times more dislocation lines than other codes. Also, previous codes could only simulate 0.1 percent strain (the change in length of a material under stress). At this point, the number of dislocations begins to grow rapidly. ParaDiS can simulate 3 percent and should be able to simulate far greater strain in updated versions.

The code is available to qualified researchers, who are free to modify it. Fifteen research groups worldwide are



Livermore's ParaDiS code has been used to model simulations in body-centered-cubic crystals, in which an atom at the center of a hypothetical cube is surrounded by identical atoms at each corner of the cube.

efficiently on two of the world's most powerful supercomputers: Livermore's Thunder and Blue Gene/L machines. ParaDiS simulations require at least 500 processors. Today, the code runs on 16,000 of BlueGene/L's 100,000 microprocessors.

The code incorporates a new theory of dislocation that is both mathematically rigorous and analytically simple. The theory is an extension of classical dislocation theory, which provides useful solutions for the behavior of dislocations associated with stress but makes calculations about individual dislocations difficult. ParaDiS removes these

Understanding Materials at Different Length and Time Scales

Materials are at the heart of most issues associated with stockpile stewardship, the National Nuclear Security Administration's program to ensure the safety and reliability of the nation's nuclear weapons. In particular, scientists want to improve their ability to predict the effects of aging on weapon parts or the likely performance of remanufactured parts. Material properties are inherently multiscale, depending on phenomena that occur at all length and time scales. These scales range from a fraction of a nanometer to meters and from nanoseconds to decades.

Multiscale modeling involves a wide array of disciplines and specialists at Livermore from the Engineering, Chemistry and Materials Science, Defense and Nuclear Technologies (DNT), Physics and Advanced Technologies, Energy and Environment, and Computation directorates. Research teams model dislocations at atomistic (nanometers), microscopic (micrometers), and meso (millimeters and above) scales. In multiscale modeling, data are passed from the smallest scale to the next scale up.

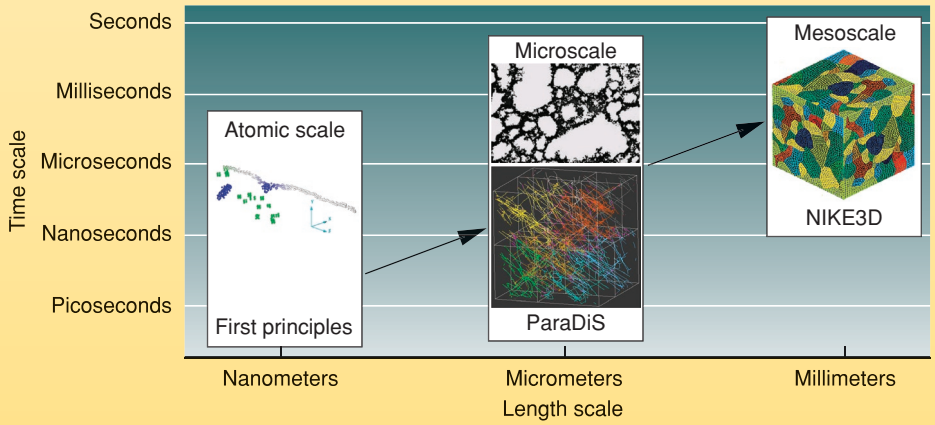
Dislocation activities (the formation, movement, and interaction of dislocation lines of misaligned atoms) occur across a range of length and time scales that must be accounted for to describe crystal plasticity accurately. Although single dislocations and reactions between a few dislocations are controlled by mechanisms at the atomistic scale, dislocations also spontaneously organize themselves into highly complex microstructures over distances of micrometers or longer during plastic deformation. The massively parallel supercomputing resources at Livermore allow researchers to connect all three scales.

Researchers begin with fundamental atomic properties to develop atomistic simulations involving many thousands of atoms. These simulation codes show the movement and interaction of individual dislocations in a perfect crystal under an applied stress.

At the microscale, scientists analyze the motion, multiplication, and interaction of dislocations, a phenomenon called dislocation dynamics. The simulations show the movement and interaction of millions of dislocations and how materials deform plastically—that is, how they change shape without breaking. The most advanced microscale code for dislocations is ParaDiS, developed by a team of Livermore researchers led by materials scientist Vasily Bulatov. By simulating thousands of dislocations and their intersecting behavior, ParaDiS bridges fundamental understanding at the atomic scale and the mesoscale.

In mesoscale modeling, individual crystals and their boundaries are resolved, but individual dislocations are not. At this scale, finite-element simulation codes such as NIKE3D examine how a system composed of multiple single crystals deforms in response to an applied stress.

When complete, comprehensive models of crystalline metals will help stockpile stewardship researchers predict with greater confidence the performance of nuclear weapons and the changes that might occur in the stockpile. In particular, multiscale modeling is important for DNT's metal dynamics research, the National Ignition Facility's target dynamics effort, and the Department of Energy's armor and antiarmor research. Advances in multiscale modeling of crystalline metals also provide data about material behavior that is of interest to industrial manufacturers.



In multiscale modeling, data are passed from the atomistic scale, to the microscopic scale, and on to the mesoscale. Different time scales are also associated with each modeling code.

calculational obstacles to allow simulations of individual dislocation lines.

For the first time, researchers can see how dislocations spontaneously organize into highly complex microstructures over distances of micrometers or greater during plastic deformation. "In a ParaDiS simulation, dislocation lines behave realistically under an applied stress," says Bulatov. "The dislocation lines multiply and move the same as they do in a physical sample. We just sit back and watch the lines advance and obtain a wealth of information."

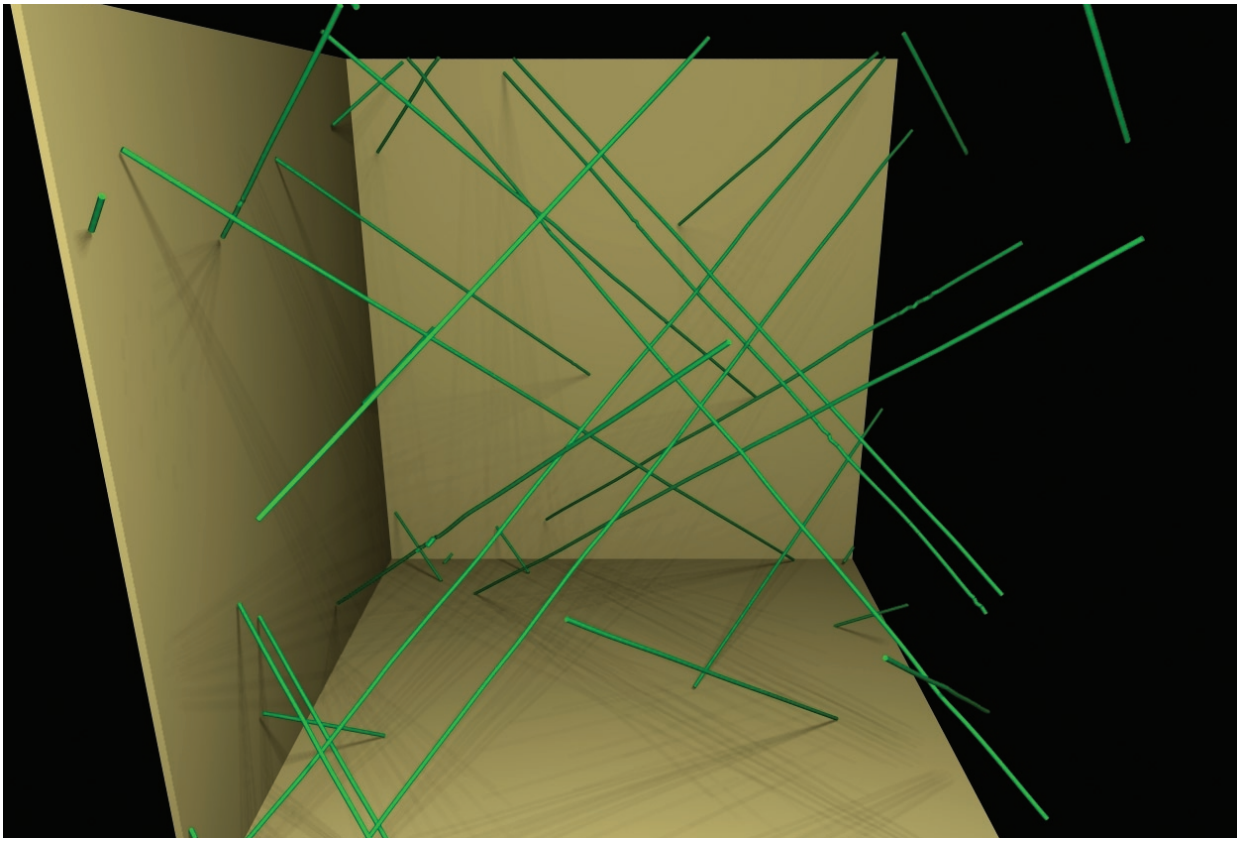
Code's Major Discovery

The power of ParaDiS was recently demonstrated when large-scale simulations revealed a new type of dislocation microstructure, one that current theory did not predict. The simulations showed that collisions among three or more dislocations result in the formation of distinctive elements previously unrecognized, called multijunctions and multinodes. "Multijunctions tie together three or more dislocation lines into a very tight knot," says Bulatov. Multinodes are located at each end of a multijunction. (See the figure on p. 8.)

Bulatov explains that during strain, two colliding dislocations may partially merge, or zip, into a junction bounded by two nodes. Transmission electron micrographs indicated that these binary junctions tie separate dislocation lines, and this process seems to confer strength in metals. The ParaDiS simulations showed that as an applied stress gradually rises, many binary junctions previously formed at a lower stress unzip. However, the multijunctions, being much stronger, endure, and new multijunctions appear. The stress required to unzip a multijunction is about four times that for a binary junction.

Multijunctions present nearly indestructible obstacles to dislocation motion and furnish new sources for dislocation multiplication. In this way, they play an essential role in the strength evolution of deforming crystalline metals. The rate at which bcc metals harden during plastic straining is defined, to a large extent, by the presence or absence of multijunctions.

Multijunctions may account for phenomena unexplained by the widely accepted theory of strain hardening caused by pair-wise dislocation interactions. In particular, multijunctions are the reason for the large, directional variation of strength observed in bcc single crystals. Indeed, multijunctions form much more rapidly when stress is applied to a crystal at certain orientations. Bulatov explains that bcc crystals exhibit various degrees of symmetry depending on the vantage point



In this ParaDiS simulation, molybdenum atoms form dislocation lines that multiply and move in response to applied stress.

of the viewer. The orientation called [001] exhibits the greatest amount of symmetry and the greatest number of multijunctions. When stress is applied along other crystal orientations with less symmetry, few if any multijunctions appear. The greater the number of multijunctions formed, the greater the amount of stress required to deform a metal (strain) before it breaks, and the harder the resulting metal. The figure on p. 9 shows this relationship using a stress–strain curve.

