June 2006

Science & Technology REVIEW

National Nuclear Security Administration's
Lawrence Livermore National Laboratory

Tomorrow's Scientists and Engineers

Also in this issue:

- **Advances in Adaptive Optics**
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- **Global Climate in Year 2300**

About the Cover

Lawrence Livermore's Student Employee Graduate Research Fellowship Program provides University of California (UC) graduate students the opportunity to conduct research at the Laboratory while earning their Ph.D.s. The students apply to the program as a team with their university thesis advisor and a Laboratory mentor. As the article beginning on p. 4 describes, the students work on fundamental science in diverse areas across the Laboratory. On the cover, UC Berkeley student Ionel Dragos Hau holds a lithium fluoride crystal similar to one he and his Laboratory mentor, Stephan Friedrich, use for a neutron spectrometer.

Cover design: Amy Henke

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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Lawrence Livermore National Laboratory

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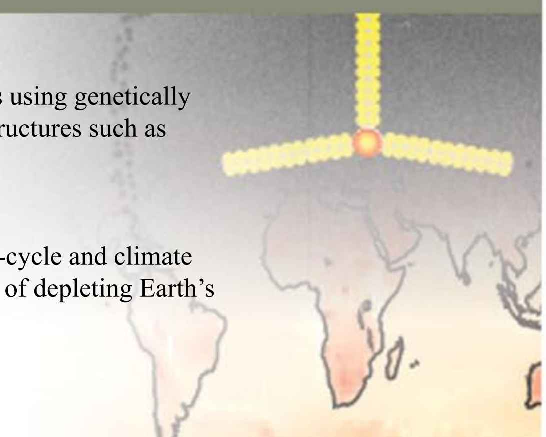

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Synthesizing noble metals under extreme conditions

Laboratory scientists, in collaboration with researchers from the Carnegie Institution of Washington and the Atomic Weapons Establishment in England, have synthesized a novel class of nitrides made from noble metals under extreme conditions. Noble metals are those that do not easily form compounds with other elements.

Using a diamond anvil cell to create high pressures and a laser to create high temperatures, the researchers made the first bulk nitride of the noble metal iridium. By combining experimental results with first-principle theoretical modeling, the scientists also have determined the structure of the known nitride of platinum as well as its bulk modulus (a measure of the material hardness). The semiconductor industry currently uses titanium nitrides because of their strength and durability. These new nitrides may prove to be even more durable than titanium.

"This work extends the scientific understanding of platinum and iridium nitrides," says lead author Jonathan Crowhurst of Livermore's Chemistry and Materials Science Directorate. "Demonstrating that these compounds exist and determining at least some of their physical properties should inspire the development of large-scale synthesis techniques to take advantage of their unusual properties." Other Livermore authors include Babak Sadigh, Cheryl Evans, James Ferreira, and Art Nelson. The research is presented in the March 3, 2006, issue of *Science*.
Contact: Jonathan Crowhurst (925) 422-1945 (crowhurst1@llnl.gov).

The evolution of icy moons

Researchers from the Laboratory, Kyushu University in Japan, and the U.S. Geological Survey found a "creep" or flow mechanism in a high-pressure form of ice that is affected by the grain size of the ice. High-pressure phases of ice are major components of the giant icy moons in the outer solar system. The convective flow of ice in the interiors of these moons has controlled their evolution and present-day structure.

Experiments were conducted in Livermore's Experimental Geophysics Laboratory under the conditions of pressure, temperature, stress, and grain size that mimic those in the deep interiors of large icy moons. Using a cryogenic scanning electron microscope, the researchers observed and measured creep as a function of grain size in a high-pressure phase of ice called "ice II." They proved that this new creep mechanism was related to grain size, something that previously had only been examined theoretically.

"These new results show that the viscosity of a deep icy mantle is much lower than we previously thought," says William Durham, a geophysicist in Livermore's Energy and Environment Directorate. The researchers conclude that it is likely the ice deforms by the creep mechanism in the interior of icy moons when the grains are up to a centimeter in size. "This newly discovered creep mechanism will change our thinking of the thermal evolution and internal dynamics of medium- and large-size moons of the outer planets in our solar system," says Durham. "The thermal evolution of these moons can help us explain what was happening in the early solar system." The team's research appeared in the March 3, 2006, issue of *Science.*
Contact: William Durham (925) 422-7046 (durham1@llnl.gov).

Oxygen breathed life into biological evolution

New research shows that many of the complex biochemical networks that humans and other advanced organisms depend on for their existence could not have evolved without oxygen. Livermore postdoctoral researcher Jason Raymond and Daniel Segrè of Boston University, who holds a joint appointment in Livermore's Biosciences Directorate, used computer simulations to study the effect of oxygen on metabolic networks, which are the biochemical systems that enable organisms to convert food and nutrients into life-sustaining energy. Their analysis shows that the largest and most complex networks—those found in humans and other advanced organisms—require the presence of molecular oxygen. The team's research appeared in the March 24, 2006, issue of *Science*.

Raymond and Segrè calculated the number of possible combinations of the thousands of enzymes and chemicals involved in all known metabolic reactions across the tree of life and came up with a "virtually limitless" number—10 to the 16,536th power. Simulating that many networks would be an impossible task even for Livermore's powerful supercomputers. To make the project manageable, the researchers used a statistical technique called Monte Carlo to randomly sample and simulate about 100,000 networks. "We found that all the types of networks fell into four different clusters of increasing size and connectivity," says Raymond. "In networks within the largest clusters, molecular oxygen was always present. Oxygen is the high-energy reactant that is needed for the growth of large, complex, multicellular organisms. Life as we know it was kick-started a few billion years ago by the oxygen-producing microbes."

The new findings also may imply that oxygen would be a good proxy for the search for intelligent life elsewhere in the universe. Furthermore, Raymond and Segrè's findings suggest that additional evolutionary secrets might be uncovered through the study of metabolic networks.
Contact: Jason Raymond (925) 423-6507 (raymond20@llnl.gov).

Maintaining Excellence through Intellectual Vitality

MEETING the ever-changing needs of national security requires constantly evaluating Livermore's programs and fostering new ideas in science and technology. An integral component of our plan for continually invigorating science and technology at the Laboratory is to recruit the brightest scientists and engineers. When Edward Teller cofounded the Laboratory, he understood that fostering an environment of intellectual vitality was necessary to maintain scientific and technological excellence. He also recognized the importance of providing next-generation scientists and engineers practical work experience while they are graduate students and postdoctoral researchers.

One of Teller's legacies is the Student Employee Graduate Research Fellowship (SEGRF) Program. For more than 40 years, this program has provided students from the University of California (UC) the opportunity to work part-time at the Laboratory while completing their dissertations. During their fellowships, the students are exposed to Livermore's multidisciplinary team approach that has been a hallmark of our successes. SEGRF, as part of a greater outreach effort managed by Livermore's University Relations Program, is among the Laboratory's most successful vehicles for recruiting tomorrow's workforce and for maintaining the intellectual vitality of our scientific and technological research.

Originally open just to students at UC Davis's Department of Applied Science, the SEGRF Program has expanded over the years to accept applications from all science and engineering departments at the 10 UC campuses. The Laboratory has been pleased with the results of the program's expansion and its continued robust performance. We are also pleased that SEGRF attracts a diverse group of students, not only in scientific and technological areas of interest but also in gender and race.

The article beginning on p. 4 reports on some of the fundamental research conducted by several current and former SEGRF students. They work with scientists and engineers across the directorates, from the National Ignition Facility Programs to Chemistry and Materials Science to Biosciences, in disciplines ranging from optical materials to detectors to advanced simulations. In one project, students are researching instruments to protect the nation from bioterrorist or radiological attacks. Students are also conducting studies to further our understanding of materials during phase transitions and under extreme temperatures and pressures. This research applies directly to our stockpile stewardship efforts to better understand metals as they age. Other research includes conditioning crystals for the National Ignition Facility and simulating the phase transitions of carbon.

The SEGRF Program is highly competitive, ensuring that we attract the brightest students. The students seed many interactions and collaborative research efforts. Students apply as a team that includes their UC thesis advisor and a Laboratory technical mentor. Some UC professors have sent us a continuing flow of high-quality students, strengthening the Laboratory's partnership with their campuses. One measure of the program's success is that over the past five years, 45 percent of the students have become Laboratory employees after completing their education.

Our next-generation scientists and engineers help us to remain a beacon of scientific inquiry and intellectual rigor. They share a passion for mission with our scientific and technical workforce that helps make it possible for Livermore to respond to new national challenges as they arise.

■ Cherry A. Murray is deputy director of Science and Technology.

A Livermore fellowship program provides students practical experience while they earn their doctorates.

Next-Generation Scientists and Engineers Tap Lab's Resources

THIS year, approximately 12,750 science and engineering students are enrolled in doctoral programs at the 10 University of California (UC) campuses. The academic requirements they must fulfill include researching and writing a thesis in their chosen field. About 50 fortunate students have been granted fellowships for up to four years to conduct research at the Laboratory using some of the most advanced facilities in the world while earning their Ph.D.s. This select group participates in Livermore's Student Employee Graduate Research Fellowship (SEGRF) Program.

The SEGRF Program traces its roots to the UC Davis Department of Applied

University of California (UC) at Davis student Erica McJimpsey works on one of the Laboratory's bioaerosol mass spectrometers.

Science (DAS), which was established at the Laboratory by Livermore cofounder Edward Teller in 1964. With a life-long commitment to science education, Teller recognized the need for a graduate program in applied science. He worked with UC administration to site a university-level education facility at the Laboratory and served as the first administrator of DAS. The SEGRF Program has supported students at DAS.

Over the years, graduate education opportunities at Livermore have grown to be broader than the disciplines emphasized in DAS. In 1999, the SEGRF Program opened to all UC Davis departments to meet the Laboratory's need for graduate students in areas such as laser physics, plasma diagnostics, fusion energy, accelerator technology, computational sciences, biosciences, materials science, and environmental and energy sciences. In 2001, the program opened to all UC campuses.

To apply for the SEGRF Program, students must pass their preliminary exams for Ph.D. candidacy, propose a project of interest to the Laboratory, and have a university thesis advisor and a Laboratory mentor. SEGRF recipients are selected from a pool of applicants by a committee of representatives from all of the Laboratory's directorates. In support of the directorates, Livermore's University Relations Program (URP) manages the SEGRF Program and facilitates interactions with UC campuses.

Paul Dickinson, who manages the SEGRF Program at Livermore, says, "To maintain the Laboratory's scientific and technological excellence, it is essential that we recruit bright, young scientists and engineers." SEGRF participants are half-time Laboratory employees during the academic year and full-time employees over the summer.

The program has achieved impressive results. Forty-five percent of SEGRF students become Laboratory employees. "Many of the other students go to other national laboratories or universities and collaborate with us on projects or become a resource for recruiting other students," says Dickinson.

Cornucopia of Experts

The Laboratory's longtime approach of using multidisciplinary collaborations to solve problems benefits the SEGRF Program. Erica McJimpsey, a UC Davis student and SEGRF participant, says, "I'm working with a team of engineers, biologists, computer scientists, physicists, and chemists, which is an advantage I wouldn't have in an academic environment." For her Ph.D. in analytical chemistry, McJimpsey is writing a dissertation on the characterization of single-particle ionization. She is working with the Laboratory's Bioaerosol Mass Spectrometry Group within the Chemistry and Materials Science Directorate.

In 2001, a Livermore team, originally funded by the Laboratory Directed Research and Development (LDRD) Program, developed the bioaerosol mass spectrometry (BAMS) system—the only instrument that can distinguish between two related but different spore species in less than 1 minute. The mass spectrometer

UC Berkeley student Ionel Dragos Hau (right) holds a lithium fluoride crystal similar to one he and his Laboratory mentor Stephan Friedrich (left) are using for a neutron spectrometer (forefront).

can also sort out a single spore from thousands of other particles. (See *S&TR*, September 2003, pp. 21–23; October 2005, pp. 8–9.) The BAMS team won a 2005 R&D 100 Award from *R&D Magazine* for developing the instrument. The Department of Defense's (DoD's) Technical Support Working Group and Defense Advanced Research Project Agency funded the Livermore team to develop BAMS for its potential use in identifying biological agents such as anthrax.

McJimpsey is working with the team to extend the spectrometer's capability for identifying signatures of proteins in individual spores. The team is using an ionization technique called matrix-assisted laser desorption ionization (MALDI) to analyze single particles and achieve greater sensitivity. In MALDI, the biomolecule of interest, often a protein, is irradiated with a laser. Because proteins are sensitive to temperature changes and can easily degrade, a chromophore (a molecule that absorbs light) is mixed with the protein to absorb the brunt of the energy from the laser.

Livermore has three BAMS instruments, one of which was modified by McJimpsey and two former SEGRF students, Scott Russell and Gregg Czerwieniec, to conduct the experiments using the MALDI technique. "At the Laboratory," says McJimpsey, "I can apply my passion for instrumentation toward an important homeland security mission." In addition to her professional goal of obtaining a DoD Presidential Management Internship to work on homeland security, McJimpsey also hopes to be a role model and mentor to minorities interested in pursuing careers in science.

In another homeland security effort, Ionel Dragos Hau, a nuclear engineering student at UC Berkeley and SEGRF participant, is working with Livermore's Advanced Detector Group to develop a novel type of neutron spectrometer as part of his thesis on neutron detection. One advantage of this neutron spectrometer is that its sensitivity is so high it can detect light elements, such as oxygen, within a heavy matrix such as plutonium. It can also detect nuclear material behind a heavy metal that would shield other types of radiation such as gamma rays. For example, if nuclear material were concealed in a lead object, the material's neutrons would interact with the lead and scatter in ways that provide a signature identifiable to the neutron spectrometer. The team uses lithium fluoride for the detector material because large crystals of it can be grown; the greater the size of the crystal, the greater the capability to detect neutrons.

