

## Virtual Electron Microscope Laboratory Demonstrated on the Internet

Ernest Orlando Lawrence Berkeley National Laboratory (LBNL) is setting up its high voltage electron microscope so that it is accessible to users on the internet. The Laboratory has created a set of interactive, online computing tools that will allow scientists to manipulate the instrument, conduct experiments, and view images online from their offices.

To sidestep the time lags that occur across computer networks, computer scientist Bahram Parvin's team is automating onsite the positioning and focusing of the microscope. This is being made possible through the development of advanced computer vision algorithms.

Parvin said, "You start with what to a computer is an indiscriminate field. You then detect and lock onto objects of interest. This is computer vision. Very soon, from a remote location, computer vision will self-calibrate the microscope, autofocus it, and compensate for thermal drift. Underlying this is a complex package of algorithms dealing with shape analysis, background measurements, wavelet transform, and servo-loop control. Essentially though, we are making the microscope smarter, making it do intuitively what users would have to do on their own."

On August 14 at the Microscopy Society of America's annual international meeting in Kansas City, LBNL scientists demonstrated the process of controlling the *in situ* electron microscope by computer. They heated an advanced alloy specimen and observed the ensuing progression of structural changes on the computer monitor.

The researchers' goal is for experimenters at remote locations to control the microscope to change magnification, scan the sample, alter its orientation, and trigger a range of experimental conditions.

## Karle, Haus Receive National Medal of Science

Eight scientists received the 1995 U.S. National Medal of Science, including Isabella Karle from the Naval Research Laboratory (NRL) and Hermann Haus from the Massachusetts Institute of Technology (MIT). The medal is awarded annually by the U.S. President in special recognition of outstanding contributions in science and engineering, many of which have directly enhanced long-term economic growth and improved standards of living.

Karle's pioneering x-ray analysis of complex crystal and molecular structures has profoundly affected the disciplines of

organic and biological chemistry. Her work has elucidated the crystal structures of numerous complex organic substances, natural products, photorearrangement products, biologically active molecules, ionophores, peptides containing many residues and supramolecular assemblies, that have significance in synthetic chemistry, medical drug design, materials design, reaction mechanisms, ion channel formation, molecular modeling programs, and energy calculations.

Karle's method systematized analyses that were formerly tedious and frustrating. From a small number of simple structure analyses published in the 1960s, her procedure has led to the analysis and publication of many thousands of structures of complicated molecules annually. All the present computerized programs for x-ray structure analyses are based on Karle's fundamental work known as the Symbolic Addition Procedure. Karle has also identified and determined the structures of a number of complex substances of chemical and biomedical significance.

Her procedures have been adopted worldwide and have contributed to the output of crystal structure analyses. More than 10,000 analyses are now published annually compared to about 150 annually in the early 1960s.

Haus's research and teaching in quantum optics has enabled scientists to make significant advances in eye surgery and instrumentation, as well as fiber optics communications. His work ranges from fundamental investigations of quantum uncertainty as manifested in optical communications to the practical generation of ultrashort optical pulses (10,000 times shorter than a nanosecond).

Fiber optical undersea cables providing rapid voice and data communications among the United States, Europe, and Asia are beneficiaries of the pioneering investigations of Haus and fellow researchers at AT&T Bell Laboratories and Nippon Telegraph and Telephone Research Laboratories, who developed the "soliton" method of transmission. Their work opens new possibilities for transmitting voice and data signals across an ocean without repeaters, thus simplifying the method and enabling higher rates of signal transmission.

## Simulations Predict Failure Mechanisms of Lubricants in Nanometer-Scale Devices

In a paper published October 27 in *Science* researchers at the Georgia Institute of Technology predict that ultrathin films of the organic lubricants used

in nanometer-scale devices may act more like solids than liquids when subjected to high pressures. The molecular dynamics simulations used also warn of possible damage from cavitation effects, as well as fatigue failure caused by repeated surface deformation. Simulations show asperities on sliding disks approaching one another at high speed.

"We believe these results could have some impact on the design and way of thinking about devices like high density disk drives that have moving parts in very close proximity lubricated by thin films," said Uzi Landman, director of Georgia Tech's Center for Computational Materials Science.

Using supercomputers to model the complex physical processes involved, the researchers studied the behavior of a thin-film hexadecane (C<sub>16</sub>H<sub>34</sub>) lubricant flowing between two gold disks sliding past each other at a relative velocity of 10 m/s. Under these conditions, the flow of liquid lubricant through the narrow space between the surfaces creates pressure high enough to cause temporary elastic deformation of the disks. Repeated deformation could ultimately lead to fatigue failure and the development of pits or cracks on the disk surface, Landman said.

More troubling are the possible effects associated with tiny surface nonuniformities, asperities, that exist on disks that appear to be smooth.