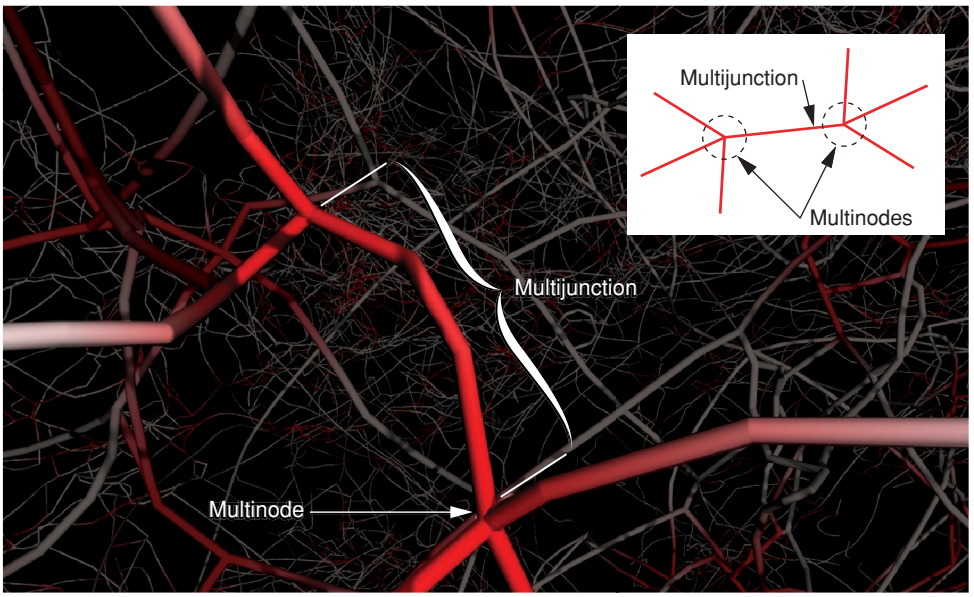
Experiments Verify Simulations

Bulatov's team was able to duplicate the surprising ParaDiS findings using atomistic calculations. These simulations created a cubic block of a perfect bcc single crystal measuring 17 nanometers on each side. The simulations showed discrete dislocation lines forming multijunctions.

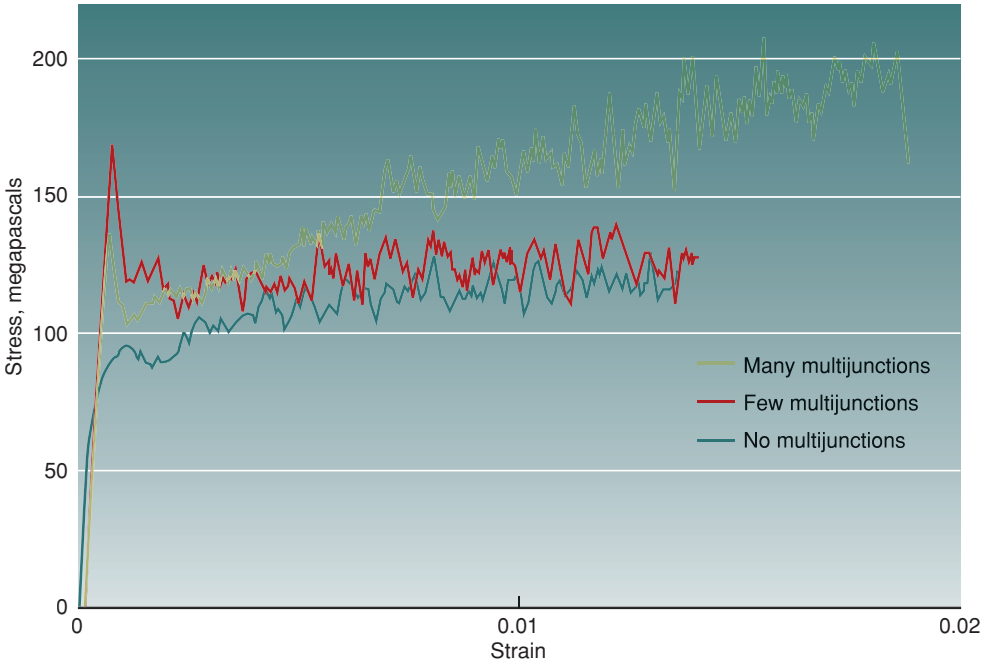
Taken together, the ParaDiS and atomistic simulations appear convincing. However, for verification, Bulatov looked to laboratory experiments and transmission electron micrographs of single-crystal molybdenum samples. In this effort, ParaDiS, like other Livermore codes, is linked closely both to theory and to data obtained from laboratory experiments. Bulatov worked with Florando and Mary LeBlanc, also of Engineering.

The engineers are conducting research on crystalline metals as part of an LDRD-funded initiative. The initiative provides large-strain data to validate ParaDiS simulations and to develop crystal-plasticity models, all as part of Livermore's multiscale modeling program on bcc metals.

The first definitive experimental work on crystals was done in the 1920s, when researchers began to understand atomic structure, crystal lattices, and the response of metals to deformation. This work was primarily one-dimensional (1D); today's research at Livermore is primarily 3D and provides the underlying physics to understand dislocation dynamics in more accurate



ParaDiS shows the eventual formation of a multijunction, which ties together three or more dislocation lines into tight knots. Multinodes are located at each end of a multijunction (see inset). Red indicates dislocations involved in multijunctions, whereas gray represents the more common binary junctions.



These stress–strain curves from a simulation of body-centered-cubic molybdenum show that the formation of multijunctions significantly increases the hardening rate (line slope). The yellow line represents stress applied along the [001] orientation, which exhibits the greatest amount of symmetry and, hence, the greatest number of multijunctions. Stress along crystal orientations with less symmetry results in few (red) or no (blue) multijunctions.

detail. Livermore researchers have been conducting experiments for more than 40 years to improve scientific understanding of crystalline solids and the way they deform. The most recent experimental series, funded by LDRD, began in the 1990s to verify advanced codes and was led by David Lassila, a materials scientist in Engineering.

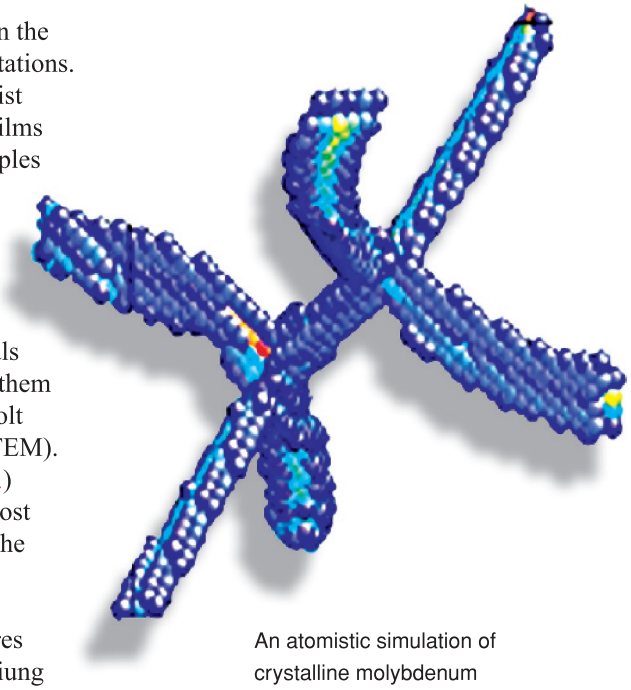
The current experiments focus on the behavior of dislocations in molybdenum and tantalum crystals. A recent series focused on whether the multijunctions seen with ParaDiS were indeed predictable by-products of bcc crystalline metals created in response to stress. The experiments matched the physical parameters simulated by the ParaDiS code.

The team obtained crystals of molybdenum and tantalum that measured about 15 centimeters tall and 1.2 centimeters in diameter. Although almost every material is composed of polycrystals—aggregates of single crystals in different orientations—researchers first need to examine how a single crystal behaves. Technologist Barry Olsen used a vacuum furnace to purify the crystals, because impurities affect a metal's strength and codes cannot yet simulate impurities. Samples of the crystal measuring 5 millimeters wide by 5 millimeters deep by 15 millimeters tall were then carefully cut at different angles using electric-discharge machining and, one by one, subjected to compression. "We needed to know how different orientations of the same crystals responded to the same amount of stress," says Florando.

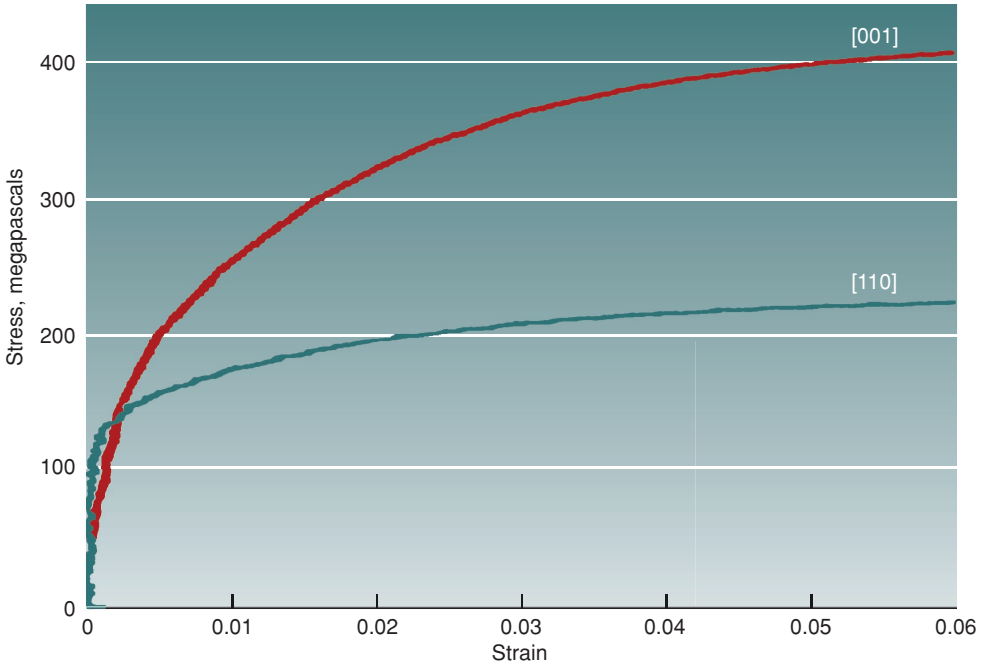
The experimenters compressed the samples to strains of 15 percent. The results showed that when stress was applied to purified crystals of different orientations, the crystals exhibited different strain-hardening behavior. The differences were probably due to multijunctions, which in the ParaDiS simulations formed preferentially in some orientations. For example, much greater stress is required to produce the same amount of strain in the [001] orientation than in other orientations.

After the experiments, technologist Ann Bliss prepared extremely thin films of the deformed crystals. Small samples measuring about 3 millimeters in diameter were cut using a diamond saw and then polished until they were transparent to high-energy electrons for imaging. The thin sections were turned over to materials scientist Luke Hsiung, who imaged them with Livermore's 300-kiloelectronvolt transmission electron microscope (TEM). (See *S&TR,* March 2001, pp. 23–25.) TEMs are special because, unlike most electron microscopes, which probe the surface of materials, they examine a material's internal structure.

Finding specific material structures using a TEM is not an easy task. Hsiung spent two weeks slowly tilting the samples to view them from slightly different angles and thereby distinguish the



An atomistic simulation of crystalline molybdenum atoms shows the formation of multijunctions and multinodes.



This stress–strain curve obtained from experiments on purified crystal samples shows that a [001] crystal orientation, which forms the most multijunctions, requires about double the stress to achieve the same amount of strain as a [110] orientation.

dislocation lines forming the multijunction. Eventually, with the help of electron diffraction experiments, Hsiung found multijunctions that looked strikingly similar to the structures seen in ParaDiS simulations.