Unlike spectrometers that collect electrical charges, this neutron detector collects heat in the form of phonons produced from a neutron reaction. A thermometer measures the rapid increase in heat, and the source of the nuclear material is revealed by the strength of the heat signal. However, because the heat has to flow out of the detector after each neutron interaction before another count can be taken, and phonons travel more slowly than electrons, the count rate is comparably lower than some types of gamma-ray detectors. Hau is working with the Livermore team to improve the spectrometer's count rate.

Laboratory postdoctoral researcher Faranak Nekoogar conducts research in ultrawideband radio-frequency identification systems.

Researchers, Authors, and Inventors

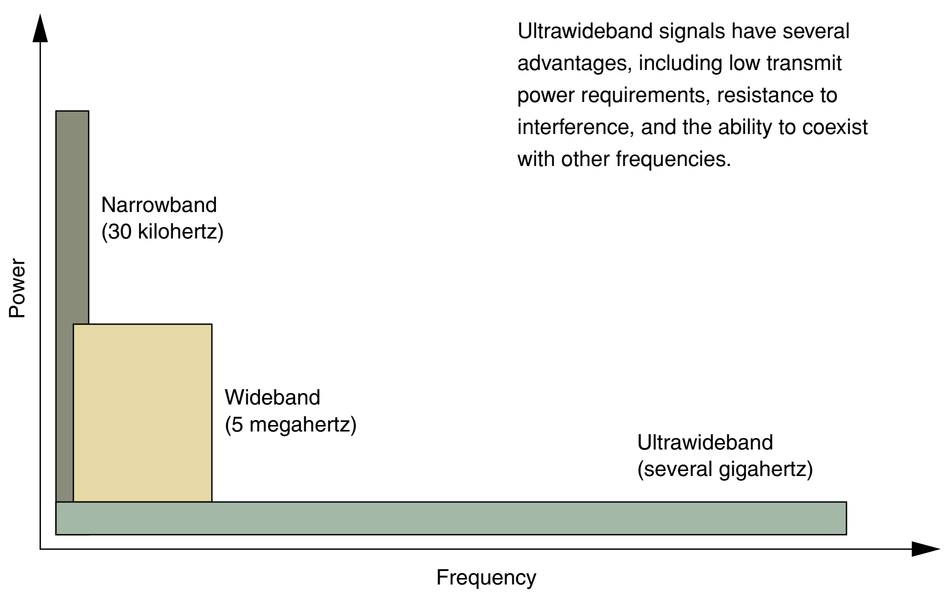
Livermore scientists and engineers benefit from the students' intellectual vitality and the fundamental research they conduct. The students greatly contribute to work that is publishable in papers, an important part of both the student's and the Laboratory scientist's career development. Some of the SEGRF students are well-seasoned authors by the time they complete their Ph.D.s. In addition to publishing articles on ultrawideband (UWB) communications, former SEGRF student Faranak Nekoogar, now a postdoctoral researcher in the Engineering Directorate, published two technical books and filed eight patents or records of inventions before completing her Ph.D.

UWB communication is fundamentally different from conventional communication systems because it employs extremely narrow (picoseconds to nanoseconds) radio-frequency pulses to communicate between transmitter and receiver. (See *S&TR*, September 2004, pp. 12–19.) Using short-duration pulses rather than continuous waveforms offers several advantages over traditional wireless technologies. They include large throughput, covertness, tamper-resistance to jamming, low transmit power, and the ability to coexist with current radio services.

A very low-power UWB radar system called micropower impulse radar (MIR) was invented in 1993 by Livermore electronics engineer Tom McEwan. It has been one of the most commercially successful licensed inventions both at Livermore and throughout the Department of Energy (DOE). Livermore won R&D 100 awards for two of the technologies that use MIR—an electronic dipstick (*S&TR*, October 1996, pp. 16–17) and a bridge inspection system (*S&TR*, October 1998, pp. 7–8). The Laboratory holds 30 MIR patents and patent filings, with Nekoogar's among them.

UWB pulses are safe to use around people and do not interfere with computers, digital watches, cellular phones, or radio and television signals. UWB technology could replace the interface between computers, printers, and entertainment devices in homes, providing a wireless network of integrated systems. Nekoogar says UWB technology could also overcome the power and range limitations of the current radio-frequency identification systems, providing more reliable monitoring of assets and people. In addition, it has potential use in tracking applications to prevent cargo-container tampering, provide situational awareness for soldiers, and help find lost children.

DoD and the Department of Homeland Security are interested in UWB technology for covert communications in mission critical applications. Nekoogar wrote her thesis on the use of UWB transmitted-reference (TR) methods that enable reliable wireless communications in harsh radio propagation conditions. For example, in the heavy metallic environment inside a ship, where conventional wireless technologies fail because multiple reflections of radio signals interfere with each other.



Ultrawideband signals have several advantages, including low transmit power requirements, resistance to interference, and the ability to coexist with other frequencies.

Nekoogar says the next step will be designing chips to carry UWB-TR systems. "We want to partner with industries that specialize in chip design." Chip design is the subject of the second book Nekoogar has authored; her first book describes the fundamentals of UWB communications.

Partnering with Industry

SEGRF students also have opportunities to partner with industry. As part of Nick Killingsworth's thesis on combustion control in homogenous charge compression ignition (HCCI) engines, the UC San Diego student works with Livermore engineers on an HCCI engine. "I had been studying HCCI technology at UC San Diego and, in particular, combustion control issues," says Killingsworth. "One day, I received an advertisement about the SEGRF Program. It was perfect timing. I contacted the Livermore team right away."

Caterpillar Inc. donated a six-cylinder, spark-ignited (SI) engine, which the Livermore team is converting to an HCCI engine in exchange for providing the company with research data. (See *S&TR*, April 2004, pp. 17–19.) The research is funded by the California Energy Commission's Advanced Reciprocating Internal Combustion Engine Program and DOE's Office of Energy Efficiency and Renewable Energy.

Combustion in HCCI engines is fundamentally different from that in SI and diesel engines. HCCI combustion involves thermal auto-ignition of a premixed fuel–air mixture, without the flame propagation found in SI engines or the mixing-controlled combustion found in diesel engines. HCCI engines can run extremely lean (low percentage of fuel and a high percentage of air), and the combustion temperature is low enough that the engine produces extremely low nitrogen oxide emissions (a few parts per million). Lean, premixed combustion also results in nearly zero particulate matter emissions.

However, HCCI engines present challenges that have kept them from commercialization. The main hurdles are combustion-timing control, low power output, and difficulty in starting when cold. At cold start, the compressed-gas temperature in an HCCI engine is low because the charge receives no preheating from the intake manifold and the compressed charge is rapidly cooled by heat transfer to the cold combustion chamber walls.

The Livermore team's novel solution is to start the engine directly in HCCI mode by preheating the intake with a gas-fired burner. Running the intake charge through the preheater while simultaneously spinning the engine with an air starter enables the HCCI engine to achieve ignition. After ignition, the combustion is self-sustaining, and the burner can be turned off.

Combustion-timing control, particularly under a range of speeds and loads, is the most challenging problem. The HCCI engine does not have a combustion trigger such as a spark plug or fuel injector. Instead, combustion is achieved by controlling the temperature, pressure, and composition of the fuel–air mixture. Multiple-cylinder engines pose an additional challenge because differences in pressure, temperature, and compression ratio invariably exist between the cylinders.

To address this problem, the Livermore team developed a thermal management system in which a controller detects cylinder-to-cylinder differences and adjusts the intake temperature of each cylinder for optimal combustion timing. Killingsworth is developing the control algorithms to regulate the opening and closing of the cylinders' valves.

The team plans to use the engine as a test bed for HCCI studies. HCCI technology can considerably improve fuel efficiency while providing unmatched flexibility in operating temperatures. At the same time, the technology will meet the stricter

UC San Diego student Nick Killingsworth (center) and his Laboratory mentors Daniel Flowers (left) and Salvador Aceves (right) are converting a Caterpillar spark-ignited engine to a homogenous charge compression ignition engine.

California standards for nitrogen oxide emissions, which go into effect next year.

Combining Talent for a Common Goal

Occasionally, former and present SEGRF students work together as a research team. Physicists Wren Carr and John Adams, both former SEGRF students and now Laboratory employees, are working with UC Davis SEGRF participant Paul DeMange. The team is conducting research relevant to the National Ignition Facility (NIF), the world's most energetic laser being constructed for the National Nuclear Security Administration's Stockpile Stewardship Program. (See *S&TR*, September 2002, pp. 20–29.)

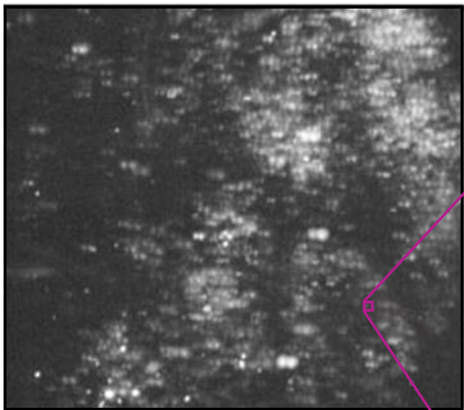
DeMange is investigating the fundamental processes associated with laser-induced damage in optical materials. His experiments have already led to five coauthored publications in journals such as *Applied Physics Letters* and *Optics Letters*. Many of DeMange's research experiments were performed using new instruments that he and Carr built to provide rapid, quantitative measurements of the density of damage sites in crystals.

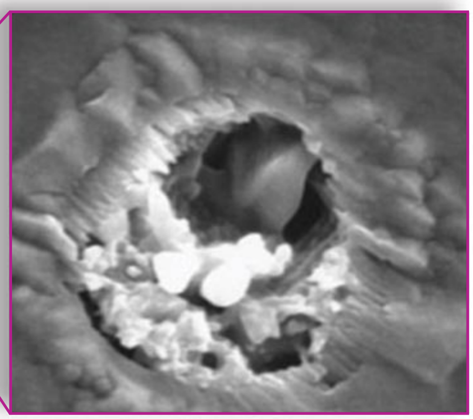
DeMange's early experiments investigated the effects of using different wavelengths to condition potassium dihydrogen phosphate crystals such as those used in NIF. Conditioning is the process of increasing a crystal's resistance to laser-induced damage by pre-exposing the crystal to subdamaging laser intensities. DeMange's results showed that the effectiveness of conditioning is sensitive to the wavelength of the laser light used, with shorter wavelengths providing a better level of conditioning. He also confirmed that exposure to two pulses of different wavelengths simultaneously resulted in more damage than that resulting from exposure to each wavelength separately.

Adams received his Ph.D. through DAS in 2002. While a SEGRF student, he discovered a widely tunable midinfrared laser material that has potential applications for remote sensing of a variety of atmospheric-borne chemicals. He also discovered a new electrooptic material for use at wavelengths near 1 micrometer, for which he earned a patent, and a new frequency-conversion material. Adams recalls being struck by the wealth of knowledge available to him as a student. "The Laboratory is so full of top-notch people that I can't imagine a better environment for a budding Ph.D. If I had a question while reading a journal article, I could often walk down the hall and ask the lead author for clarification. Or, if a piece of equipment broke, an expert was always around to help me. To have access to these resources as a student was phenomenal."

Adams and DeMange's studies are providing Carr with data he needs as

Laboratory physicists Wren Carr (center) and John Adams (right) collaborate with UC Davis student Paul DeMange (left) on the investigation of laser-induced damage in optical materials for the National Ignition Facility.





A scanning electron microscope image of a crystal shows the damage imprint left by a laser beam.

principal investigator for a $1.5 million LDRD project studying conditioning in crystals to mitigate laser-induced damage. Carr says, “Part of the purpose of the LDRD effort is to better understand the laser parameters that govern conditioning of crystals.” His work has focused on studying the mechanisms involved in energy deposition by low-intensity, visible, and near-ultraviolet laser light in a material, the mechanisms that govern laser-induced damage, laser machining, and laser conditioning.

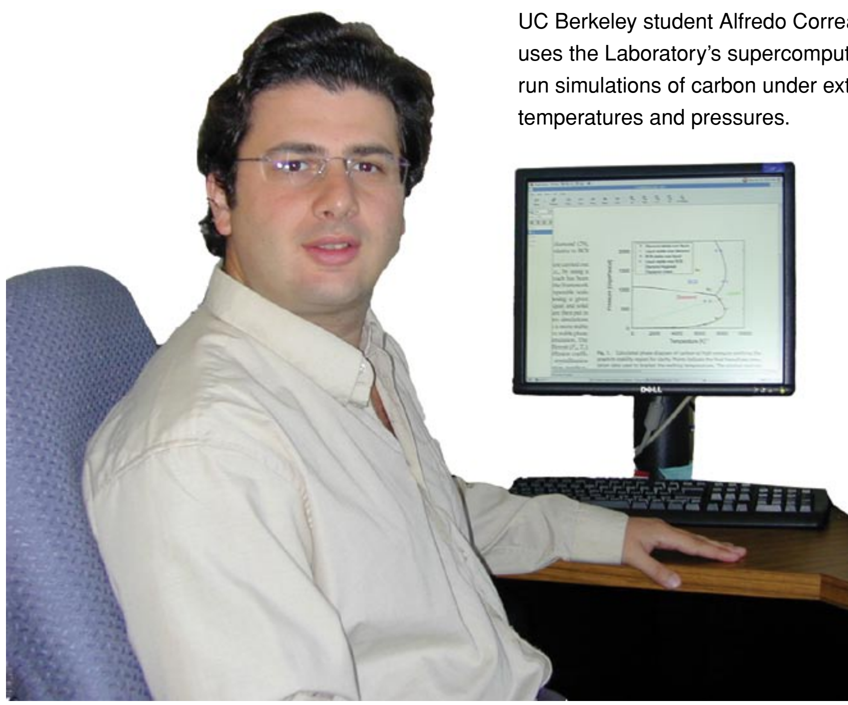
While a SEGRF student, Carr demonstrated that damage induced by a laser pulse a few nanoseconds long results in a tiny region inside the crystal reaching a temperature of 12,000 kelvins and a pressure of 250,000 atmospheres of pressure, far higher than had been theorized. The damage sites, which are only a few micrometers in diameter, were examined using a scanning electron microscope and were found to have the same general structure of craters made by underground explosions with 20 orders of magnitude more energy.