Samples of the deformed crystals are also being analyzed at the Advanced Light Source (ALS). Lassila and Florando are collaborating with University of California, Berkeley professor William Morris, Jr., and graduate student Karen Magid, who are using the ALS for a 3D study of dislocation structures. The ALS data can provide maps of the dislocation structure that are several hundred micrometers square, a much greater scale than the TEM observations.

Simulation Is a Full Partner

Bulatov notes it is quite unusual for a code to predict a phenomenon in a material that is later verified by experiment. "ParaDiS predicted something that no one before had seen, or at least recognized." Although dislocation theory is more than seven decades old, previously no one had discovered the connection between multijunctions and metal hardening. "We're sure other investigators have seen multijunctions in electron microscopes, but they didn't understand what they were seeing," says Bulatov.

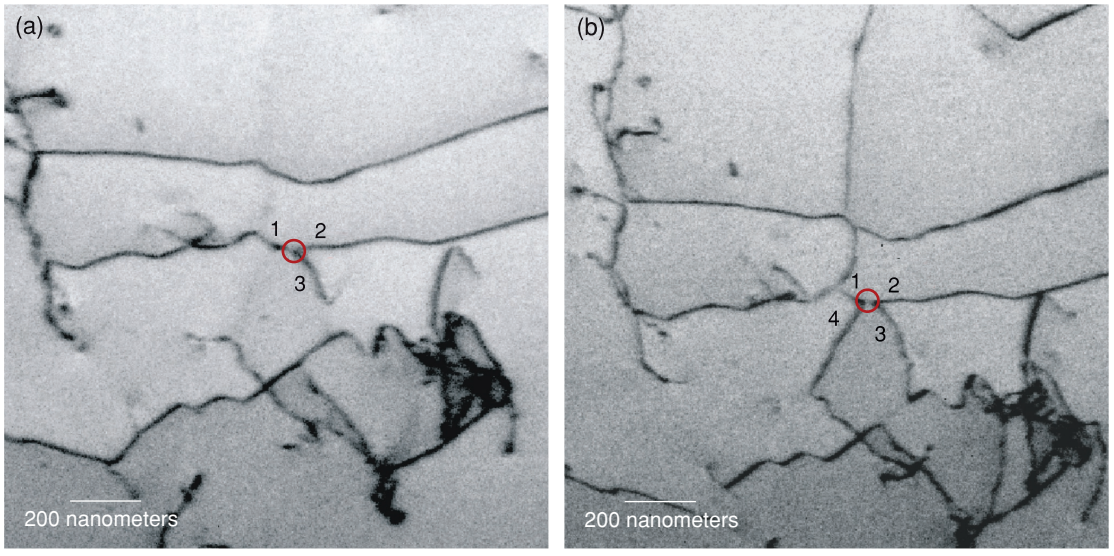
ParaDiS underscores the role of simulation as a full partner with theory and experiment. Bulatov notes that some scientists are skeptical about a code's ability to predict new phenomena. "We watch the simulations with no preconceived notions; we just observe and let the model teach us about the structure of crystals. Others often use codes to confirm what they intuit."

Not surprisingly, the Livermore team is planning additional ParaDiS simulations of bcc single crystals. Bulatov anticipates that by 2006, deformation simulations with 10-percent strain will become standard using BlueGene/L. The result will be greater understanding of multijunctions and multinodes. More complex multijunctions and multinodes appear to exist; some ParaDiS simulations have produced multinodes with five, six, and more arms, and TEM observations have located six-armed nodes.

Once again, experiments on different orientations of purified crystals will be compared to the simulations, as part of the continuing interaction between simulation and experiment. In addition, Bulatov predicts the existence of multinodes and multijunctions in face-centered-cubic crystals (a different form of crystalline organization) and believes that confirmation of their existence by simulation, experiment, and TEM observations will validate the predictions.

Multijunctions represent a potentially outstanding hardening mechanism. If a method to create multijunctions efficiently were developed, it could be important to industry as a new mechanism to harden metals.

According to Florando, new experimental techniques are needed to accurately measure the deformation behavior of single crystals subjected to



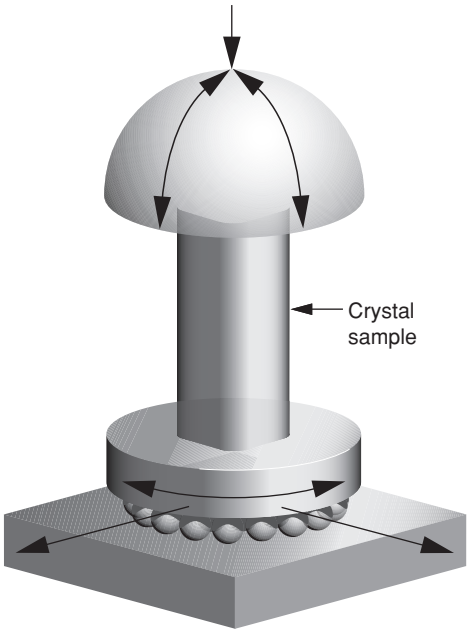
These images of a molybdenum crystal sample were taken with a transmission electron microscope at different viewing angles. (a) Three dislocation lines appear to form a multijunction (circled), but when the crystal sample is examined with a slightly different tilt, (b) an additional fourth line can be seen.

large extents of strain. In response, the experimental team is performing six-degrees-of-freedom (6DOF) experiments, unique to Livermore, which provide data on single crystals as they advance from elastic (reversible) deformation to plastic (nonreversible) deformation, the point when dislocations start to move. The experiments allow the crystals to deform essentially unconstrained in six directions because the bottom of the sample can move as the sample is being compressed. This unconstrained motion prevents the internal crystal planes from rotating during deformation.

The new experimental setup includes a 3D imaging method to measure strains with high-resolution video cameras taking images at 20 frames per second. So-called full-field optical techniques are becoming popular as a method to measure deformation, especially in materials that exhibit nonuniform behavior. The imaging technique measures the deformation that occurs in single crystals better than conventional strain gauges. ParaDiS will eventually include the data derived from the 6DOF experiments.

"We're helping researchers understand simulations. In turn, simulations are helping us understand our experiments," says Lassila. "It's the synergy between simulation and experiment that allows progress to be made." For Bulatov, the rapid acceptance of ParaDiS in the materials science community shows that researchers are well on their way to unraveling the mysteries of how metals harden.

—Arnie Heller



Livermore engineers have developed six-degrees-of-freedom experiments, which provide data on the deformation of single crystals. The experiments allow the crystal to deform essentially unconstrained in six directions because the bottom of the sample can move as the sample is being compressed.

Key Words: Advanced Light Source (ALS), Advanced Simulation and Computing (ASC) Program, BlueGene/L, body-centered-cubic (bcc) metals, dislocation dynamics, multijunction, multinode, Parallel Dislocation Simulator (ParaDiS), six degrees of freedom (6DOF), stockpile stewardship, Thunder, transmission electron microscope (TEM).

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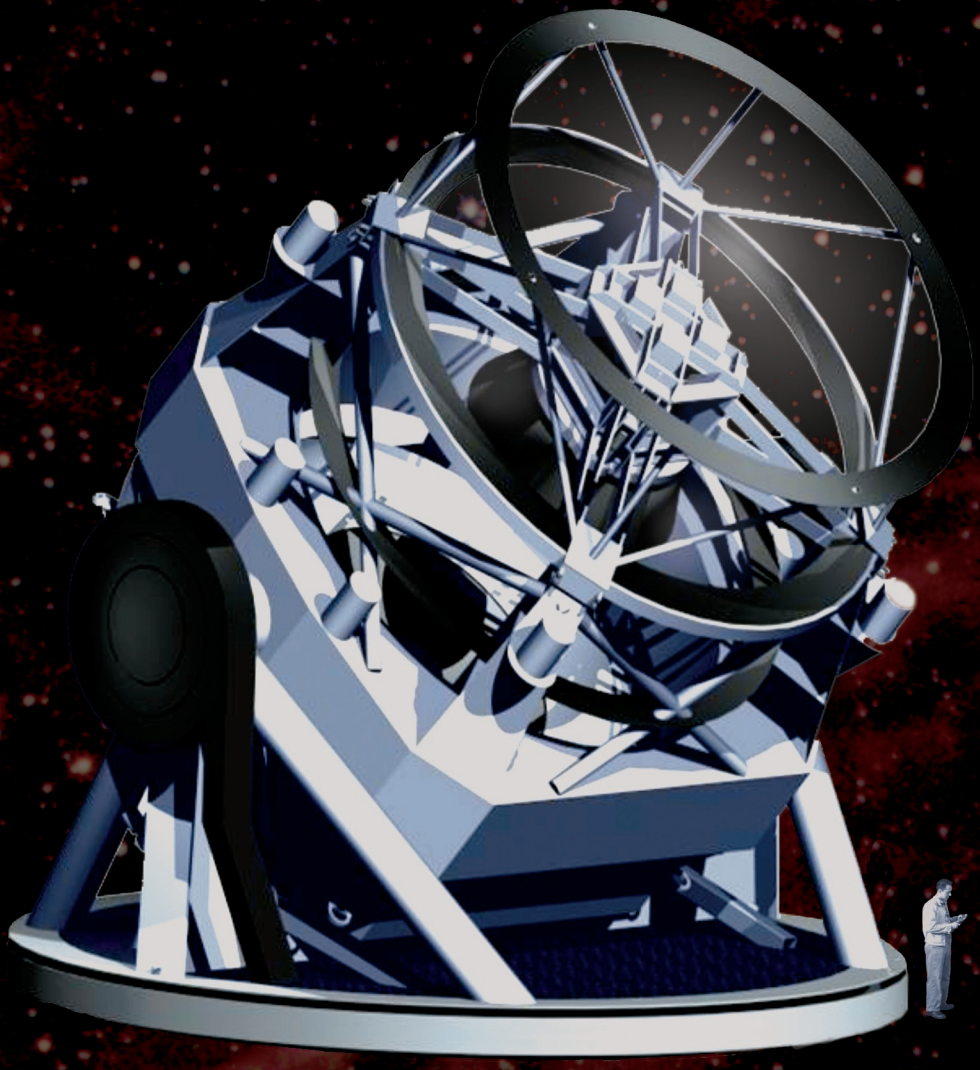
A Wide New Window on the Universe



The Large Synoptic Survey Telescope (LSST) will feature an 8.4-meter-aperture primary mirror, a 10-square-degree field of view, and a camera with more than 3 billion pixels.

FOR decades, ground-based astronomy has consisted mostly of a lone astronomer earning the right to train a powerful telescope for a few nights on an extremely small patch of sky. If the astronomer is fortunate, a celestial discovery will be shared many months later with colleagues through a journal article or private correspondence.

Lawrence Livermore is a major partner in a new telescope project that promises to forever change that scenario—and all of astronomy—by taking advantage of advanced optical manufacturing techniques, digital imaging, supercomputer data processing, and the Internet. The ground-based Large Synoptic Survey Telescope (LSST), scheduled for completion in 2012, will provide, for the first time, digital imaging of objects, including changing events, in deep space across the entire sky. Data from LSST's astronomical surveys will be accessible almost immediately to astronomers and the public on the Internet.

Over a span of three nights, LSST will construct a complete, detailed map of the sky using a telescope with a 8.4-meter primary mirror and an enormous detector. Of particular importance, the telescope will record objects that change or move, from exploding supernovae billions of light years away to comets passing close to Earth. The first complete survey produced by LSST may also provide clues about so-called dark matter and dark energy and new information about the nature and origin of the universe. Finally,

By making frequent, detailed maps of the sky, the proposed Large Synoptic Survey Telescope will change astronomy forever.

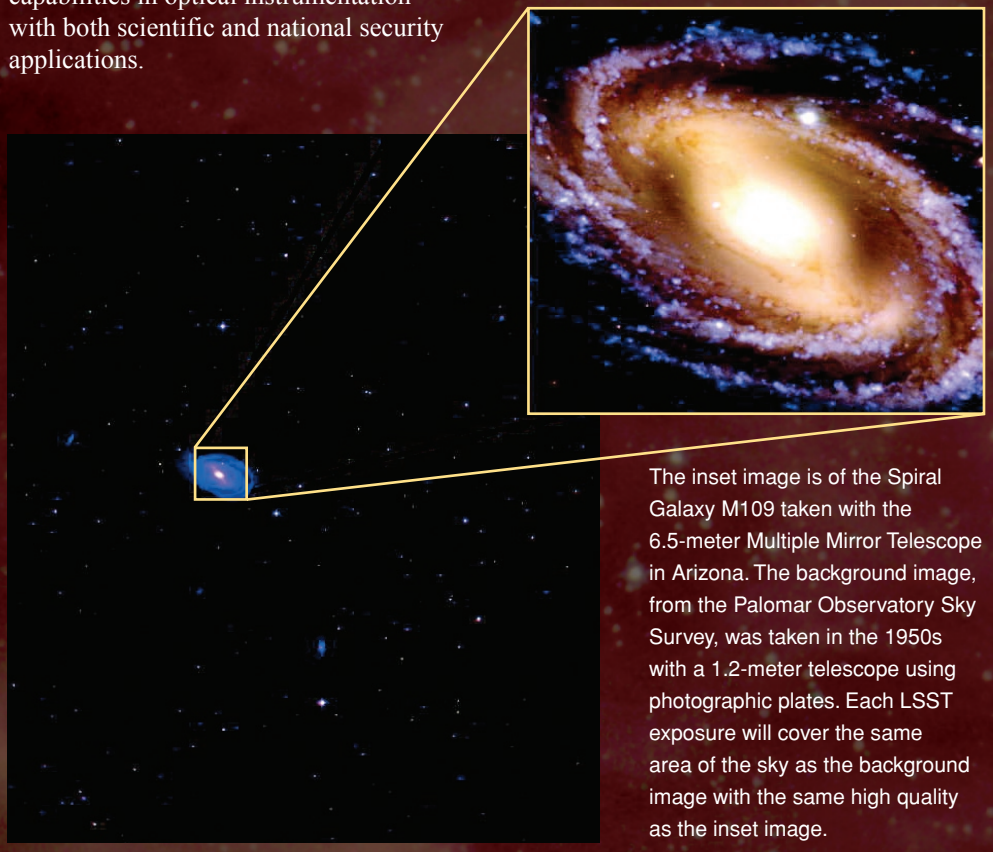
LSST will catalog near-Earth objects to provide insight into the formation of the solar system and to warn Earth's inhabitants in the event of a potential collision with an asteroid.

Although a few telescopes with 8-meter-aperture mirrors exist, they are optimized to look deeply at small parts of the sky. Their small field of view makes it extremely unlikely that a single observation will catch a transient event. Furthermore, such an instrument would take many years to map the entire sky. Current all-sky maps made with smaller telescopes are limited in depth (faintness) and detail. LSST will overcome these drawbacks by mapping the entire sky deeply, rapidly, and continuously with a 10-square-degree field of view. What's more, when the telescope detects an object of interest, such as an exploding supernova, it will send out an alert for more specialized telescopes to follow up with higher resolution images.

Livermore researchers are participating in all aspects of the LSST project, from management to research efforts. For example, Bill Goldstein, associate director of the Physics and Advanced Technologies (PAT) Directorate, is on the governing board of the nonprofit LSST Corporation. Physicist Don Sweeney is the LSST project manager and manages the entire LSST effort from the project offices in Tucson, Arizona. Astrophysicist Kem Cook is a key member of the LSST science team and heads the Laboratory's LSST-related astrophysics research activities. Engineer Jim Brase is managing Livermore's participation.

Brase heads PAT's Optical Science and Technology Division, which develops advanced detectors for both astronomical research and national security. Most of the LSST research and development work is supported by Livermore's Laboratory Directed Research and Development (LDRD) Program, which is enabling scientists and engineers to develop new capabilities in optical instrumentation with both scientific and national security applications.

Brase says, "Astronomers traditionally apply for time on a remote telescope, but LSST will change everything." The telescope will be completely automated, building a huge database of celestial objects every night. Science will be done by astronomers doing "data mining," that is, finding unique features on LSST images they have downloaded from the Internet to their office computers. In this



The inset image is of the Spiral Galaxy M109 taken with the 6.5-meter Multiple Mirror Telescope in Arizona. The background image, from the Palomar Observatory Sky Survey, was taken in the 1950s with a 1.2-meter telescope using photographic plates. Each LSST exposure will cover the same area of the sky as the background image with the same high quality as the inset image.

way, scientists worldwide will have near-real-time access to astronomical developments that occur anywhere in the sky.

Livermore Is a Pioneer

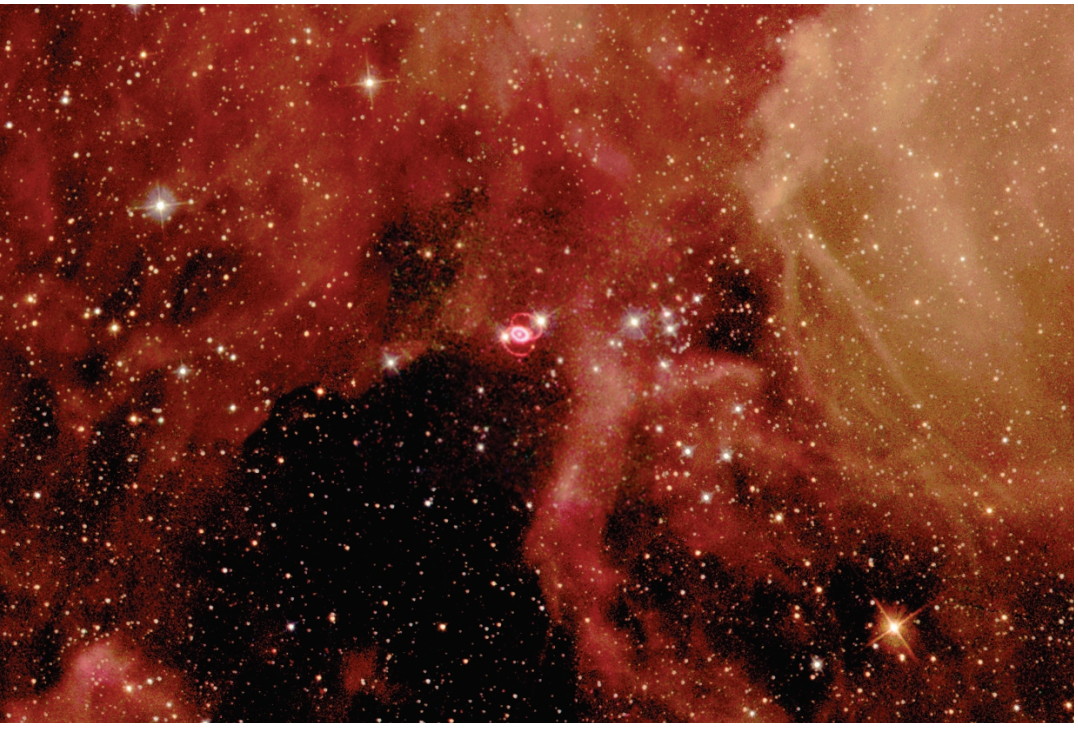
Livermore helped pioneer wide-field, time-domain astronomy with the MACHO (Massively Compact Halo Object) project. Cook was a MACHO project founding member. Originally funded by LDRD, the project was a digital-imaging study in search of cosmic dark matter. (See *S&TR*, April 1996, pp. 6–11.) A key feature of the project was that astronomical events called gravitational microlensing were identified as they were happening, allowing detailed study by networks of telescopes. "The universe is an exciting place with major events occurring on time scales of minutes," says Cook. "We've missed almost all of these events in the past. LSST will do the first good job of watching the universe change on a large scale."

LSST will incorporate several technologies developed, for the most part, at Livermore. These include fabrication techniques for large optics developed for the recent generation of telescopes and the National Ignition Facility (NIF); detector technologies that allow cameras to capture wide-angle images on focal planes coated with billions of high-sensitivity pixels; and the technologies and tools for computing and storing large amounts of data.

The telescope will benefit from Livermore's experience with optics, precision engineering, astrophysical research, and computing. NIF, currently being assembled at Livermore, will be the world's largest optical instrument. NIF scientists and engineers have worked with vendors to push the development of advanced optical components and coatings. Livermore scientists have also designed optics for land- and space-based telescopes and surveillance systems. Research in astrophysics is conducted at the Laboratory through its branch of the University of California's Institute for Geophysics and Planetary Physics. Livermore is also a world leader in supercomputing and in the managing, storing, and analyzing of enormous amounts of data.

The LSST project has been identified as a scientific priority in reports by several national panels. The effort to build the telescope is overseen by the nonprofit LSST Corporation, a collaboration of universities, national laboratories, and scientific organizations. The LSST team is considering three possible sites for the telescope: Las Campanas or Cerro Pachon in Chile and San Pedro Martir in Baja California, Mexico. The site will be selected in a year or so.

The estimated cost of LSST is about $300 million: $30 million for design and $270 million for construction. The funding will come from a partnership of private and federal sources. The LSST Corporation has already raised $25 million of private funding to jump-start the project and begin items such as the mirrors. The remainder is proposed to come from the National Science Foundation and the Department of Energy. The National Science Foundation recently announced that it will fund a 4-year, $14.2-million design and development project for LSST.



Astronomers predict LSST will detect more than 100,000 supernova explosions. This National Aeronautics and Space Administration (NASA) image shows Supernova 1987A in the Large Magellanic Cloud, a nearby galaxy. Astronomers witnessed the explosion of this star on February 23, 1987. The supernova remnant, surrounded by inner and outer rings of material, is set in a forest of diffuse gas clouds. (Photo courtesy of NASA.)

Optics Benefit from NIF

Livermore physicist Scot Olivier oversees the development of LSST camera optics, including lenses, filters, and mirror wavefront sensors as well as the mechanisms for keeping these components free of distortion. Olivier says, "We're leveraging our experience in

extreme ultraviolet lithography, precision engineering, adaptive optics, and NIF optics. The astronomical community has never built refractive optics for a camera this large or this powerful. We'll have the advantage of working with the same vendors who manufactured optics for NIF."

Layton Hale, a precision engineer, is devising the mechanisms that will hold optical components securely in place. The telescope's mount is being designed to ensure accurate tracking and repointing of the telescope quickly and repeatedly to adjacent locations.