Are Diamonds Really Forever?

Laser-induced damage in optical materials is one example of modifications that result from extreme conditions. Studying materials exposed to extreme conditions often requires the use of simulations. SEGRF students have opportunities to conduct research using some of the fastest supercomputers in the world. Alfredo Correa-Tedesco, a theoretical physics student at UC Berkeley, uses the Laboratory’s 11-teraops (trillion operations per second) Multiprogrammatic Capability Resource (MCR) and 23-teraops Thunder machines to run three-dimensional simulations of carbon at high pressures and temperatures. Correa-Tedesco’s work is part of a study to determine carbon’s phase diagram.

Carbon is one of the most abundant elements in the universe. In its elemental form, carbon is found in coal, graphite, diamond, bucky balls, and nanotubes. These are materials with very different properties, yet at the microscopic level, they differ only by the geometric arrangements of atoms. Little is known about the phase boundaries and melting properties between different crystalline phases of carbon and liquid carbon. Experimental data are scarce because of difficulties in reaching a million atmospheres of pressure and thousands of kelvins in the laboratory.

Correa-Tedesco uses Qbox, a first-principles code developed by physicist Francois Gygi, formerly at Livermore and now at UC Davis. Qbox can simulate hundreds of atoms at a time



UC Berkeley student Alfredo Correa-Tedesco uses the Laboratory’s supercomputers to run simulations of carbon under extreme temperatures and pressures.

and allows the team to model the transition between two phases in a single simulation cell. "Modeling the coexistence of two phases is difficult," says Correa-Tedesco. "We need the supercomputing capabilities of MCR and Thunder. It takes three to four days and 400 processors of MCR for results, but it could take a year or more for such a simulation without them."

The team determined the solid–liquid and solid–solid phase boundaries of carbon for pressures up to 20 million atmospheres and more than 10,000 kelvins. "We expected to determine just the melting transition for one solid phase," says Correa-Tedesco. "Instead, we found the melting transitions for two solid phases of carbon and the transition between two phases of solid." The results will help researchers devise models of Neptune and Uranus, including an estimate of the planets' core temperatures.

The results will also provide valuable data for experimental studies used to characterize materials at extreme pressures. One of the experimental methods involves using a diamond anvil cell (DAC), which is a small mechanical press that forces together two brilliant-cut diamond anvils. (See *S&TR,* December 2004, pp. 4–11.) The diamond tips press on a microgram sample of a material to create extremely high pressures. Diamonds are used because they are the hardest known solid and can withstand ultrahigh pressures. They also permit x rays and visible light to pass unhampered through their crystalline structure.

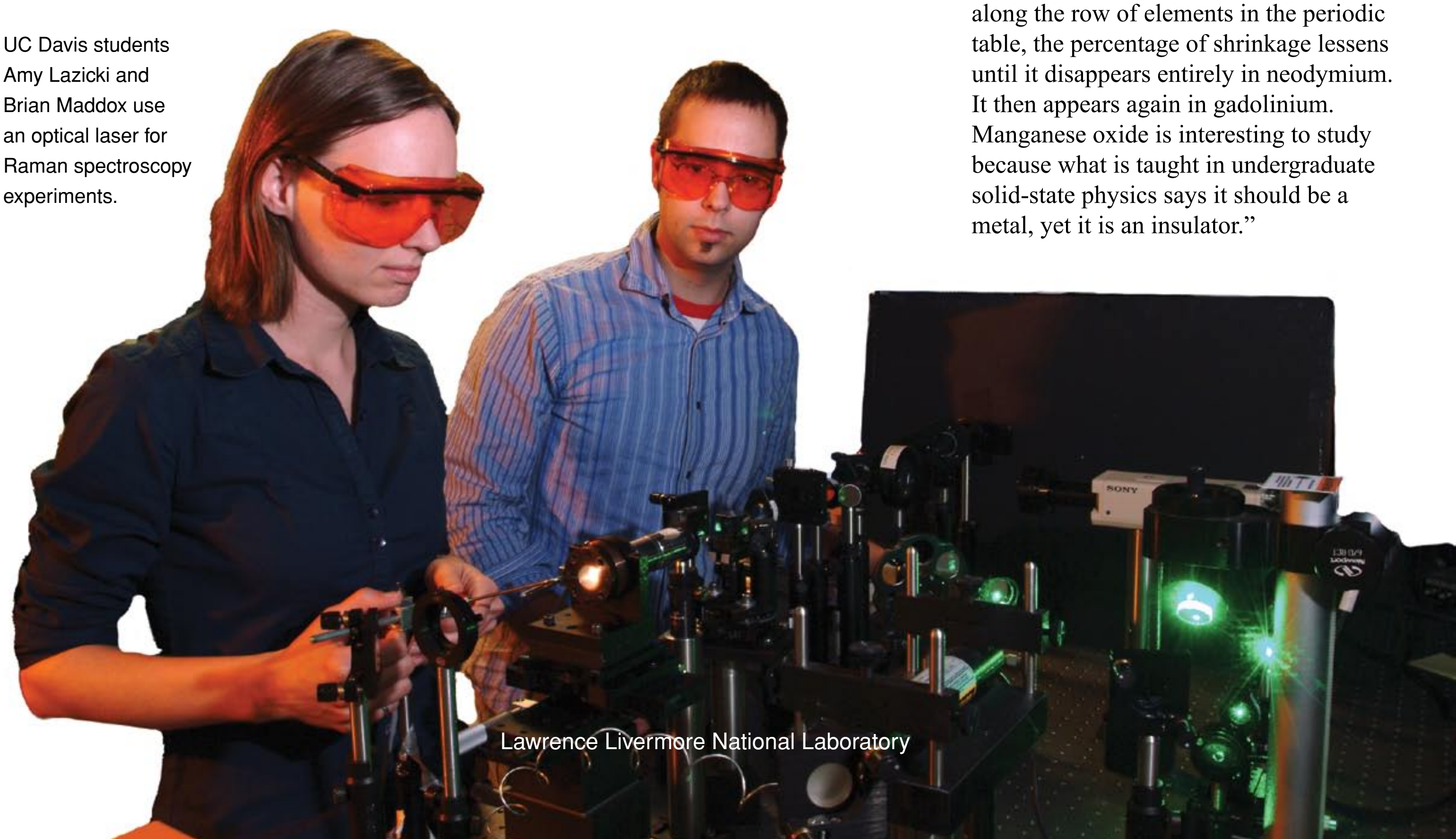
Because diamond is a form of carbon, understanding phase transitions of carbon provides insight on diamonds used in DAC. "Experimentalists are interested in knowing the limits of diamond, for example, at what temperature and pressure the diamond will be destroyed," says Correa-Tedesco. "They also want to know other characteristics about diamond, such as whether it becomes conducting at high temperatures."

The team discovered that diamond remains insulating—that is, resistant to the movement of its electrons—in the solid phase, while it metallizes at melting. Under extreme pressures, certain electrons, which are normally tightly held within an atom's inner electron bands or shells, can move about, resulting in changes in material properties and molecular structures. The transition is marked by a reduction in the sample's volume as the crystalline lattice shifts to accommodate the new electronic configuration.

Resolving Theoretical Mysteries

Two SEGRF students from UC Davis, Brian Maddox and Amy Lazicki, are combining a DAC with x-ray diffraction techniques to study the effects of pressure on the electronic structure of certain materials during the phase transitions. Maddox works in the Physics and Advanced Technologies Directorate studying transition metal compounds, such as manganese oxide, and rare-earth metals, such as the lanthanides cerium, gadolinium, and praseodymium, all of which exhibit large volume collapses at high pressure. The lanthanides are important to study because the same volume shrinkage occurs in the actinides, which are the elements belonging to the row in the periodic table below the lanthanides and include the nuclear weapon metals plutonium and uranium.

Maddox says, "When we apply pressure to cerium, its volume shrinks by about 17 percent. However, the structure of the material doesn't change. As we move along the row of elements in the periodic table, the percentage of shrinkage lessens until it disappears entirely in neodymium. It then appears again in gadolinium. Manganese oxide is interesting to study because what is taught in undergraduate solid-state physics says it should be a metal, yet it is an insulator."



UC Davis students Amy Lazicki and Brian Maddox use an optical laser for Raman spectroscopy experiments.

One of the theories to explain the volume shrinkage is the Mott transition theory. The theory proposes that pressure could drive manganese oxide from its anomalous insulating state to a metallic state. Until the invention of the DAC, experimental methods for detecting this type of transition of a substance at high pressure were not available. Maddox's experiments may help determine if the Mott transition theory is correct.

Maddox conducts his experiments using elastic x-ray scattering techniques, such as angle-dispersive x-ray diffraction (ADXRD), and inelastic x-ray scattering techniques, such as x-ray emission spectroscopy and resonant inelastic x-ray scattering. For many years, researchers have conducted inelastic scattering experiments on large samples at room temperature. However, until advancements were made in the synchrotron—a particle accelerator that boosts the velocity of electrons to nearly the speed of light—the techniques could not be applied to high-pressure samples inside a DAC. In ADXRD experiments, researchers send a beam of highly focused x rays through a sample in the DAC and record the diffraction pattern on an image plate detector, which is sensitive to x rays. Changes in the diffraction pattern reveal how a material's structure responds to pressure. Maddox used the synchrotron at Argonne National Laboratory's Advanced Photon Source (APS) to conduct his experiments on manganese oxide. The results showed a transition at 300 kelvins and 1.07 million atmospheres of presure. "These results confirmed that the compound exhibits similarities to transitions in the lanthanides and actinides as has been predicted," says Maddox.

Lazicki also uses the APS synchrotron and a DAC to conduct ADXRD and x-ray Raman spectroscopy experiments on lithium compounds, such as lithium oxide and lithium nitride, which are analogs to hydrogen-containing materials. X-ray diffraction techniques, including ADXRD, require more than one electron to map the position of an atom's electrons. Hydrogen has only one electron, so researchers often use hydrogen's nearest neighbor lithium, which has three electrons, to further their understanding of the nature of hydrogen compounds.

The team's results for lithium nitride showed the first experimental evidence that this compound undergoes a phase transition near 395,000 atmospheres of pressure. "The transformation represents a state that is uncommonly stable and compressible up to at least 2 million atmospheres of pressure," says Lazicki. "Lithium nitride is also one of the most difficult materials to metallize, with the metallization transition predicted to occur at 80 million atmospheres of pressure."

Maddox notes that although he works with an experimental group at Livermore, his advisors at Davis are theoretical physicists working on computational models. Maddox and Lazicki's data are useful feedback for their studies.

Maintaining Vision of Excellence

Over the years, the SEGRF Program has provided hundreds of young scientists and engineers a springboard to their professional careers. In exchange, the students have helped vitalize the Laboratory's research efforts and conducted studies of important fundamental science.

After graduation, many of the students remain at Livermore to contribute toward its national security missions. Dickinson notes, "The program has proven to be an important recruiting vehicle for building and maintaining scientific and engineering excellence at Livermore."

—Gabriele Rennie

Key Words: bioaerosol mass spectrometry (BAMS) system, Department of Applied Science (DAS), diamond anvil cell (DAC), homogenous charge compression ignition (HCCI), matrix-assisted laser desorption ionization (MALDI), neutron spectrometer, potassium dihydrogen phosphate, Qbox, Student Employee Graduate Research Fellowship (SEGRF) Program, ultrawideband (UWB) communications.