Optical engineer Lynn Seppala designed LSST's mirrors and camera lenses. The optical-system design features three deeply curved mirror surfaces that collect light from objects as faint as 24th magnitude in a 10-second exposure, which is equivalent to the brightness of a golf ball at the distance from Earth to the Moon. Light gathered by the 8.4-meter primary mirror is reflected back up to the 3.4-meter convex secondary mirror and then down to the 5.2-meter tertiary mirror. Light is then bounced upward again through a series of three lenses to the camera detector suspended within the telescope structure. In a unique design choice, the primary and tertiary mirrors will be fabricated from a single piece of glass, 8.4 meters in diameter and more than a meter thick at the edge.

Wide Field of View

Three mirror surfaces allow high image quality over a wide field of view. The mirrors will provide a field of view encompassing 10 square degrees of sky, roughly 50 times the area of a full Moon. This field of view is more than 20 times that of existing large telescopes, yet LSST's light-gathering capability will be among the best in the world.

The tertiary mirror fits neatly into a hole of the primary mirror, offering the opportunity to construct a novel hybrid mirror. In January 2005, LSST Corporation awarded a contract to the University of Arizona's Steward Observatory Mirror Laboratory to begin fabrication of the hybrid primary and tertiary mirrors. Sweeney says, "Combining the primary and tertiary mirrors on a single 8.4-meter-diameter optical substrate is an engineering challenge never before undertaken."

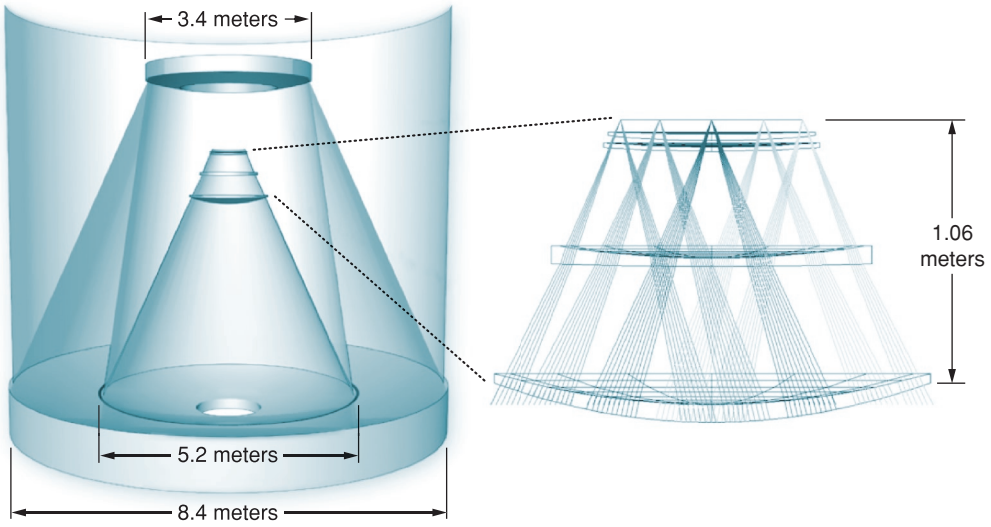
All LSST mirrors will be "active," that is, deformable by tiny actuators that ensure the mirrors maintain their proper shape. When the telescope points to a different area of the sky, or as temperature fluctuates during the night, the mirrors tend to bend, which would compromise their ability to focus a clear image.

Livermore researchers are designing a computer-controlled, wavefront-sensing system, in which the mirrors' shapes will be measured and adjusted by hundreds of actuators once every 60 seconds to within 10 nanometers of accuracy. The active optics and wavefront sensing system will also counter the turbulence in the atmosphere that degrades the quality of images from ground-based telescopes. According to Sweeney, "The completed LSST optical system will be the fastest, most compact system of this scale ever built for an advanced research telescope."

Livermore-built adaptive optics systems are used on large telescopes such as the University of California's (UC's) Lick Observatory on Mount Hamilton near San Jose and the Keck Telescope in Hawaii. In fact, nearly every large telescope in the world now has an existing or planned adaptive optics system.

Combining 1,000 Digital Cameras

To capture images produced over such a wide field, LSST will use a camera with three lenses, measuring 1.6, 1.0, and 0.7 meters in diameter. The camera will be combined with a charge-coupled device (CCD) and cover a 64-centimeter-diameter flat focal plane. The CCD will be the world's largest and contain more than 3 billion pixels. It is being designed as a circular mosaic of about 200 individual detectors, each comprising about 16 million pixels. Olivier says the combined detector will represent a huge extrapolation of consumer digital photography technology. "It's similar to combining 1,000 digital cameras, but unlike consumer digital cameras, this detector will be sensitive to more



Light gathered by the 8.4-meter primary mirror is reflected up to the 3.4-meter convex secondary mirror and then down to the 5.2-meter tertiary mirror. Light is then bounced upward again through a series of three lenses to the camera detector suspended within the telescope structure.

wavelengths." In particular, the detector will be sensitive to the near-infrared portion of the electromagnetic spectrum. It will thus detect light that has been "redshifted." (In an expanding universe the colors of stars moving away are shifted toward the red end of the spectrum.)

The camera will record images in five colors using 70-centimeter-diameter filters, the largest telescope filters ever manufactured. Five filters—green, red, blue, and two in the near-infrared region of the electromagnetic spectrum—will be inserted between both the second and third lenses. Sweeps of the sky in different colors will help provide information about the distance to each galaxy and the mass and evolutionary state of stars. Livermore engineers are leveraging NIF experience to design an automated system that will change the filters in 2 seconds or less.

The CCD-camera effort also involves participation by the Stanford Linear Accelerator Center (SLAC), Brookhaven National Laboratory, Harvard University, the University of Illinois, the National Optical Astronomy Observatory (NOAO), and UC Davis.

Negating Atmospheric Turbulence

Livermore physicists Leslie Rosenberg and Steven Asztalos, both researchers of

Scientific Missions

The Large Synoptic Survey Telescope (LSST) will compile a complete map of the entire sky, advance understanding of the nature and origin of the universe, and discover transient events. "No one knows what we'll discover," says Livermore physicist Jim Brase. For example, a new source brightening over a period of a few days with a particular color signature might be identified as one of several hundred thousand supernovae that LSST is expected to discover each year, located in galaxies billions of light years from the Milky Way. Other transient events include gamma-ray bursts and other unusual violent objects.

In one pass across the visible sky (14,000 square degrees, or about three nights of observation), LSST will detect and classify 840 million persistent objects. Astronomers worldwide will use the Internet to access the enormous—and ever-increasing—database of objects. A single 15-second exposure will detect sources at 24th magnitude with only a 10-percent error in magnitude. At this level of brightness, the most common objects in the sky are galaxies—60,000 of them per square degree across the sky.

Many parallel scientific missions can be conducted with this massive collection of data. For example, LSST will uncover new information about dark matter via weak gravitational lensing and supernovae studies. Dark matter (which dominates the mass of the universe) and dark energy are unseen phenomena whose existence has been inferred. A better understanding of these forces will help researchers determine how the universe is evolving.

LSST will help astronomers learn more about near-Earth objects such as comets and asteroids. These objects are composed of the material from which the solar system formed and thus hold important clues to the origin of the Sun and planets. Current efforts to find near-Earth objects are limited because asteroids and comets reflect little light, and telescopes do not have adequate light-gathering capacity or wide-area coverage. Astronomers estimate a one-in-10,000 chance exists that a 1- to 2-kilometer meteoroid will strike Earth within the century and cause enormous devastation. Therefore, asteroids represent a threat worth identifying and assessing.

LSST will also study the Kuiper Belt, the origin of most comets. The Kuiper Belt is a collection of minor planets orbiting beyond Neptune. It is the remnant of the disk of material that once orbited the Sun and produced the planets and their moons about 5 billion years ago.

NASA's Galileo Spacecraft took this image of the asteroid 951Gaspra. The asteroid measures 19 by 12 by 11 kilometers and is similar to those whose impacts could cause mass extinctions on Earth. It is one of thousands of near-Earth objects that will be imaged by LSST. (Image courtesy of NASA.)

dark matter, are analyzing the potential capability of LSST to provide images that would allow astronomers to learn more about the mysterious distribution of invisible dark matter and energy in the universe. "LSST will be taking images at incredible distances to the outer edges of the universe," says Rosenberg, who coordinates researchers from Livermore, UC Davis, SLAC, and NOAO.

To better understand dark matter, and to some extent dark energy, scientists depend on the phenomenon of gravitational lensing, the deflection of light by either visible matter or invisible dark matter. Astronomers study many images over several weeks to detect the subtle elongations caused by weak gravitational lensing. "We'll need to obtain incredible image quality from LSST because the changes caused by intervening dark matter are so small," says Rosenberg.

Unfortunately, atmospheric turbulence can mimic the elongation signal caused by gravitational lensing. Therefore, astronomers need to understand atmospheric turbulence so they can differentiate between elongations caused by the atmosphere and those caused by dark matter. In this respect, LSST's 15-second exposures pose a problem. At much shorter exposures, the irregular effects of atmospheric turbulence are frozen; however, at 15 seconds, they mostly average out. With LDRD funding, Rosenberg and Asztalos are completing a 3-year effort to evaluate the capability of LSST for detecting gravitational lensing in the presence of atmospheric turbulence.

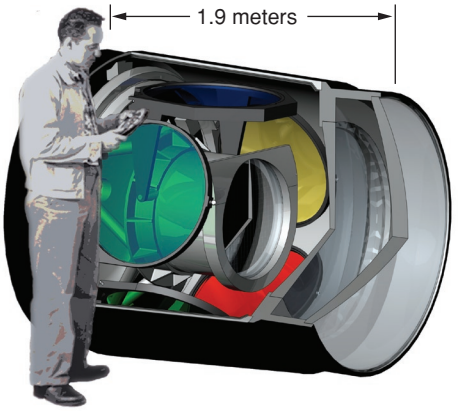
In May 2005, a team that included Livermore researchers traveled to Chile to acquire atmospheric data recorded from 4- and 8-meter telescopes as well as distant images of the universe taken by the telescopes. These data are the most comprehensive to date and have allowed Asztalos to simulate what an LSST image would look like by modifying a software program originally developed by astronomers at the California Institute of Technology. The program, which has been shared with other collaborators, models the sky, atmosphere, and LSST instrument. The simulations incorporate atmospheric-caused elongations.

"Our understanding of atmospheric effects based on results to date give us confidence that LSST can meet our goals to detect weak gravitational lensing," says Rosenberg. "However, we want to increase that confidence."

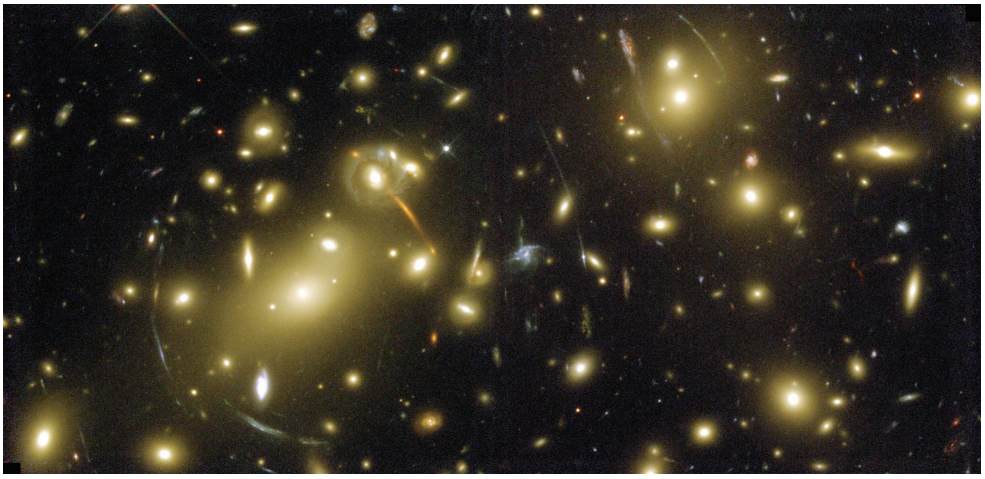
If LSST achieves the project's goals, it will be able to map out dark matter to enormous distances from Earth. In addition, by estimating distances to dark-mass concentrations, astronomers will be able to map dark energy. "Without a doubt, as soon as LSST sees first light, it will be the premier cosmology survey instrument," says Asztalos.