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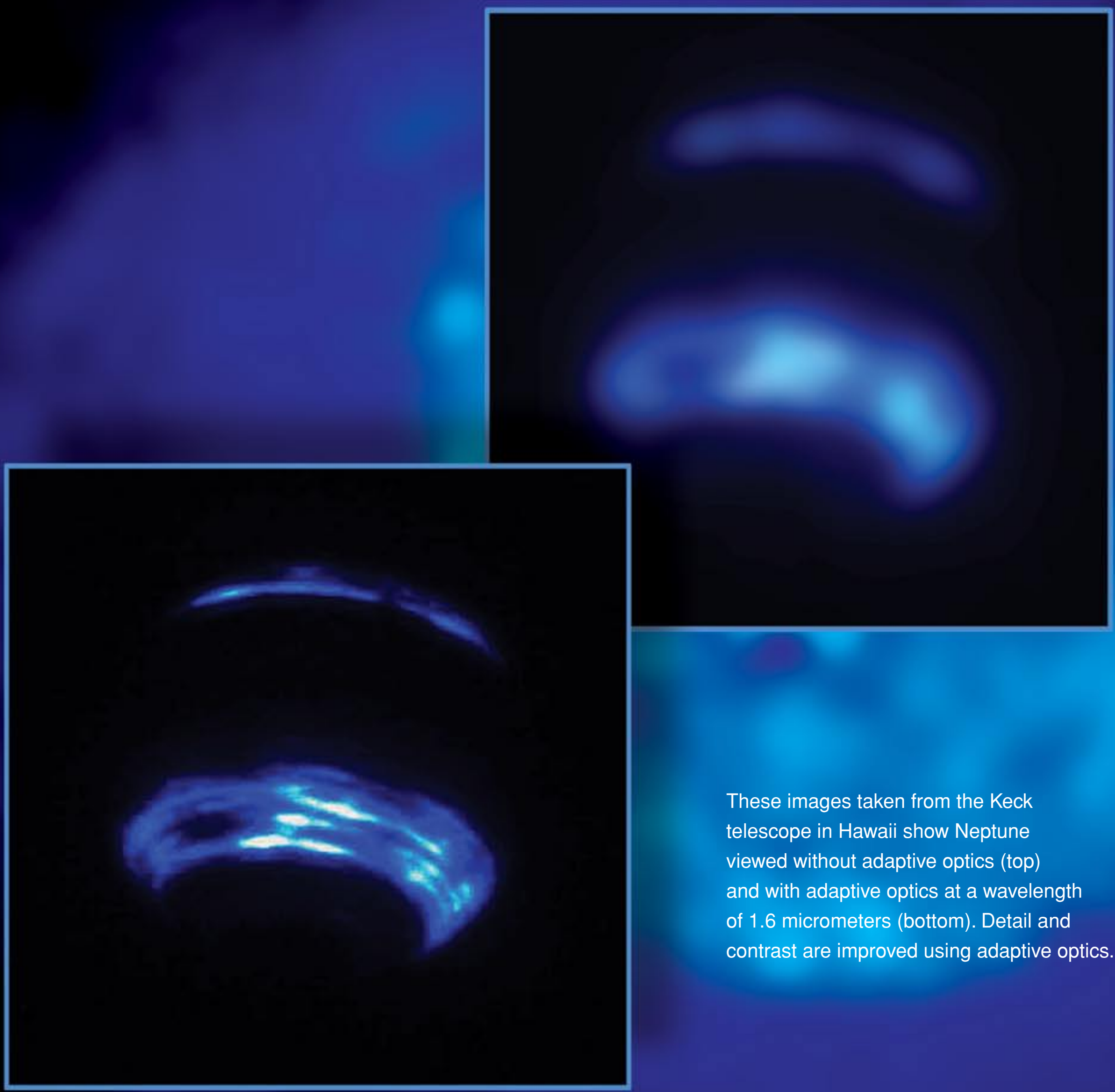
ADAPTIVE OPTICS PROVIDE A CLEARER



These images taken from the Keck telescope in Hawaii show Neptune viewed without adaptive optics (top) and with adaptive optics at a wavelength of 1.6 micrometers (bottom). Detail and contrast are improved using adaptive optics.

The Center for Adaptive Optics, with strong participation by Livermore researchers, advances a revolution in how we see.

FROM astronomers training their telescopes on the faintest pinpoints of light to newspaper readers straining to read small print, the demand persists for images that are clear and sharp. The Center for Adaptive Optics (CfAO), a National Science Foundation Science and Technology Center, is showing how to sharpen images with adaptive optics (AO) systems. Founded in 1999, the center researches AO in the fields of astronomy and vision science so that astronomers can more clearly visualize distant galaxies, stars, and planets and physicians can better diagnose eye diseases and more accurately prescribe corrective lenses. (See the box below.)

Adaptive Optics: A Short Primer

Whenever light from stars passes through the atmosphere, it becomes distorted by layers of air with different temperatures and densities. As a result, we see a shimmering or twinkling orb instead of the distinct and steady pinpoint of light seen from space.

Adaptive optics (AO) corrects the wavefronts of light, "straightening" them so that stars, galaxies, and other celestial objects gain resolution and contrast. AO systems work best with longer wavelength light, that is, light in the infrared region of the electromagnetic spectrum. Conceived in the 1950s by astronomers, AO was developed in the 1970s for laser beam propagation as part of the U.S. Strategic Defense Initiative.

Current AO systems use a wavefront sensor to sample the light that is being collected by the telescope's primary mirror. Only about 1 percent of the sky contains stars sufficiently bright to be of use as a reference beacon for an astronomical AO system. An alternative to a natural star is an artificial star made by a laser. Laser guide stars use a laser trained in the vicinity of the astronomical object of interest. The wavefront sensor takes hundreds or thousands of samples per second of the atmosphere-distorted light from the natural or artificial reference beacon, while sending the data to a computer that controls a deformable mirror. The mirror is adjusted by many tiny actuators, canceling the distortions of the atmosphere while it images the object of interest.

One way to escape the adverse effects of Earth's atmosphere is to place telescopes in space. However, spaced-based observatories, such the National Aeronautics and Space Administration's Hubble Space Telescope, are extremely costly to build and operate and must be compact for launching. Land-based telescopes equipped with the latest AO systems have the potential to provide several times greater resolution than Hubble in the infrared region.

The center is headquartered at the University of California at Santa Cruz (UCSC), one of the world's leading institutions for research in astronomy and astrophysics. UCSC is the home of UC Observatories, which operates the Lick Observatory on Mount Hamilton in California and is one of the partners in the Keck Observatory on the dormant volcano Mauna Kea in Hawaii.

The CfAO is one of the National Science Foundation's 13 Science and Technology Centers, the first of which was established in 1987 to fund fundamental research and create educational opportunities. The centers also encourage technology transfer, provide innovative approaches to interdisciplinary research, and emphasize partnerships.

The CfAO directly funds researchers nationwide and administers a growing network of partners that include universities, national laboratories, observatories, medical research centers, and private industry. Center partners develop AO systems that combine advanced technologies such as precision optics, wavefront sensors, deformable mirrors, lasers, and control systems. The center also helps transfer information about developments in AO from research laboratories to commercial entities and the broader scientific community.

Livermore physicist Scot Olivier, who is the center's associate director of knowledge transfer and partnerships, says, "Frequent interchanges occur between the center, universities, and private industry." Olivier also leads Livermore's 20-member Adaptive Optics Group. "Through its partnerships with industry," says Olivier, "the center is building an industrial base; researchers can now buy equipment that didn't exist just a few years ago, such as silicon-based MEMS [microelectromechanical systems] for deformable mirrors."

Other Livermore researchers also play a major role in the CfAO organization and participate in its activities. Claire Max, Livermore astrophysicist and UCSC professor of astronomy and astrophysics, is the center's director. Former Livermore engineer Don Gavel is the center's associate director of AO for extremely large telescopes. About 10 other Livermore employees, as well

Laboratory for Adaptive Optics

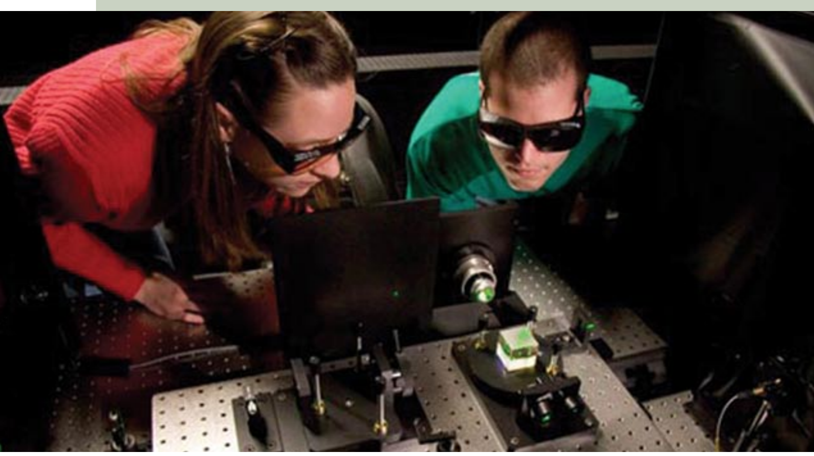
In August 2002, the Center for Adaptive Optics (CfAO) at the University of California at Santa Cruz received a six-year, $9.1-million grant from the Gordon and Betty Moore Foundation to establish a Laboratory for Adaptive Optics. This new facility, the first comprehensive university laboratory dedicated to adaptive optics (AO) in the U.S., supports the center's mission to advance and disseminate AO technology.

Researchers use the laboratory to develop prototypes of advanced AO equipment and concepts and test them in a controlled laboratory setting. The laboratory also serves as a training facility where researchers and students gain experience with AO equipment.

The laboratory currently focuses on developing equipment for extreme AO to directly image planets around nearby stars and on multiconjugate AO to account for the effects of turbulence at different levels in the atmosphere and over a much larger area of the sky. Livermore astrophysicist Bruce Macintosh will use the laboratory to integrate and test the Gemini Planet Imager, which is designed for the Gemini South Telescope to look for planets around other stars. Multiconjugate AO will be featured on the planned Thirty Meter Telescope.

Claire Max, director of the CfAO, notes that the center previously did not have laboratories or experimental facilities directly associated with it. "The Laboratory for Adaptive Optics gives us a capability that will be the foundation for many future projects and significant advances in AO systems," says Max.

"We test new components and new algorithms under controlled conditions and compare different ways of optimizing the performance of adaptive optics systems," says Max. "One of the problems with testing equipment on a telescope is that one never knows exactly what the atmosphere is doing during the test, whereas in the laboratory one can simulate what the atmosphere might do."



At the Laboratory for Adaptive Optics, researchers develop prototypes of advanced adaptive optics equipment and concepts and test them in a controlled laboratory setting. The laboratory also serves as a training facility for researchers and students. Pictured are graduate students Katie Morzinski (left) and Mark Ammons.

as a Student Employee Graduate Research Fellowship participant (see the article on p. 4), are involved in center-sponsored research. In addition, every year several college students complete internships at Livermore under center sponsorship. Livermore research on AO technology supports several of the Laboratory's national security projects such as long-range surveillance for homeland security and high-power lasers for stockpile stewardship.

In the field of astronomy, CfAO researchers equip existing telescopes with innovative AO systems, and they design advanced AO systems for planned extremely large telescopes. In astronomical AO systems, light is first detected from either a bright star or a laser guide star, which serves as a reference beacon shining through the atmosphere. The system's wavefront sensors then analyze the distortions of the light caused by atmospheric aberrations. These distortions are removed by the adjustment of an "adaptive" component, usually a deformable mirror, allowing for a sharper view of the fainter, more distant celestial object of interest.

The vision-science instruments designed by center-affiliated researchers use AO in ways somewhat similar to telescopes. A laser is focused on a retina, and the reflected light is analyzed by a wavefront sensor. Actuators fed by data from the sensor continually change the surface of a deformable mirror to provide the necessary compensations for obtaining a clear image of the optical structures in the eye.

AO for Giant Telescopes

One of the CfAO's major efforts is to study the requirements for extremely large optical telescopes, whose primary mirrors range from 30 to 100 meters in diameter. AO for these giant telescopes will allow scientists to achieve major advances in their knowledge of the universe. The center is developing long-range partnerships

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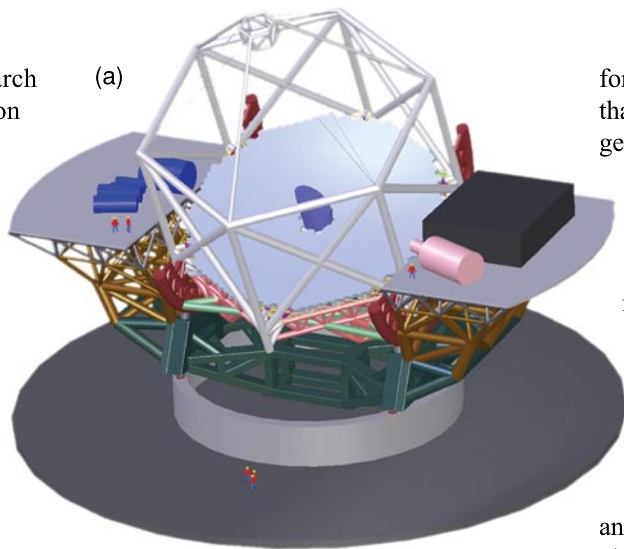

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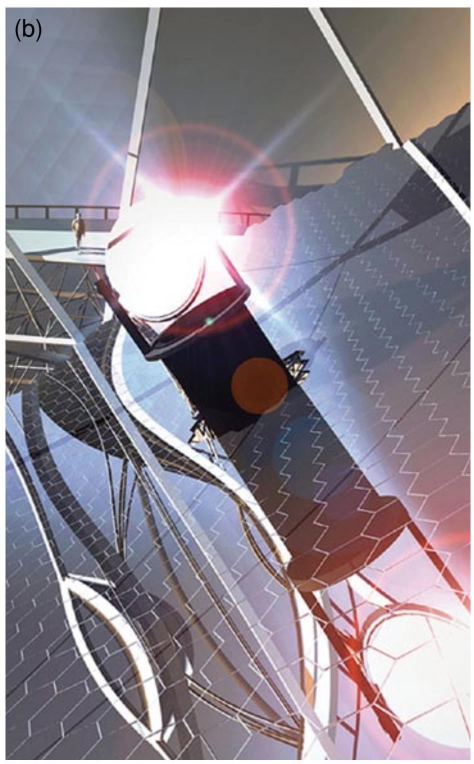


(a) The Center for Adaptive Optics is playing an important role in the Thirty Meter Telescope (TMT) Project, which will allow astronomers to detect the most distant objects in the universe. (Image courtesy of the TMT Project/Todd Mason, Mason Productions.) (b) The design of the 30-meter-diameter telescope is based on more than 700 hexagonal-shaped mirror segments. (Image courtesy of the TMT Project.)

for working on key AO technologies that will be required to operate this new generation of telescopes. The technologies include improved deformable mirrors, wavefront sensors, and artificial guide stars.

The center is playing a key role in the Thirty Meter Telescope (TMT) Project, a collaboration between UC, the California Institute of Technology, anda number of Canadian universities. The optical–infrared telescope will allow astronomers to resolve detail in early galaxies and planetary systems and detect the faintest and most distant objects in the universe. The center's new Laboratory for Adaptive Optics is used for developing one of TMT's AO systems. (See the box on p. 16.)

The TMT design is based on more than 700 hexagonal-shaped mirror segments that stretch 30 meters in diameter. The design fulfills the conceptual goals of the Giant Segmented Mirror Telescope, which was identified by the National Academy of Sciences as the highest priority, ground-based facility for the first decade of the 21st century. Livermore astrophysicist Bruce Macintosh has completed a feasibility study for extrasolar planet detection using TMT. Full-science operations of the telescope are scheduled to begin as early as 2015 on a site to be chosen in 2007.

Laser Guide Stars

The CfAO is developing advanced technologies for laser guide stars that produce artificial reference beacons in the atmosphere. A new generation of laser guide stars, some of which are being developed by Livermore physicist Deanna Pennington, will be combined into multiconjugate AO systems. These systems will deploy multiple lasers and wavefront sensors that compensate for distortions at different altitudes over a wider area.

Pennington is working on fiber lasers that will replace the dye lasers used on the world's first two fully functional laser-guide-star AO systems. Both of those AO systems—one on the 3-meter Lick telescope and the other on the 10-meter Keck 2 telescope—were designed by Livermore scientists. The new lasers are similar to the laser used on the front end of the National Ignition Facility at Livermore and are an adaptation of lasers used in the telecommunications industry. Guide-star AO systems based on fiber lasers will be much more compact, robust, and cost-efficient. A prototype system is planned for deployment on a telescope within two years.

The center is also helping astronomers pursue astronomical science projects using laser guide stars. Max is using Lick and Keck observatories to study the formation of galaxies in the early universe. She is also developing methods and procedures for efficient use of the laser-guide-star AO systems, methods for data analysis, and ways to study nearby galaxies with active black holes in their cores.

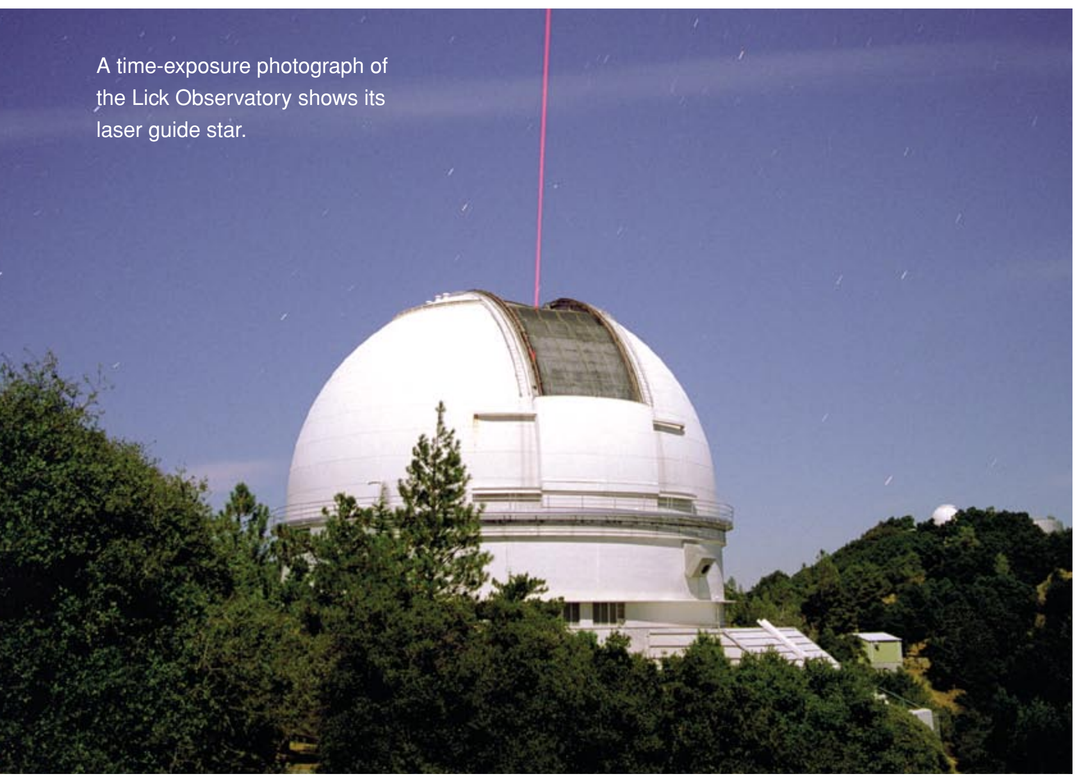
Looking for Planets

Effectively probing the environments of distant stars in a search for planets requires the development of next-generation, high-contrast AO systems. These systems are sometimes referred to as extreme AO. Macintosh says direct imaging of planets is challenging because planets such as Jupiter are a billion times fainter than their parent stars. "Detection of the youngest and brightest planets is barely within reach of today's AO systems," he says. "To see other solar systems, we would need new tools."

In 2005, Livermore was selected as the lead institution to build the Gemini Telescope Planet Imager for the Gemini South Telescope. The Gemini Observatory is a multinational institution that operates two 8-meter-diameter optical–infrared telescopes, one in Hawaii (north) and one in Chile (south).

Livermore will partner with seven universities and institutions in the U.S. and Canada to build the new instrument. "The Gemini Planet Imager will be the most advanced AO system in the world," says Macintosh. The system will have a 2-centimeter-square deformable mirror with 4,000 actuators. This deformable mirror will be made of etched silicon MEMS, similar to microchips, rather than the large reflective glass mirrors used on older AO systems. The new mirror will correct for atmospheric distortions by adjusting its shape 2,500 times per second with an accuracy of better than 1 nanometer. When the imager is operational in 2010, astronomers will be able to detect planets 30 to 150 light years from our solar system.

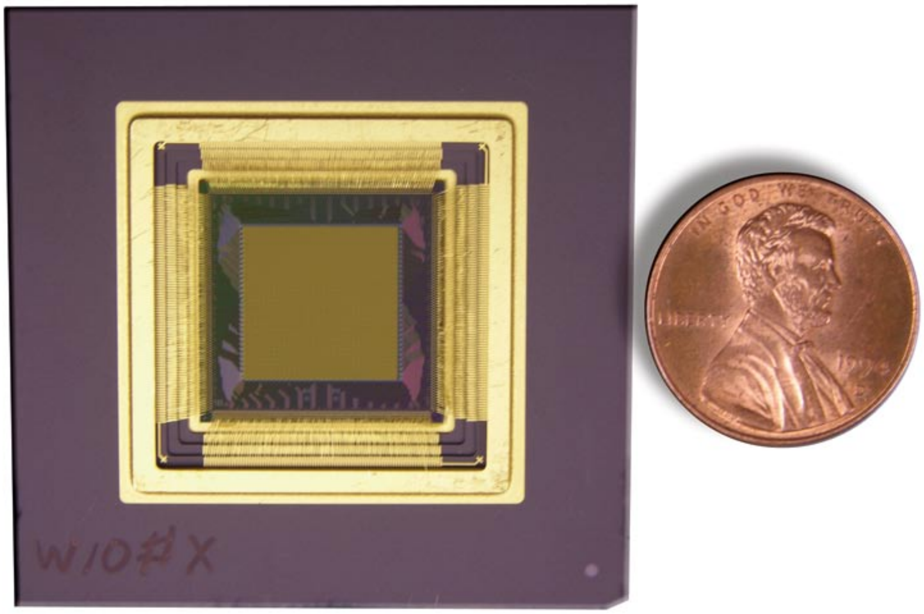
Macintosh, the lead developer of the Gemini Planet Imager, has been working with the center's Laboratory for Adaptive Optics, which features an extreme AO test bed. The Gemini Planet Imager will use an imaging infrared spectrograph to detect and characterize extrasolar planets. The goal is to find young, extrasolar planets orbiting nearby stars, using advanced infrared image-processing techniques to separate planets from other, much brighter celestial objects and system "noise." With funding from Livermore's Laboratory Directed Research and Development Program, Macintosh is currently using existing AO to probe dust and possible planets in nearby solar systems, and he is developing technology needed for Gemini.



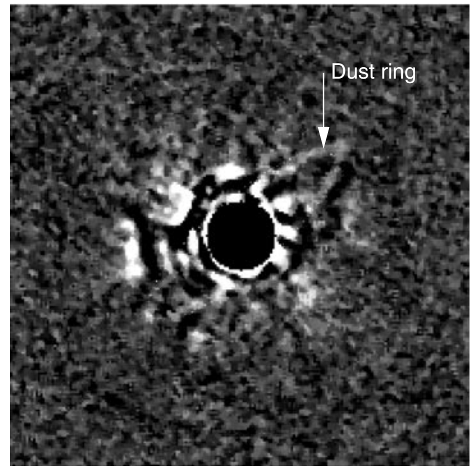
A time-exposure photograph of the Lick Observatory shows its laser guide star.

Revolutionizing Vision Science

Technology derived from AO research for astronomy is being adapted to measure aberrations in the eye. AO promises to revolutionize vision science by allowing physicians to measure the optical imperfections of the living eye with unprecedented thoroughness and accuracy. Physicians will also be able to diagnose tiny retinal defects before they become a threat to healthy vision. In all, the CfAO has spawned more than a dozen vision-science AO instruments.



This prototype deformable mirror made of an etched silicon microelectromechanical system has 1,024 actuators that adjust the shape of the mirror hundreds of times per second.



Livermore astrophysicist Bruce Macintosh used the Keck telescope and adaptive optics to obtain this image of the young star HR4796. The image shows a tilted dust ring. The star is masked out by an occulting spot. The image has been processed to highlight the ring, which results in white and black artifacts close to the star.

The vision instruments direct a weak laser beam into the retina, and the perturbed wavefront of the light reflected off the retina is then analyzed with a sensor. Data from the sensor is used to adjust the shape of an adaptive mirror so it compensates for the distortions. The resulting image can be used to provide prescriptions for eyeglasses and contact lenses as well as a more accurate diagnosis of retinal disease.

AO is poised to transform the phoropter, the standard binocular device used to test vision and calculate lense prescriptions. A team of Livermore physicists and engineers, with other collaborators, has developed an optical instrument called the MEMS-based adaptive optics phoropter (MAOP). The device received a 2003 R&D 100 Award from *R&D Magazine* for being one of the most significant high-technology inventions of the year. (See *S&TR*, October 2003, pp. 12–13.)

The instrument uses a wavefront sensor that measures the aberrations in a patient's eyes and then adjusts the surface of an adaptive mirror to correct the visual flaws. The MAOP can detect and correct for aberrations that conventional phoropters cannot. In this way, results from the MAOP can be used to design contact lenses that produce 20:10 eyesight or to guide laser surgery for vision correction. (These enhanced corrections cannot easily be incorporated into eyeglasses because different portions of the lenses are used for different gaze directions.) Bausch & Lomb, an industrial partner of the CfAO, is conducting clinical trials of the instrument.

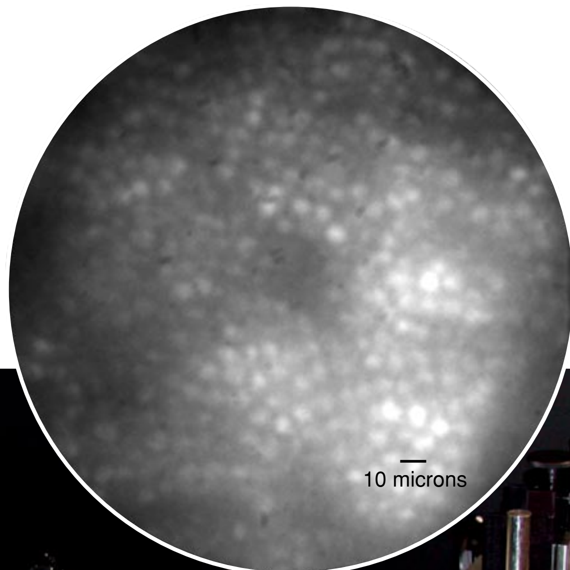
With support from the Department of Energy, the National Institutes of Health, and the National Science Foundation, researchers are incorporating AO technology into vision instruments so clinicians can more effectively diagnose such retinal diseases as glaucoma and macular degeneration. One such instrument is the scanning laser ophthalmoscope (SLO), which scans a low-power laser beam across the retina to build up an image. When confocal imaging is added to the SLO, image contrast increases as the focal length is adjusted and images are recorded at different depths within the retina. With the addition of an AO system, the instrument produces error-free images of the internal structures of retinal cells with improved resolution. In this way, ophthalmologists can watch individual blood cells moving through tiny blood vessels in the retina and, as a result, detect retinal diseases earlier.