Data-Management Hurdle

Effectively managing the large amount of LSST data is the most challenging aspect of ensuring the project's overall scientific success, according to Brase. Livermore computer scientist Celeste Matarazzo is leading a data-management team that includes computational experts from Livermore, Johns Hopkins University, SLAC, and UC Davis and San Diego. The Livermore group, led by computer scientist Ghaleb Abdulla, takes advantage of extensive Laboratory experience in building large-scale



LSST's camera will record images in five colors using 70-centimeter-diameter filters. Five filters—green, red, blue, and two in the near-infrared region of the electromagnetic spectrum—will be inserted between the second and third lenses. This schematic shows the filters surrounding the third camera lens.



NASA's Hubble Space Telescope imaged the Abell 2218 massive cluster of galaxies located about 2 billion light years from Earth. The cluster is so massive that its gravitational field distorts light rays passing through it from faraway objects, as seen in the elliptical-shaped celestial objects. This phenomenon is called strong gravitational lensing. Weak grativational lensing is more subtle and must be measured by computer analysis.

computer and data-storage systems, performing data-intensive computing, maintaining large databases, and developing astronomical applications.

LSST will spend about 30 seconds observing a field of view before it is repointed to the next field. "The telescope must do sophisticated processing within that 30 seconds," says Brase. For example, each image will be corrected for geometric distortions and ambient light from the night sky and mapped to a coordinate system. Any variations in sensitivity across the detectors will also be corrected. Stars and galaxies will be identified, and then the image will be added to data previously collected from the same location in the sky to build a very deep master image. All of these tasks will be done without human intervention.

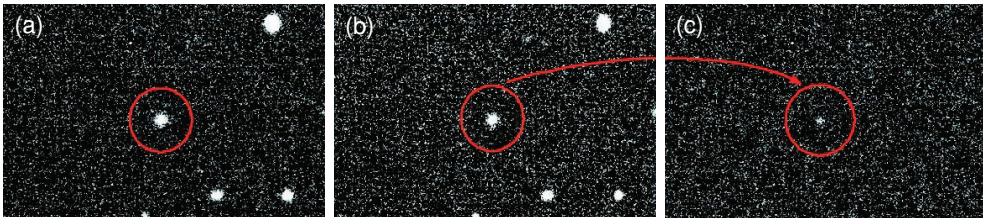
Changes in an image will be revealed using image subtraction and a comparison against the database of known objects, allowing the type of change to be classified. If an object is moving or changing in brightness, the telescope will send out an alert to both ground- and space-based telescopes with the sky coordinates of the object of interest. One challenge is developing procedures for sending out automatic alerts. "We don't want to send out false alerts," says computer scientist Jim Garlick.

Abdulla notes that Livermore is building pipelines to efficiently process images by breaking the image up and processing each piece in parallel. Such a technique makes effective use of massively parallel supercomputers with thousands of microprocessors.

LSST will create 24 gigabytes of data every 30 seconds, a sustained data rate of 1,200 megabytes per second, unprecedented in astronomical data gathering. By comparison, the highest data rate in current astronomical surveys is about 4.3 megabytes per second. More than 30 terabytes of data must be processed and stored each night. One year's worth of data from LSST will require the storage of more than 30 petabytes (10^{15} bytes). In comparison, the Hubble Space Telescope produces about 1 terabyte each year. Much of the science that will be done by astronomers will be accomplished with queries to this database. Garlick says that although the LSST data rate is challenging, "Big systems at Livermore move data around at comparable rates."

Large computers will be located adjacent to the telescope. At least one supercomputer center in the U.S. will help process the huge amount of data. The chosen supercomputer will be similar to Livermore's MCR or Thunder machines. Livermore computer scientist Don Dossa is chief architect of LSST's computer system.

"We'll be combining high-performance computing and databases in a new way," says Abdulla. The Livermore team is anticipating how scientists will query the image database, especially when the same patch of sky will be imaged thousands of times.



LSST will use image subtraction to discover supernovae. In this example, image (a) is subtracted from image (b) (taken three weeks later) to reveal that a supernova has exploded (c). Once LSST detects a supernovae, it will send out alerts to astronomers worldwide. (Photo courtesy of the ESSENCE project, National Optical Astronomy Observatory.)

Excitement Building

As the work on LSST gains momentum, excitement in the astronomical community is building. By rapidly making complete digital sky maps, LSST will change astronomy forever.

Brase notes that image-probing techniques similar to those being developed for LSST are also important for other areas of science, such as satellite observations, biology, and oceanography. In addition, the software tools developed to mine the LSST data resource will find wide application. Livermore's national security mission will benefit because LSST technologies have application to national and homeland security. For example, the LSST optical design serves as a prototype for future wide-field surveillance systems. Also, investments in astrophysics have enabled new capabilities for nuclear proliferation detection, such as lightweight nanolaminate optics, adaptive optics, multigigapixel camera systems, tools for image analyses, and data-search algorithms.

In just a few years, people worldwide will be turning to the Internet to find the latest digital maps of the universe.

—Arnie Heller

Key Words: adaptive optics, asteroid, comet, dark energy, dark matter, gravitational lensing, Kuiper Belt, Large Synoptic Survey Telescope (LSST), National Ignition Facility (NIF), near-Earth objects, supernovae, wavefront sensing.

For further information contact Jim Brase (925) 422-6992 (brase1@llnl.gov).

Built for Speed
Graphics Processors for General-Purpose Computing

Dave Bremer, a member of the Graphics Architectures for Intelligence Applications team, holds a commercial graphics processing card. These units used for virtual entertainment are providing low-cost solutions for high-performance data processing.

WHILE computer gamers are eagerly awaiting the next generation of platforms, the computer scientists of Lawrence Livermore's Graphics Architectures for Intelligence Applications (GAIA) project are tracking the rapidly changing technology, but for a different reason. A team, led by John Johnson of the Computation Directorate, is researching graphics processing units (GPUs)—the highly specialized, low-cost, rendering engines at the heart of the gaming industry—to determine how they might be programmed and used in applications other than virtual entertainment.

"Graphics processors are accelerating in performance much faster than other microprocessors," says Sheila Vaidya, project leader for GAIA. "We have an opportunity to ride the wave of innovations driving the gaming industry." These processors—traditionally designed for fast rendering of visual simulations, virtual reality, and computer gaming—could provide efficient solutions to some of the most challenging computing needs facing the intelligence and military communities. Real-time data-processing capabilities are needed for applications ranging from text and speech processing to image analysis for automated targeting and tracking.

Gaming the System

The GAIA team, including collaborators from Stanford University, the University of California at Berkeley and Davis, and Mississippi State University, is researching graphics processors used in the computer gaming and entertainment industries to determine how they might be used in knowledge-discovery applications of relevance to national security.

Why bother with this class of processors when plenty of central processing units (CPUs) exist to do the heavy-duty work in high-performance computing? Two words: speed and cost.

The ever-growing appetite in the three-dimensional (3D) interactive gaming community has led to the development and enhancement of GPUs at a rate faster than the performance of conventional microprocessors predicted by Moore's Law. This acceleration in improved performance will likely continue as long as the demand exists and integrated-circuit technologies continue to scale.

During the past 2 years, the GAIA team has implemented many algorithms on current-generation CPUs and GPUs to compare their performance. The benchmarks that followed showed amazing performance gains of one to two orders of magnitude on GPUs for a variety of applications, such as georegistration, hyperspectral imaging, speech recognition, image processing, bioinformatics, and seismic exploration.

GPUs have a number of features that make them attractive for both image- and data-processing applications. For example, they are designed to exploit the highly parallel nature of graphics-rendering algorithms, and they efficiently use the hundreds of processing units available on-chip for parallel computing. Thus, one operation can be simultaneously performed on multiple data sets in an architecture known as single-instruction, multiple data (SIMD), providing extremely high-performance arithmetic capabilities for specific classes of applications. Current high-end GPU chips can handle up to 24 pipelines of data per chip and perform hundreds of billions of operations per second.

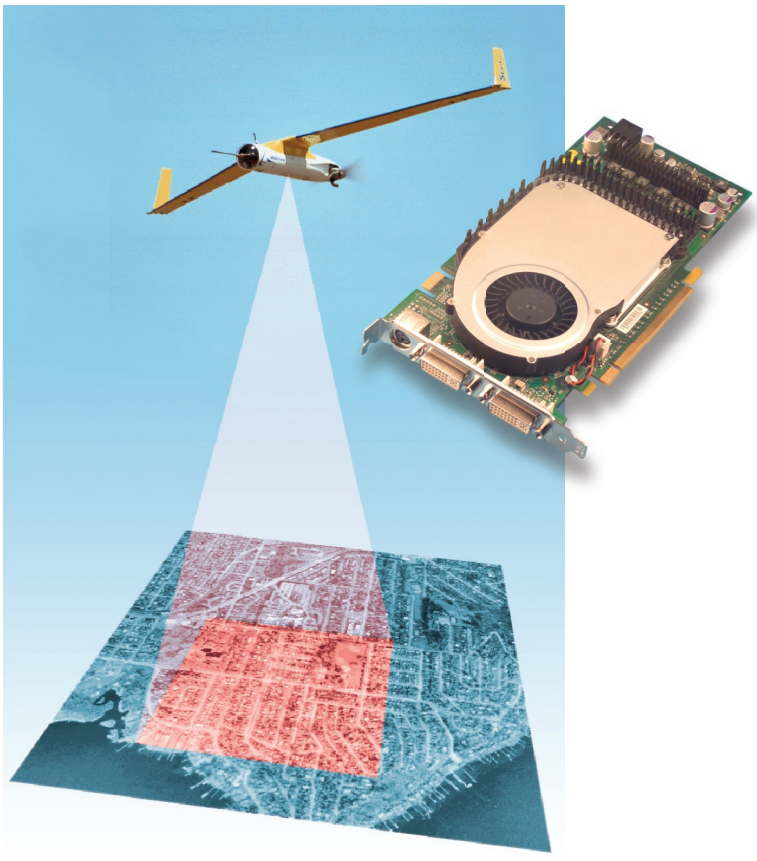
Today's commercial GPUs are relatively inexpensive as well. "National retailers charge a few hundred dollars for one, compared to the thousands of dollars or more that a custom-built coprocessor might cost," says Johnson.

The performance of these GPUs is impressive when compared with that of even the newest CPUs. "A modern

CPU performs about 25 billion floating-point operations per second," says Johnson. "Whereas a leading-edge GPU, such as the NVIDIA® GeForce™ 7800 GTX video card or the upcoming successor to the ATI Radeon® X850, performs six times faster at half the cost of a CPU." These GPUs are optimized for calculating the floating-point arithmetic associated with 3D graphics and for performing large numbers of operations simultaneously.