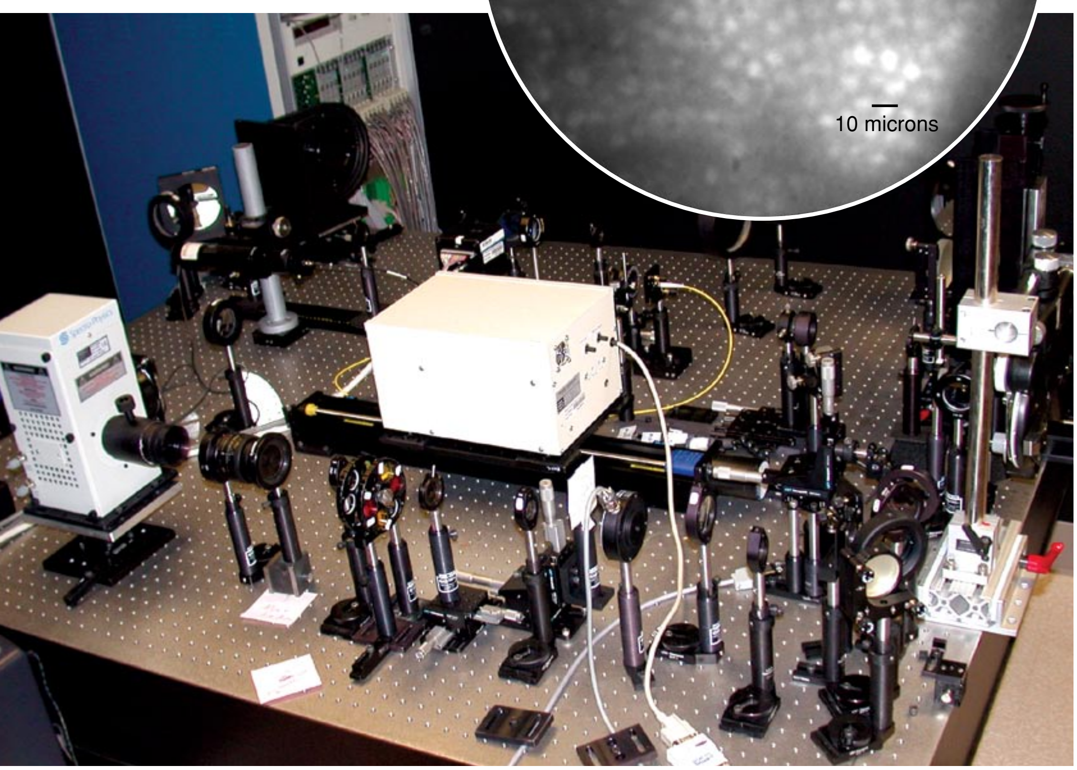
Another technique, optical coherence tomography (OCT), is used increasingly among ophthalmologists to diagnose and monitor retinal disease. OCT makes noninvasive measurements of the thickness of retinal layers, such as the nerve-fiber layer that thins in patients with glaucoma. Several groups nationwide have combined AO with OCT to make possible the first noninvasive three-dimensional (3D) visualization of the human retina at the cellular level.

"Adaptive optics is currently the only option for studying living retinal tissue at the cellular level," says Olivier. He notes that an AO system can compensate for tiny fluctuations in eye muscles, which means during an examination, the eye would not have to be temporarily paralyzed.

Livermore's AO Group is involved in two, five-year Bioengineering Research Partnerships (BRPs) funded by the National Institutes of Health. Both efforts are outgrowths of CfAO-funded research at Livermore and elsewhere to develop instruments for high-resolution retinal imaging. The goal is to develop and test clinical ophthalmic instruments using MEMS AO devices to revolutionize the diagnosis and treatment of the diseases that cause blindness and to develop techniques for vision correction in the general population.

The first BRP is led by the University of Rochester and includes UC Berkeley, Livermore, Indiana University, and the University of Southern California's Doheny Eye Institute. In this effort, Livermore's AO Group is developing a portable, MEMS-based, AO confocal scanning laser ophthalmoscope for use at the Doheny Eye Institute.





This adaptive optics ophthalmoscope is being used by medical researchers at the University of California at Davis to view individual retinal cells (inset), allowing for the early detection of retinal diseases such as glaucoma and macular degeneration.

The second BRP is led by UC Davis Medical Center and includes Indiana University, Duke University, and Livermore. In this effort, Livermore's AO Group is combining MEMS technology with OCT instruments developed at the partner universities to improve the ability to visualize the retina in 3D with cellular-level resolution.

Enhancing Scientific Literacy

One of the center's charters from the National Science Foundation is advancing education, especially among student groups that are underrepresented in science and engineering. Many of the CfAO's educational activities take place in Hawaii because a number of major observatories are located on Maui and the island of Hawaii.

A major educational thrust is aimed at the professional development of graduate students and postdoctoral researchers. The center runs an annual, weeklong professional development workshop on Maui. For example, in February 2006, graduate students, postdoctoral researchers, faculty members from Hawaiian community colleges, and staff from Hawaii-based observatories met to learn teaching skills. The group formed into small teams to prepare science curriculum for high-school and college students. "We want scientists to become more effective science communicators and educators," says Lisa Hunter, the center's associate director for education.

Center educators also work to motivate high-school and college students interested in science and engineering. Eight-week summer internships for college students are held on the islands of Maui and Hawaii and on the mainland. The Maui internship program is directed at helping students gain entry into the local high-technology workforce. The program on the island of Hawaii emphasizes working in technical positions on island observatories or gaining admission into graduate school in a technical field.

The mainland program is open to college students from underrepresented groups and begins with a one-week intensive short course at UCSC. Taught by CfAO graduate students and postdoctoral researchers, the course provides background in AO-related topics, such as spectroscopy, and prepares students for performing research. Students then begin internships at Lawrence Livermore, UC Berkeley, UC Los Angeles, UCSC, or the University of Rochester. "These students receive a lot of support from the center and a lot of encouragement from us," says Olivier. At the completion of their research project, the students make a presentation to their peers at UCSC. About 10 students have completed internships at Livermore, and many of them have gone on to graduate school.

The center also offers a four-week summer course for high-school students considering a technical degree. The course, which covers vision, astronomy, and optics, is taught by CfAO scientists. A weeklong AO summer course is offered for graduate students and professionals.

The Center for Adaptive Optics operates eight-week summer internship programs for college students on the islands of Maui and Hawaii and on the mainland. Students assigned to Livermore work under an Adaptive Optics Group researcher. John Ruiz from the University of Houston and Aftan Alameda from San Antonio College were two of the 2005 Livermore interns.

Accomplishments Are Gratifying

Olivier says it is gratifying that the center has encouraged collaboration between researchers, fostered interactions between astronomers and vision scientists, and advanced educational opportunities for students. "We have come a long way," says Max. "Our educational programs both in Hawaii and on the mainland are recognized for their quality and diversity of participants. In astronomy, adaptive optics is a feature of many more scientific papers. The challenge of lasers for guide stars is not as daunting as it was several years ago. The performance of MEMS deformable mirrors is approaching the specifications required by astronomers and vision scientists. And vision scientists have developed new AO instruments and received international recognition."

Olivier notes the importance of partnerships as AO technology becomes more firmly established in astronomy, vision science, and military applications. For example, under a Defense Advanced Research Projects Agency initiative, Livermore teamed with academic institutions and industry to develop extremely fast and secure long-range communication links and aberration-free, 3D imaging and targeting systems using MEMS devices.

For Livermore researchers, technologies developed in support of the center help advance a wide range of work in remote sensing and large optical systems for national security missions. Livermore-developed techniques that allow an optical system to adapt to changing atmospheric conditions can be used to control the wavefront in high-energy laser systems. For example, a wavefront sensor concept developed for extreme AO is being used in Livermore's Solid-State Heat Capacity Laser. (See *S&TR*, April 2006, pp. 10–17.)

The advancements may help scientists discover new planets and understand the origin, formation, and composition of stars, planets, and galaxies. They may also provide better vision for pilots, enhance military surveillance, and save the sight of thousands of people through early detection and treatment of retinal diseases. It seems that few things are as important as seeing clearly.

—Arnie Heller

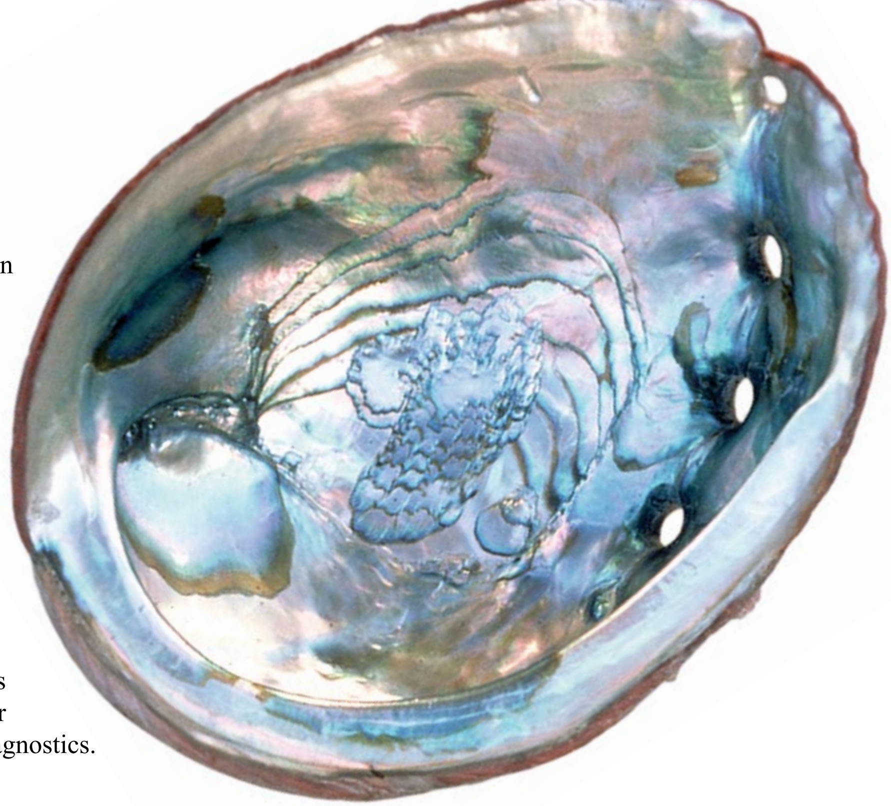
Key Words: adaptive optics (AO), Center for Adaptive Optics (CfAO), fiber laser, Gemini Observatory, Keck Observatory, Laboratory for Adaptive Optics, laser guide star, Lick Observatory, MEMS-based adaptive optics phoropter (MAOP), microelectromechanical systems (MEMS), National Science Foundation, optical coherence tomography (OCT), scanning laser ophthalmoscope (SLO), Science Technology Center, Thirty Meter Telescope (TMT), vision science.

For further information contact Scot Olivier (925) 423-6483 (olivier1@llnl.gov).

Wired on the Nanoscale

If you think viruses are only good (or not good) for causing the common cold, flu, and other ailments, then you're in for a surprise.

Scientist Yu Huang, a Lawrence fellow at Livermore, spent a year and a half at the Massachusetts Institute of Technology learning a technique for creating metallic and semiconducting nanostructures using genetically engineered viruses. Among the structures she has created are tiny gold nanowires that may be used to make single-molecule devices. The technique allows the scientist the final word in determining the size and shape of the structures at a level that has been difficult to control with other techniques. Future applications for single-molecule devices include light-emitting displays, optical detectors and lasers, fast interconnects, nanometer-scale computer components, magnetic storage, sensors, and medical diagnostics.



An abalone shell is an example of a structure found in nature that is created by an organism binding to and assembling inorganic materials in its environment.

Building with Viruses

As the sizes of electronic devices continue to shrink, the need for control over minutely small dimensions—even down to single molecules and atoms—increases. Huang and other researchers are following nature's lead to solve this technological problem. "Our goal is to build structures at the molecular level from the bottom up, just as nature does," says Huang.

In nature, some organisms have evolved the ability to bind to and assemble inorganic materials with nearly perfect alignment, orientation, and shape, in a complex yet beautifully controlled fashion. The proteins expressed from particular genes in living bone, shells, diatoms, and certain bacteria can bind to inorganic materials creating elegant structures with great precision on scales from the nanoscopic to macroscopic. An abalone shell is one example of this process in nature.

For the past few years, Huang and other scientists have been researching the process, using bacteria, viruses, and other organisms as the first building blocks for generating devices on the nanoscale. Whereas organisms in nature must make do with their own genes and proteins and whatever materials are accessible in their environments, scientists can turn to special protein libraries called peptide combinatorial libraries and splice in genes that express specific proteins. This technique allows the researchers to choose which proteins will coat the surface of a given organism and, in turn, which inorganic materials will bind to the organism. The use of specific genes and proteins allows the possibility of controlling the self-assembly of multiple electronic components on a single device.

A Golden Opportunity

Huang has been using the M13 bacteriophage, a virus that infects bacteria. M13 is a circular single-stranded DNA molecule encased in a flexible cylinder that is coated with the protein pVIII. In addition, at one end of the M13 virus are five copies of the protein pIII, and at the other end of the virus are five copies of two other proteins.

Huang uses the M13 bacteriophage virus to create one-dimensional (1D) nanostructures, such as gold nanowires, and more complex

2D and 3D structures. In addition, she has taken the process a step further by connecting such structures to each other. Using viruses as "scaffolds" from which to build these structures allows scientists to take advantage of the growth process perfected by nature.

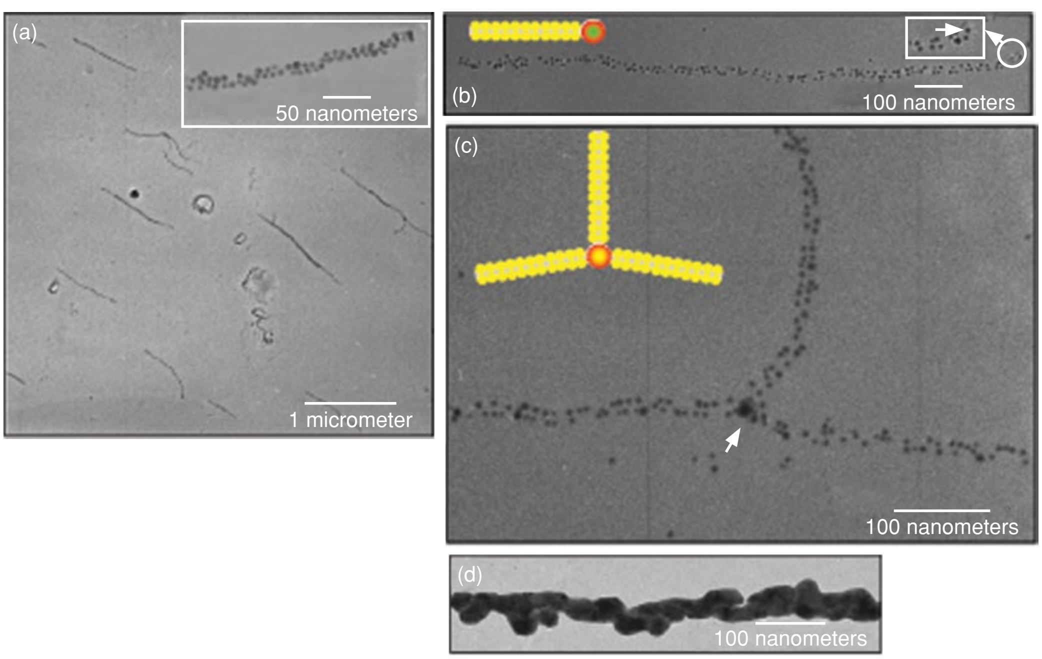
Huang began by modifying two genes (gIII and gVIII) in the genome of the M13 bacteriophage. The modified gVIII gene expresses a modified pVIII protein that has a high affinity for binding to gold. The modified gIII gene expresses a modified pIII protein that binds well to streptavidin (a protein routinely used to purify DNA binding proteins). The modified pVIII protein coats the length of the genetically engineered bacteriophage clone, and the modified pIII protein expresses at just one end of the clone.

Huang then used the modified virus as a building block on which to bind and assemble 1D gold nanocrystal arrays. Solutions containing the genetically modified bacteriophage virus were mixed with a suspension that held gold nanoparticles. Images taken with a transmission electron microscope (TEM) showed that the gold nanoparticles had assembled around the modified bacteriophages (called 8–3 bacteriophages because of their modified proteins pVIII and pIII) into wirelike structures. A closer look revealed that the gold nanoparticles were actually arranged in an ordered 1D array on the pVIII proteins along the axis of the virus.

Huang then assembled a more complex structure using the modified pIII proteins at one end of the bacteriophage to bind to gold particles coated with streptavidin. TEM images showed that an array of 5-nanometer-diameter gold particles had formed on the modified pVIII proteins, and streptavidin-coated 15-nanometer-diameter gold particles had bound to the pIII proteins on the end.

"We can easily extend this process to other materials and structures," notes Huang. For example, when the streptavidin-coated gold was replaced with streptavidin-conjugated cadmium selenide quantum dots, the result was arrays with quantum dots bound to the modified pIII proteins and gold nanoparticle arrays bound to the modified pVIII proteins. "We can connect more than one bacteriophage to a quantum dot and create complex structures," says Huang.

She also created continuous metallic nanowires—originally 1D arrays of separate gold nanocrystals—with average diameters of 40 nanometers and lengths of 100 nanometers. The process involved using electroless deposition to coat the existing gold nanoparticle arrays with additional gold. Huang conducted studies of these wires to evaluate their capability to transmit electricity. Measurements indicated that the wires, indeed, can act as conductors for considerable amounts of electrical current at the nanoscale. "These experiments indicated that a wire built on modified pVIII proteins could be used to transmit electricity to another nanostructure, such as a quantum dot built on the pIII proteins at the end of the virus," she explained. "The approach is one solution to the interconnection problem found in studies of quantum objects." Other studies are under way to thoroughly



Transmission electron microscopy images of a genetically engineered 8–3 bacteriophage virus show the formation of nanostructures. (a) Distinct wirelike structures are self-assembled into one-dimensional arrays along the axis of the virus. (b, c) More complex structures are created from gold nanoparticles and streptavidin-coated gold particles and quantum dots, using the modified virus as a starting building block. White indicates the virus structure, yellow dots are gold nanoparticles, the green dot is a quantum dot, and red indicates the streptavidin coating. (d) This continuous metallic nanowire began as one-dimensional arrays of gold nanoparticles bound to the genetically engineered virus. After 5 minutes of electroless deposition, enough additional gold particles were deposited to thicken the wire to the point where it could transmit a small electric current.

characterize the bacteriophage-based wires and detail their electrical performance.

From Livermore to Beyond

Huang came to Livermore from Harvard's Department of Chemistry as part of a prestigious postdoctoral program called the Lawrence Fellowship Program. The purpose of the fellowship is to pursue cutting-edge science and stimulate cross-fertilization of ideas. Lawrence fellows have the freedom to pursue research with ample resources to support their efforts. (See *S&TR*, November 2002, pp. 12–18.) "One thing I found very attractive about the Laboratory is that many opportunities exist to exchange ideas and work with scientists of different disciplines," Huang notes.

Huang has recently completed her three-year fellowship and is preparing to move on to an assistant professorship position at the University of California at Los Angeles (UCLA). Harry Radousky, deputy director of Livermore's University Relations Program, views Huang's appointment as a success for the Laboratory both now and in the future. "The program attracts some of the brightest scientists to the Lab and promotes university collaborations," he says. "We see situations such as Huang's as a success story—our hope being that our fellows will find a place either here at the Laboratory or at prestigious universities, where they will strengthen collaborative ties between the Laboratory and their institution."

Huang is indeed planning future collaborations with her Livermore colleagues. They plan to genetically engineer viruses to produce precise nanostructures and better understand the pathogenesis of kidney-stone formation. She intends to establish a research program at UCLA that focuses on developing complex material structures with molecular precision through genetic control of biological scaffolds. The program will investigate these structures' fundamental properties and explore their use as functional nanosystems for various applications such as molecular electronics and drug delivery.

—Ann Parker

Yu Huang's research, conducted at Lawrence Livermore and at the Massachusetts Institute of Technology as a Lawrence fellow, will continue when she takes on a new position at the University of California at Los Angeles.

Key Words: bacteriophage, biological scaffolds, DNA, genetic engineering, Lawrence Fellowship Program, nanosystems, nanotechnology, nanowires, quantum dots, virus.

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Too Hot to Handle

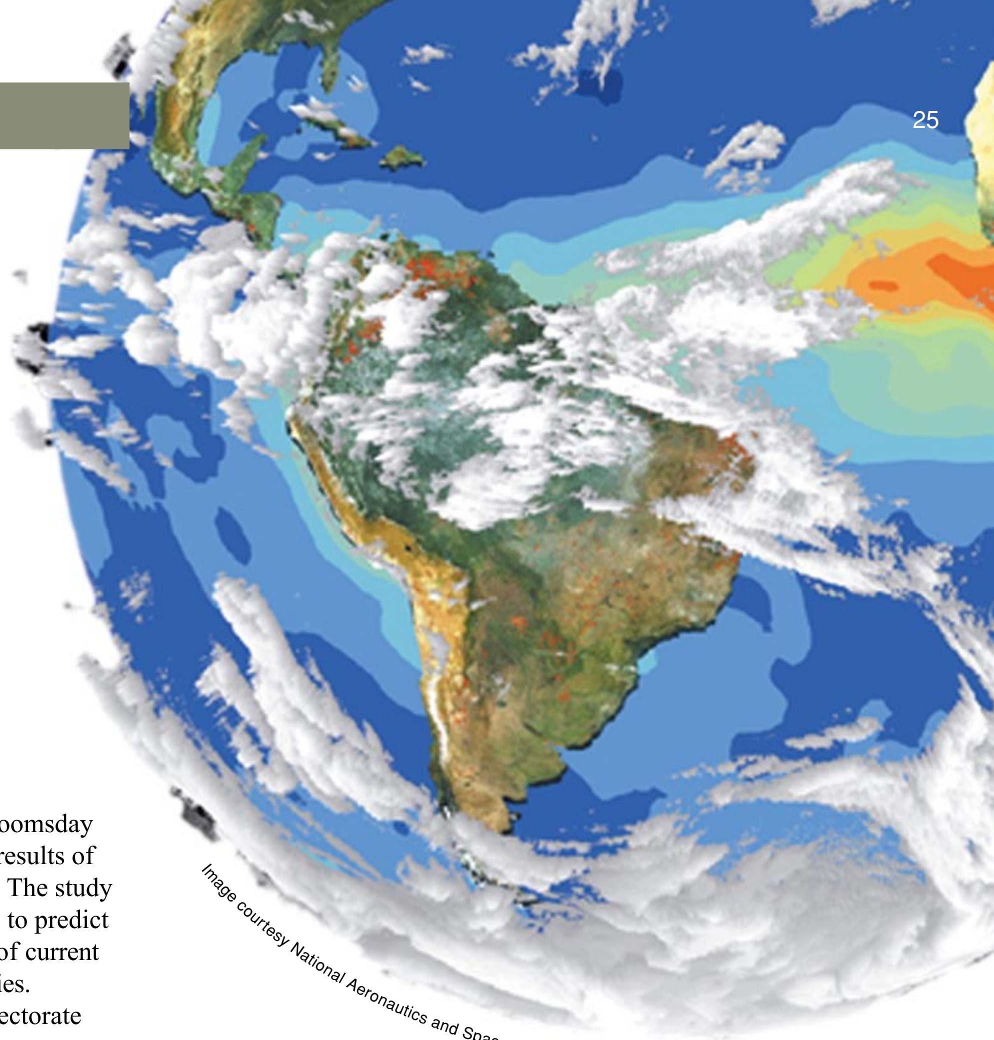


Image courtesy National Aeronautics and Space Administration.

IF humans deplete the world's supply of fossil fuels in the next 300 years as they are on track to do, they will be faced with many more challenges than just finding alternative energy sources.

According to Livermore physicist Govindasamy Bala, humans inhabiting polar regions would have to figure out new methods of subsistence as their ice and tundra landscapes turn into boreal forests as a result of temperatures spiking more than 20°C. Even more striking, residents of certain islands that rise only a few meters above sea level would be looking for a new home entirely, as their communities slowly disappear beneath a rising sea.

Although these scenarios sound like material for a doomsday plot straight out of Hollywood, they do, in fact, reflect results of computer simulations recently conducted at Livermore. The study is the first to combine climate and carbon-cycle models to predict out to 300 years the long-term, global climate effects of current and future energy usage and resource management policies.

Bala's team within the Energy and Environment Directorate also includes physicists Arthur Mirin and Michael Wickett. Physicist Ken Caldeira, formerly a Laboratory employee, collaborates from the Carnegie Institution. The study, funded by the Laboratory Directed Research and Development Program, supports the Department of Energy's (DOE's) mission priorities in energy and environment. This work is one of Livermore's programs that contribute to the scientific and technological basis for secure, sustainable, and clean energy resources.

How Did We Get Here from There?

When fossil fuels are burned to create the energy we need to run our cars, heat our homes, and power industry, they emit carbon dioxide—a heat-trapping gas also commonly known as greenhouse gas. The scientific community has reached near consensus that the accumulation of such gases in Earth's atmosphere is causing a global warming trend. How soon we will see, and be affected by, the consequences of this gradual warming continues to be a source of debate.

Climate data show some warming has already occurred. "Over the 20th century, the average global temperature has increased more than half a degree," says Bala. What many climate researchers would like to know is where the trend is going and how fast it is getting there.

To predict the outcomes of different energy- and resource-usage scenarios, scientists depend on computer models that are of increasingly higher resolution, include better physics models, and are validated with observations. Bala underscores the value of Livermore's massively parallel computing capabilities in pushing this research ahead. "These simulations require very high-capability computing," says Bala, whose team has used nearly every supercomputing machine in the DOE complex to run several climate codes. Beyond running simulations to study scenarios, the Laboratory plays a broader role in climate research for DOE. Livermore's Program for Climate Model Diagnosis and Intercomparison develops methods and tools for diagnosing, validating, and comparing the global climate models used for predicting climate change.

We're Getting Warmer

Climate model simulations performed in the past have been limited to predicting the effects of this trend out only 100 years or so. Bala's study included data that looked forward to 2300.

The resulting predictions, which are intended to give a big-picture view, showed an average increase in global temperature of 8°C by 2300 and implied that the Greenland ice sheet could completely melt, triggering a sea level rise of 7 meters over the next several centuries. The simulations also pointed to a 20°C warming over the Arctic by 2300. "What is alarming about this recent study is that severe changes to the distribution of terrestrial vegetation can also occur much more rapidly than we previously thought," says Bala.

Of even more concern, he says, is that the team was conservative with some of the input used in the simulation code. "This model did not consider changing land use such as deforestation and the expansion of metropolitan areas," he says. "These factors would have an even greater effect on the global temperature if they were included."

Bala's team couples both climate and carbon-cycle simulations to model climate change. This coupling has produced data that Bala believes are more accurate than past studies, which have relied just on climate models. "The coupling realistically represents the interaction between climate and the carbon cycle, and our model simulated atmospheric carbon dioxide concentrations and surface mean temperature changes that are in line with observations over the 20th century," says Bala.