GPUs also feature a high on-chip memory bandwidth, that is, a large data-carrying capacity, and have begun to support more advanced instructions used in general-purpose computing. When combined with conventional CPUs and some artful programming, these devices could be used for a variety of high-throughput applications.

"GPUs work well on problems that can be broken down into many small, independent tasks," explains GAIA team member Dave Bremer. Each task in the problem is matched with a pixel in an output image. A short program is loaded into the GPU, which is executed once for every pixel drawn, and the results from each execution are stored in an image. As the image is being drawn, many tasks are being executed simultaneously through the GPU's numerous pipelines. Finally, the results of the problem are copied back to an adjacent CPU.



The use of graphics processing units (inset) for real-time georegistration of high-resolution wide-area imaging was demonstrated by Livermore's Sonoma project. Graphics processing on remote-collection platforms, such as in the one in this aircraft, reduces the volume of data transferred to users, enabling real-time analysis.

However, general-purpose programming on GPUs still poses significant challenges. Because the tasks performed on a GPU occur in an order that is not controlled by a programmer, no one task can depend on the results of a previous one, and tasks cannot write to the same memory. Consequently, image convolution operations work extremely well (100 times faster) because output pixels are computed independently, but computing a global sum becomes very complex because there is no shared memory. "Data must be copied in and out of the GPU over a relatively slow transmission path," says GAIA team member Jeremy Meredith. "As a result, memory-intensive computations that require arbitrary access to large amounts of memory off-chip are not well suited to the GPU architecture."

Today's GPUs are power hungry. But designers, faced with the growing demand for mobile computing, are rapidly evolving chip architectures to develop low-power versions that will approach the performance of high-end workstations.

What's in the Pipeline

"GPUs are beginning to more closely resemble CPUs with every evolution," notes Johnson. "The drawbacks for general-purpose programming are being tackled by the industry, one by one." Next-generation CPU architectures are adopting many features from GPUs. "Emerging architectural designs such as those found in Stanford's Merrimac and the IBM–Toshiba–Sony Cell processor look similar to the architecture of GPUs," says Johnson. "These designs could be the next-generation technology for real-time, data-processing applications. Our work with GPUs will help us evaluate and deploy the emerging devices."

The Cell processor, which is a crossover GPU–CPU chip, is scheduled to hit the gaming market soon. But the Cell might also prove to be useful in defense and security computing environments. The scientists of GAIA—just like the gamers—are eager to test and scale its limits.

—Ann Parker

Key Words: central processing unit (CPU), general-purpose programming, Graphics Architectures for Intelligence Applications (GAIA) project, graphics processing unit (GPU), knowledge discovery, streaming architectures.

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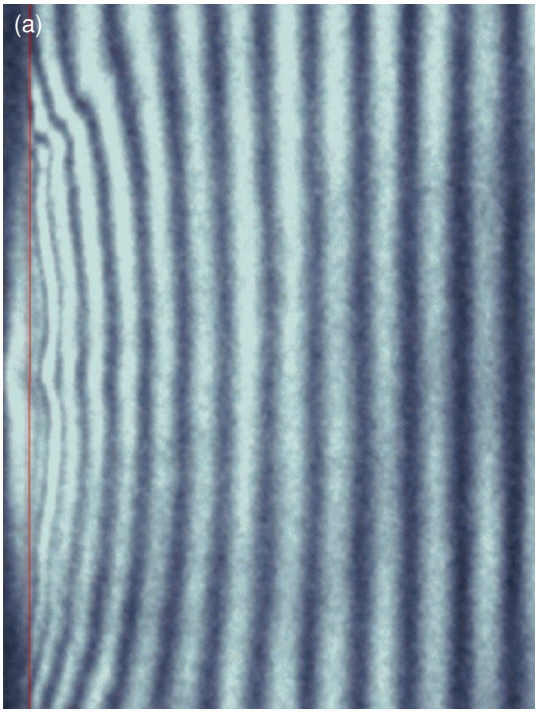
Negative Plasma Densities Raise Questions

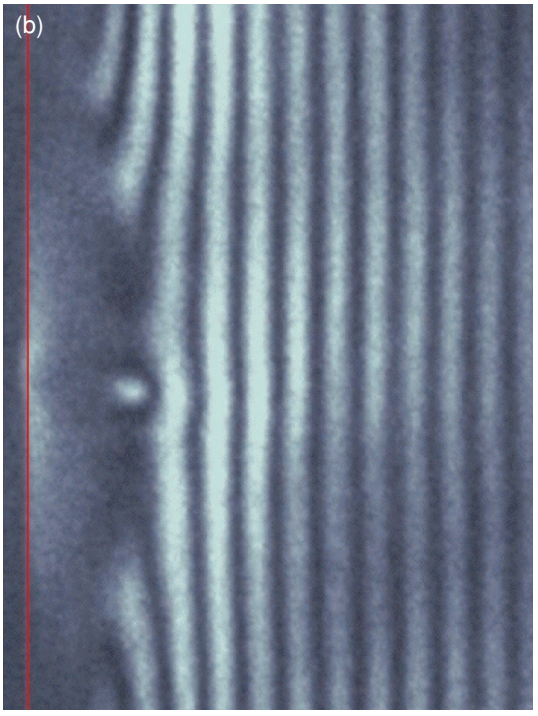
NEARLY all the matter encountered on Earth is either a solid, liquid, or gas. Yet plasma—the fourth state of matter—comprises more than 99 percent of the visible universe. Understanding the physical characteristics of plasmas is important to many areas of scientific research, such as the development of fusion as a clean, renewable energy source.

Lawrence Livermore scientists study the physics of plasmas in their pursuit to create fusion energy, because plasmas are an integral part of that process. When deuterium and tritium are heated to the extreme temperatures needed to achieve and sustain a fusion reaction (about 100 million degrees), the electrons in these light atoms become separated from the nuclei. This process of separation is called ionization, and the resulting collection of negatively charged free electrons and positively charged nuclei is known as a plasma. Although plasmas and gases have many similar properties, plasmas differ from gases in that they are good conductors of electricity and can generate magnetic fields.

For the past decade, x-ray laser interferometry has been used in the laboratory for measuring a plasma's index of refraction to determine plasma density. (The index of refraction for a given material is defined as the wavelength of light in a vacuum divided by the wavelength of light traveling through the material.) Until now, plasma physicists expected to find an index of refraction less than one. Researchers from Livermore and Colorado State University recently conducted experiments on aluminum plasmas at the Laboratory's COMET laser facility and observed results in which the index of refraction was greater than one.

This surprising result implied a negative electron density. Livermore physicist Joseph Nilsen and his colleagues from Livermore and the University of Notre Dame have performed sophisticated calculations to explain this phenomenon. Previously, researchers believed that only free electrons contributed to the index of refraction. Nilsen and his colleagues posit that bound electrons attached to the ions in plasmas can greatly affect the index of refraction and make it greater than one. Furthermore, if the effect of bound electrons is ignored when analyzing experimental results from x-ray interferometry, the electron density of plasmas may be indeterminate or significantly under- or overestimated.





(a) An interferogram of aluminum plasma captured 0.2 nanosecond after the plasma is created shows the expected fringe shifts bending to the right, away from the high-density plasma region. (b) An interferogram captured 3.2 nanoseconds later shows an anomalous negative fringe shift with fringes bending to the left, toward the high-density plasma region.

Electrons: Bound Versus Free

According to Nilsen, plasma physicists in the past who have used optical lasers to probe plasmas have assumed that the index of refraction, which is used to determine plasma density, can be calculated using only the number of free electrons. Using the significantly shorter wavelength 14.7-nanometer x-ray laser, Nilsen's colleagues probed plasmas many orders of magnitude denser and hotter than those probed using optical lasers. When a plasma's density is measured by x-ray laser interferometry, the interferometer splits the x-ray beam into two paths, with one beam propagating through the plasma and then recombining with the second reference beam. When recombined, the beams display the interference pattern, which is captured by a charge-coupled device camera. The image, or interferogram, appears as a series of alternating light and dark bands, or "fringes," with the fringes bending away from the region of high density.

Fringe shift is calculated as the distance between light bands. For instance, if the bend is equivalent to the distance between two bands, then the number of fringe shifts is 1. The resulting number of fringe shifts (N_{fringe}) is subsequently used in calculations that incorporate other variables, such as wavelength, index of refraction, and number of free electrons, to determine plasma density.

Experimentalists have been using this technique with assumed reliability for many decades. However, occasionally researchers have observed negative fringe shifts—fringes that bend toward the high-density region. "The bands appear," says Nilsen, "as if they are being sucked into a black hole of high-density plasma." Other scientists who have observed this phenomenon thought the anomalies were due to equipment or experimental error. Because they had no explanation for their observations, no findings were published.

That was not the case with Nilsen and his colleagues. "We wanted to figure out why the fringe was bending the wrong way," says Nilsen. "The negative fringe shift implied a negative plasma density, which we knew was not physically possible." The more likely explanation was a greater contribution of bound electrons to the index of refraction. As it turns out, x-ray lasers interact more with bound electrons than do optical lasers. In a small number of experiments using a tabletop x-ray laser on warm, dense plasmas, Nilsen's colleagues found that as the plasma cools, more anomalies appeared in the collected data, confirming the importance of considering bound electrons.

Doing the Numbers

Nilsen and his colleagues realized that because the contribution of the bound electrons to the index of refraction was so significant, the standard formulas for plasma density needed to be recalculated. So, Nilsen and Livermore physicist Jim Scofield took on the challenge of recalculating the formulas using x-ray interferometry. According to Nilsen, their goal was to calculate the index of refraction for any material at any temperature, density, or photon energy. "We revised the numbers using both theoretical and experimental results."

To date, the new calculations have been incorporated into a number of computer codes, including the Inferno and OPAL codes, which are used to predict such physical characteristics of plasmas as opacity and equations of state. Gaining a better understanding of these characteristics brings scientists closer to myriad insights on subjects from thermonuclear charges to radiation transport to the evolution of stars.

—Maurina S. Sherman

Key Words: bound electrons, free electrons, fringe shifts, index of refraction, plasma density, x-ray interferometry.

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

Patents

Microfluidic Fuel Cell Systems with Embedded Materials and Structures and Method Thereof

Jeffrey D. Morse, Klint A. Rose, Mariam Maghribi, William Benett, Peter Krulevitch, Julie Hamilton, Robert T. Graff, Alan Jankowski

U.S. Patent 6,921,603 B2

July 26, 2005

In this process for fabricating microfluidic systems with embedded components, micrometer-scale features are molded into the polymeric material polydimethylsiloxane (PDMS). Micromachining is used to create a mold master, and the liquid precursors for PDMS are poured over the mold and allowed to cure. PDMS is then removed from the mold and bonded to another material, such as PDMS, glass, or silicon, after a simple surface preparation step is taken to form sealed microchannels.

Compact Refractive Imaging Spectrometer Utilizing Immersed Gratings

Scott A. Lerner, Charles L. Bennett, Jay V. Bixler, Paul J. Kuzmenko, Isabella T. Lewis

U.S. Patent 6,922,240 B2

July 26, 2005

This compact imaging spectrometer has an entrance slit for directing light, a first means for receiving the light and focusing the light, an immersed diffraction grating that receives the light from the first means and defracts the light, a second means for receiving the light from the immersed diffraction grating and focusing the light, and an image plane that receives the light from the second means.