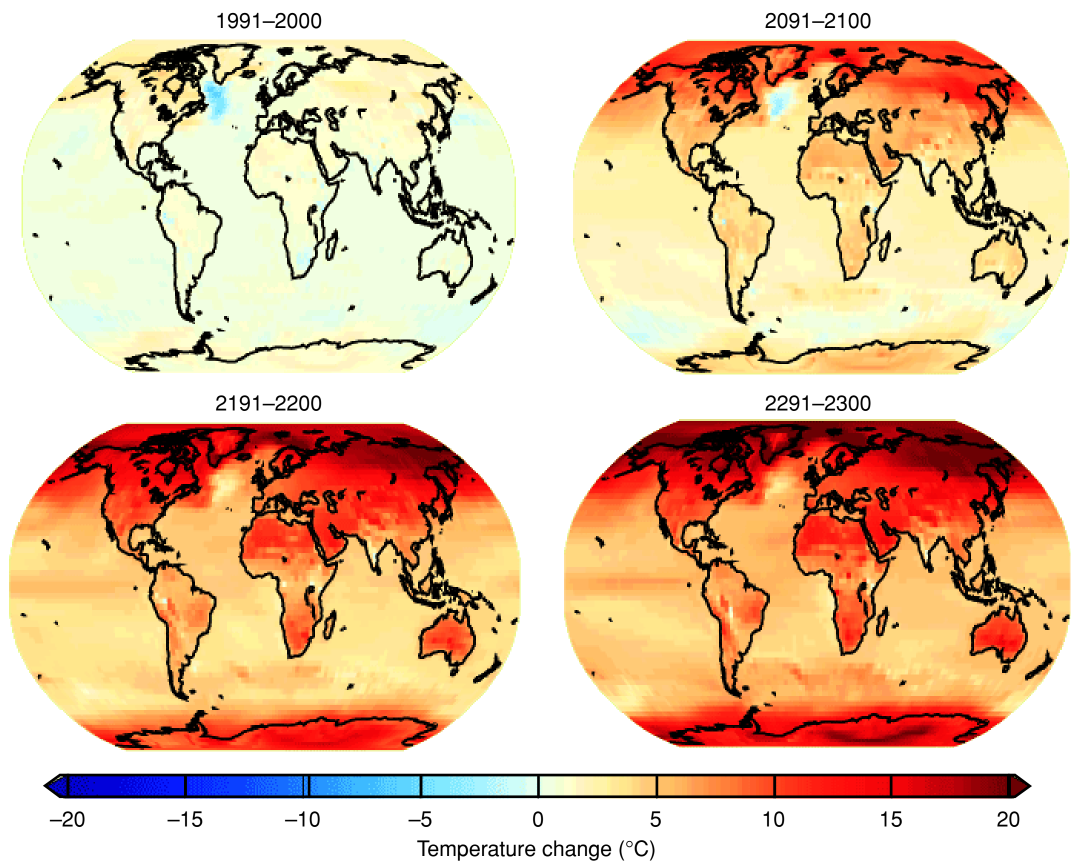
Carbon Sinks and Acid Oceans

Atmospheric carbon dioxide emissions from the burning of fossil fuels affect the carbon content of both terrestrial and oceanic systems—and both of those carbon reservoirs affect climate and vice versa. The flow of carbon dioxide through the atmosphere and the terrestrial and marine ecosystems is referred to as the carbon cycle. Bala's model predicts that Earth's level of atmospheric carbon dioxide will nearly quadruple by the year 2300.

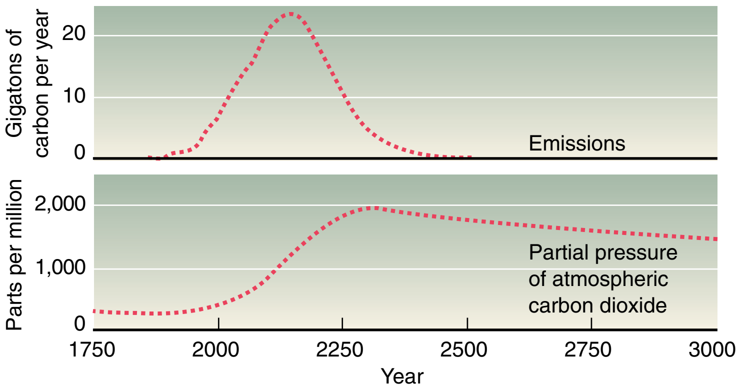
Carbon dioxide, however, does not remain indefinitely in the atmosphere. It is taken up by terrestrial carbon sinks—living biomass and soils—and, in large part, the oceans. Indeed, about 80 percent of carbon dioxide eventually ends up in the oceans. Bala's simulations show a significant increase in the acidity of the oceans when fossil-fuel stores are depleted. "This phenomena will occur even if climate change does not happen," says Bala.

The acidification of the oceans is expected to be quite damaging to marine life. And, in typical ecosystem fashion, the destruction of certain marine organisms is likely to feed back into the climate cycle. In question is the fate of marine organisms, such as corals, that are made of calcium carbonate shells and skeletal materials. These organisms normally act to regulate ocean chemistry and, in turn, the ocean's ability to absorb carbon dioxide from the atmosphere. Observations have already shown that even a few degrees of ocean warming threaten the existence of some coral reefs. Scientists predict that the destruction of these coral systems would hamper the ocean's ability to adequately absorb atmospheric carbon dioxide.

Bala's simulations predict that eventually the ability of oceans to absorb carbon dioxide would decline, and about 45 percent of the emitted carbon dioxide would remain in the atmosphere. The



Computer modeling data of the global surface-temperature change over the next 300 years indicate the Arctic will be warmer by 20°C in 2300. All plots are referenced to preindustrial times (1891–1900).



Determining how large the concentrations of atmospheric carbon dioxide will be in the future depends on how much fossil fuel is emitted. The top curve shows the emission rate of carbon dioxide and supposes all the estimated conventional fossil-fuel resources will be depleted by the year 2500. The bottom curve shows the resulting carbon dioxide concentrations up to year 3000. Ocean absorption of carbon dioxide is taken into account, but climate and land carbon changes are not.

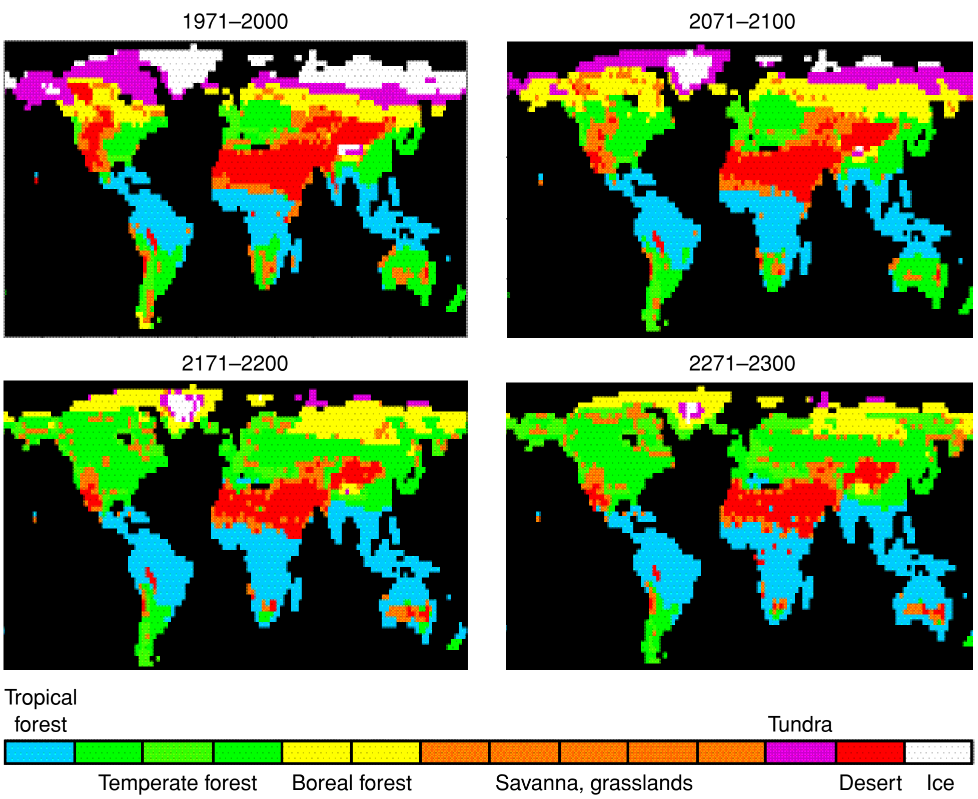
model also shows that the warming trend would reduce terrestrial uptake and the ability of soils to retain carbon dioxide. Moreover, the warmer climate would change the distribution of terrestrial vegetation on a large scale. For example, tropical and temperate forests would expand, with Arctic tundra transforming into boreal forests by 2200.

No Time to Lose

If this study were only a cautionary tale, it would be enough to make individuals and policy makers alike take pause and commit to reversing the trend. However, as Bala points out, it is now evident that damage has already been done. “We have what is called ‘committed warming,’ which is already set in motion,” says Bala. “No matter what we do—even if we completely stop burning fossil fuels today—we are committed to further increases in global temperature. Although a consensus does not yet exist on the amount of committed warming, a recent study estimates that it could be about 0.6°C. Our present trajectory is risking severe environmental damage that could last many hundreds of years.”

Computer simulations using integrated models offer a glimpse into the future and an opportunity to mitigate damage yet to come. “We are just in the beginning of this integrated assessment,” says Bala. “Many challenges are ahead.”

—Maurina S. Sherman



Simulations of the changes in global dominant vegetation types show that northern ice caps will begin vanishing this century and tundra regions will disappear within 200 to 300 years.

Key Words: carbon cycle, carbon dioxide emissions, carbon sink, climate modeling, deforestation, fossil-fuel depletion, global climate change, global warming, greenhouse gases, land use, oceanic acidity, vegetation change.

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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

Method of Producing a Hybrid-Matrix Fiber Composite
Steven J. DeTeresa, Richard E. Lyon, Scott E. Groves
U.S. Patent 7,018,578 B2
March 28, 2006
Fiber composites produced using matrix hybridization have an enhanced stiffness and compressive performance with toughness and durability suitable for compression-critical applications. The hybrid-matrix fiber composites are made of two chemically or physically bonded matrix materials. The first matrix material is used to impregnate multifilament fibers formed into ribbons. The second matrix material is placed around and between these fiber ribbons. Both matrix materials are cured and solidified.

Safety and Performance Enhancement Circuit for Primary Explosive Detonators
Ronald W. Davis
U.S. Patent 7,021,218 B2
April 4, 2006
A safety and performance arrangement is enhanced for primary explosive detonators. This arrangement includes a circuit containing an energy-storage capacitor and preset self-trigger to protect the primary explosive detonator from electrostatic discharge (ESD). The circuit does not discharge into the detonator until a sufficient level of charge is acquired in the capacitor. The circuit parameters are designed so that normal ESD environments cannot charge the protection circuit to a level to achieve discharge. The performance of the detonator is also improved because of the close coupling of the stored energy.

Abstracts

Next-Generation Scientists and Engineers Tap Lab's Resources

Lawrence Livermore's Student Employee Graduate Research Fellowship (SEGRF) Program provides University of California students the opportunity to conduct research at the Laboratory using some of the most advanced facilities in the world while they earn their Ph.D.s. The students work on fundamental science in diverse areas. For example, SEGRF students are part of homeland security efforts such as the bioaerosol mass spectrometry system developed for its potential use in identifying biological agents and a neutron spectrometer that identifies gamma rays and neutrons in nuclear material. Students are also conducting research on ultrawideband communications systems, which could replace the interface between computers, printers, and entertainment devices. Another team is converting a spark-ignited, six-cylinder engine to a homogenous charge compression ignition engine, which could considerably improve a vehicle's fuel efficiency and lower nitrogen oxide emissions. In research relevant to the National Ignition Facility, a team of present and former SEGRF students is investigating the processes associated with laser-induced damage in optical materials. In addition, SEGRF students are performing three-dimensional simulations of carbon at high pressure and temperature. Another team of students is combining a diamond anvil cell with x-ray diffraction techniques to study the effects of pressure on the electronic structure of certain materials similar to elements that are important in stockpile stewardship. SEGRF students are also conducting experiments on lithium compounds that are analogs to hydrogen-containing materials.

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Adaptive Optics Provide a Clearer View

Founded in 1999, the Center for Adaptive Optics researches adaptive optics (AO) in the fields of astronomy and vision science so that astronomers can more clearly visualize distant celestial objects and physicians can better diagnose eye diseases and more accurately prescribe corrective lenses. The center is headquartered at the University of California at Santa Cruz. It directly funds researchers nationwide and administers a growing network of partners that include universities, national laboratories, observatories, medical research centers, and private industry. Center partners develop AO systems that tie together advanced technologies including precision optics, wavefront sensors, deformable mirrors, lasers, and control systems. The center also plays an important role in transferring information about developments in AO from research laboratories to commercial entities and the broader scientific community. Lawrence Livermore researchers are major participants in the center's organization and activities.

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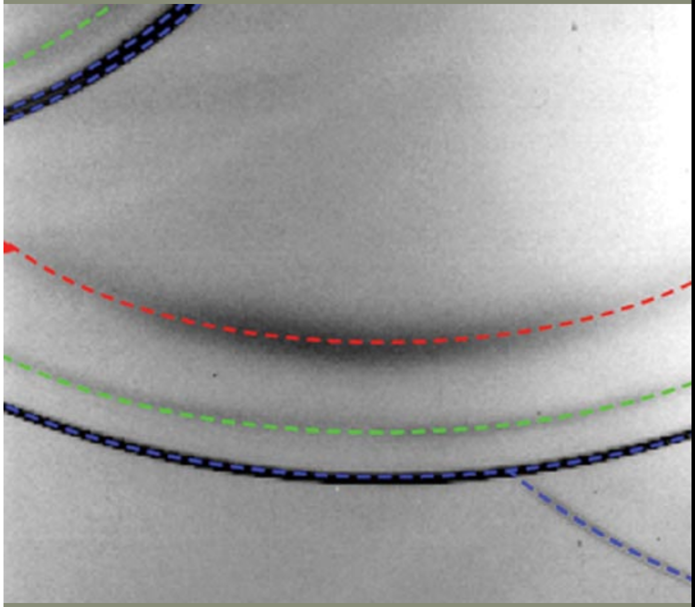
On the Frontier of Materials Science



Researchers are examining the changes that occur in a metal's lattice structure under extreme pressures.

Also in July/August

- *Using the microlensing technique, scientists discover a rocky, Earth-like planet orbiting a dim star.*

- *Livermore technology is on duty to detect any instance of bioterrorism.*

- *A pioneering simulation on BlueGene/L provides an atom-by-atom demonstration of solids forming under high temperatures and pressures.*

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