Controlling and Operating Homogeneous Charge Compression Ignition (HCCI) Engines

Daniel L. Flowers

U.S. Patent 6,923,167 B2

August 2, 2005

A homogeneous charge compression ignition engine system includes an engine that produces exhaust gas. A vaporization means vaporizes fuel for the engine, and an air-induction means provides air for the engine. An exhaust-gas-recirculation means recirculates the exhaust gas. A blending means blends the vaporized fuel, exhaust gas, and air. An induction means inducts the blended vaporized fuel, exhaust gas, and air into the engine. A control means controls the blending of the vaporized fuel, exhaust gas, and air. It also controls inducting the blended vaporized fuel, exhaust gas, and air into the engine.

Thio-, Amine-, Nitro-, and Macrocyclic Containing Organic Aerogels and Xerogels

Glenn A. Fox, Thomas M. Tillotson

U.S. Patent 6,924,322 B2

August 2, 2005

Organic aerogels and xerogels are formed by a solgel reaction using starting materials that exhibit similar reactivity to the most commonly used resorcinol starting material. The new starting materials, including thio-, amine-, and nitro-containing molecules and functionalized macrocyclic molecules, will produce organic xerogels and aerogels that have improved performance in the areas of detection and sensor technology and water-stream remediation. Further development of these new organic aerogels and xerogels will yield material that can be extracted more easily than current organic aerogels.

Direct-Patterned Optical Waveguides on Amorphous Silicon Films

Steve Vernon, Tiziana C. Bond, Steven W. Bond, Michael D. Pocha, Stefan Hau-Riege

U.S. Patent 6,925,216 B2

August 2, 2005

An optical waveguide structure is formed by embedding a core material within a medium of lower refractive index (that is, the cladding). The optical index of refraction of amorphous silicon (a-Si) and polycrystalline silicon (p-Si), in the wavelength range between about 1.2 and 1.6 micrometers, differ by about 20 percent, with the amorphous phase having the larger index. Spatially selective laser crystallization of a-Si provides a mechanism for controlling the spatial variation of the refractive index and for surrounding the amorphous regions with crystalline material. In cases where an a-Si film is interposed between layers of low refractive index, for example, a structure composed of a silicon–oxygen substrate (SiO_2), Si film, and SiO_2 film, the formation of guided wave structures is particularly simple.

Apparatus and Method for Reducing Drag of a Bluff Body in Ground Effect Using Counter-Rotating Vortex Pairs

Jason M. Ortega, Kambiz Salari

U.S. Patent 6,926,345 B2

August 9, 2005

An aerodynamic-based drag reduction apparatus and method for bluff bodies, such as tractor-trailer trucks, uses a pair of lift surfaces extending to lift surface tips and located alongside the bluff body, for example, on the opposing left- and right-side surfaces. In a flow stream substantially parallel to the longitudinal centerline of the bluff body, the pair of lift surfaces generates a pair of counterrotating trailing vortices that join in the wake of the bluff body in a direction orthogonal to the flow stream. The confluence draws or turns the flow stream in and around behind the trailing end of the bluff body, raising the pressure on a base surface at the trailing end and thereby reducing the aerodynamic base drag.

Solid-Phase Microextraction Field Kit

Peter J. Nunes, Brian D. Andresen

U.S. Patent 6,929,778 B2

August 16, 2005

This field kit is used to collect, isolate, and concentrate trace amounts of residue from high explosives and biological and chemical weapons agents found in air, soil, vegetation, swipe, and liquid samples. The kit includes a number of solid-phase microextraction fiber and syringe assemblies. It also includes a sampling port, a protective cap for the fiber, an extractor for the protective cap, spare parts, a protective glove, and an instruction manual. The kit is enclosed in a hermetically sealed transportation container.

High-Power Laser Having a Trivalent Liquid Host

Earl R. Ault

U.S. Patent 6,931,036 B1

August 16, 2005

This high-power laser features a lasing chamber and a semiconductor-pumping device with trivalent titanium ions dissolved in a liquid host within the lasing chamber. Because the host is a liquid, it can be removed from the optical cavity when it becomes heated, avoiding the inevitable optical distortion and birefringence common to glass and crystal hosts.

Ion Mobility Sensor
Jackson C. Koo, Conrad M. Yu
U.S. Patent 6,933,496 B2
August 23, 2005
This ion mobility sensor can simultaneously detect both ions and molecules. Thus, one can measure the relative arrival times between various ions and molecules. Different ions have different mobility in air, and the ion sensor enables measurement of ion mobility. One can identify the various ions and molecules from these measurements. The ion mobility sensor, which uses a pair of glow discharge devices, can be designed for coupling with an existing gas chromatograph, where various gas molecules are already separated and the number of each kind of molecules is relatively small. In such a case, a conventional ion mobility sensor cannot be used.

Process for Direct Integration of a Thin-Film Silicon P-N Junction Diode with a Magnetic Tunnel Junction
Daniel Toet, Thomas W. Sigmon
U.S. Patent 6,933,530 B2
August 23, 2005
This process for direct integration of a thin-film silicon p-n junction diode with a magnetic tunnel junction is used in advanced magnetic random-access-memory cells of high-performance, nonvolatile memory arrays. The process is based on pulsed laser processing for the fabrication of vertical polycrystalline silicon electronic device structures, in particular p-n junction diodes, on films of metals deposited on low-temperature substrates such as ceramics, dielectrics, glass, or polymers. The process preserves underlayers and structures onto which the devices are typically deposited, such as silicon integrated circuits. The process involves the low-temperature deposition of at least one layer of silicon, either in an amorphous or a polycrystalline phase, on a metal layer. Dopants may be introduced in the silicon film during or after deposition. The film is then irradiated with short-pulse laser energy that is efficiently absorbed in the silicon, resulting in the crystallization of the film and simultaneously in the activation of the dopants by ultrafast melting and solidification. The silicon film can be patterned either before or after crystallization.

Free-Space Optical Communications Using Holographic Conjugation
Eddy A. Stappaerts
U.S. Patent 6,934,475 B2
August 23, 2005
A beacon beam is transmitted from a receiver to a transmitter. The transmitter generates and transmits a conjugate beacon beam back to the receiver, which is then interfered with a local oscillator beam to form a hologram. The hologram is used to configure a spatial light modulator as a diffraction grating. A conjugate communications laser beam containing information is subsequently transmitted to the receiver. The diffraction grating deflects the conjugate communications beam to a fixed and known direction, whereupon it is directed through a spatial filter. Because the direction of the conjugate communications beam is fixed and known, the diameter of the filter aperture can be minimized to accept the communications beam, while rejecting most of the background light. A high-speed detector directly detects the filtered conjugate communications beam. The detector output is transmitted to a demodulator, which extracts the information carried by the beam.

Awards

Livermore scientists **William Pitz** and **Charles Westbrook** of the Chemistry and Materials Science Directorate, along with other team members, received the **Society of Automotive Engineers** (SAE) **2003 Arch T. Colwell Merit Award**. The award was given for the paper entitled "Effects of Oxygenates on Soot Processes in DI Diesel Engines: Experiments and Numerical Simulations," which they coauthored with Charles Mueller, Lyle Pickett, and Dennis Siebers of Sandia National Laboratories. The paper was one of 11 honored at the SAE 2005 World Congress in Detroit in April.

Pitz says the recognized work is the result of "a productive and ongoing collaborative effort" with the Sandia researchers. The experiments and investigations were performed at Sandia, while the computer simulations were done at Livermore. Westbrook says that Livermore's computing resources have been used for the past 30 years to simulate chemical kinetics of hydrocarbon oxidation in automotive environments. He and Pitz are currently using chemical kinetic modeling to study the effects of different types of fuels in automotive engines.

The award, established in 1965, is named for the late Arch T. Colwell, who served SAE in many capacities for nearly 50 years. It annually recognizes the authors of papers of outstanding technical or professional merit. Papers are judged primarily for their value as new contributions to existing knowledge of mobility engineering.

Abstracts

Materials Scientists Discover the Power of ParaDiS

The strength of most crystalline materials, including metals, derives from the motion, multiplication, and interaction of defects called dislocation lines. Dislocation dynamics—the interaction among dislocation lines—is believed to be responsible for strain hardening, a property of metals in which a material's strength increases as deformation increases. By combining advances in supercomputing and materials experiments and characterization, Livermore scientists are providing insight on dislocation dynamics and how materials deform and fail in body-centered-cubic (bcc) metals, such as molybdenum and tantalum. A new Livermore code, called Parallel Dislocation Simulator (ParaDiS), models in unprecedented detail the mechanisms of dislocations. Results from the code's simulations indicate the presence of multijunctions, which tie together three or more dislocation lines into tight knots. Multijunctions were seen in images taken with a transmission electron microscope. At the same time, Livermore engineers have been conducting research on crystalline metals to validate ParaDiS simulations and to develop crystal-plasticity models, all as part of Livermore's multiscale modeling program of bcc metals.

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A Wide New Window on the Universe

The ground-based Large Synoptic Survey Telescope (LSST), scheduled for completion in 2012, will provide, for the first time, digital imaging of objects, including changing events, in deep space across the entire sky. Data from LSST's astronomical surveys will be accessible almost immediately to astronomers and the public over the Internet. LSST will have an 8.4-meter-aperture primary mirror and an enormous detector. The telescope will inventory celestial objects billions of light years away as well as near-Earth objects such as asteroids, comets, the Milky Way, dark matter, and dark energy. Lawrence Livermore researchers are participating in all aspects of the LSST project, from management to research efforts.

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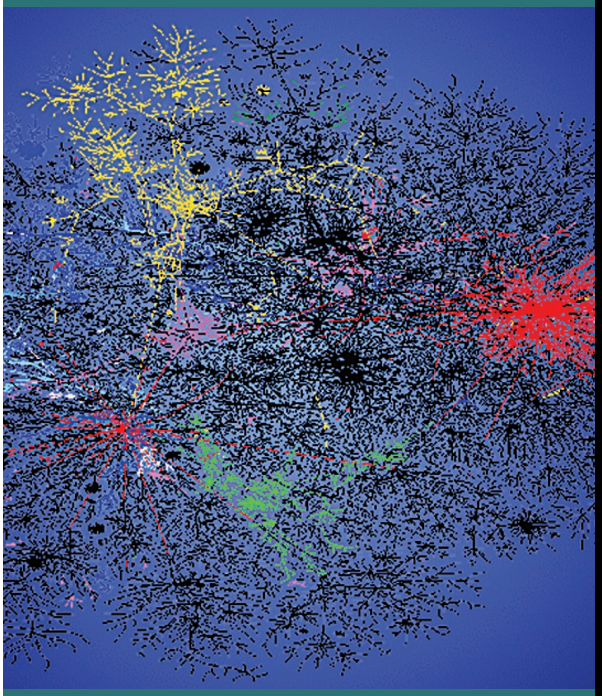
U.S. Government Printing Office: 2005/570-077-10013

Modeling the Future



Livermore scientists have developed a tool that simulates how changing demands may affect the nuclear weapons complex.

Also in December

• Radio astronomers search the universe for black holes that emit new stars.

• A study combining experiments with simulations demonstrates how food mutagens promote hormone-sensitive cancers.

• Engineers are certifying that Livermore's Site 300 facilities will protect high explosives if lightning strikes.

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