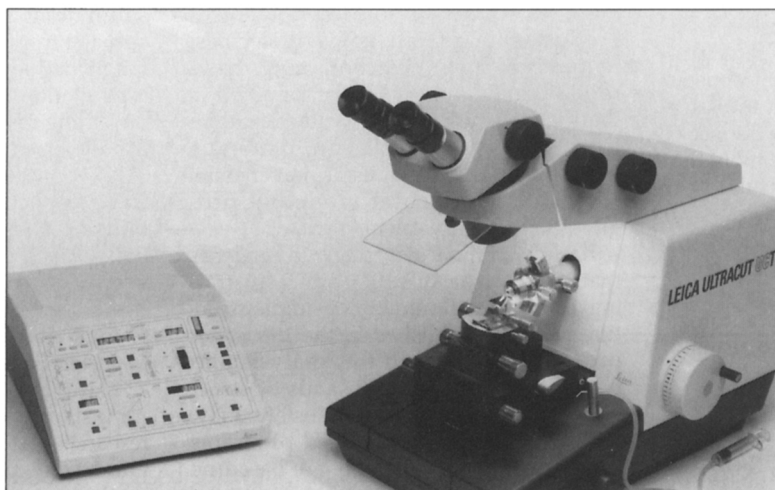
Landman and colleagues Jianping Gao and W. D. Luedtke studied three instances in which asperities passed close enough together to affect the lubricating film. The first involved a separation of approximately 17.5 Å; the second a "near-overlap" of 4.6 Å, and the third a situation in which the ridges overlapped and collided.

In the first instance, the increased confinement in the region between the approaching asperities caused the lubricant to organize into distinct layers that resembled the ordered structure of a solid. As the pressure continued to increase, the viscosity of the liquid film increased as the molecules flowed out of the gap one layer at a time. This quantized layered structure of the lubricant molecules caused an oscillation in the force required to maintain the relative sliding velocity between the disk surfaces.

In the second instance of a much smaller separation, the pressure imposed on the lubricant became large enough to elastically deform and flatten the asperities, helping to smooth the surface of the disks. Pressures of 200,000 to 300,000 atm could be created as the lubricant is squeezed out of the gap.

In the third instance, all of the lubricant molecules were forced out of the gap and

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the asperities collided, briefly forming a metallic junction and transferring material before separating. The high pressures created by the collision caused the liquid lubricant to change into a near-solid phase.

Landman said, "You come to the point at which the lubricant molecules are arrested. There is not enough time for them to escape the confined region that is being produced. This can cause the lubricant to undergo a phase change to an ultra viscous fluid or a soft solid. Under extreme circumstances, the liquid can become a glassified solid that develops a significant resistance to shear. This could bring about seizure and a disk crash."

Another potentially harmful effect is the cavitation that can occur after the asperities collide. When they separate as the disks continue their rotation, lubricant molecules are slow to fill the widening gap, creating a cavitation phenomena that may be harmful because, according to Landman, "their collapse releases sufficient energy to damage the surface through the propagation of supersonic shock waves and the release of heat."

In addition to the cases of nonuniform surface asperities, Landman said the normal starting and stopping of a disk drive could also alter the space between moving surfaces and create increased pressure. As reader heads are placed closer and closer to disk surfaces to gain spatial resolution, this problem could become more of concern. In the process of deformation and collision, the action of the elastohydrodynamic lubrication may liberate wear particles. Landman does not know, yet, how these particles may affect the device and degrade the lubricant.

**Recently Announced CRADAs**

**Southwire Company** (Carrollton, Georgia) and **Oak Ridge National Laboratory** (Oak Ridge, Tennessee) signed a two-year agreement of about \$870,000 for Phase I of a project to develop a superconducting electrical transmission cable that will enable electric power companies to deliver energy with greater efficiency, higher power density, and lower costs than now possible.

**Rare-Earth Solid-State Lasers Extended into Mid-IR**

Researchers at the Naval Research Laboratory (NRL) have developed a technique to extend the range of rare-earth solid-state lasers into the mid-infrared (IR) range. According to Steven R. Bowman, one of the principal investigators of this research, solid-state lasers based on rare-earth ions have been restricted to wavelengths shorter than 3  $\mu\text{m}$  because of rapid fluorescence quenching resulting from multiphonon relaxation. He said, "To extend the range of solid-state laser sources farther into the mid-IR, we have explored the optical properties of rare-earth ions doped into unconventional host crystals."

The researchers developed two mid-IR lasers at 5 and 7  $\mu\text{m}$  by using praseodymium in lanthanum trichloride, a low phonon energy host crystal. They grew optical quality crystals using a modified Bridgeman-Stockbarger technique. The researchers were able to identify laser transitions and energy transfer processes that activate the laser channels. "Through

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this technique, optically pumped material at 2.0  $\mu\text{m}$ , using a pulsed, diode-pumped thulium laser, resulted in the longest wavelength reported to date for any rare-earth laser," Bowman said.

### Palladium-Coated Tantalum Sandwich Extracts Hydrogen

Researchers in the Materials Science and Technology Division of Los Alamos National Laboratory have developed a metallic membrane that purifies hydrogen. The membrane consists of a thin foil of tantalum 13  $\mu\text{m}$  thick, coated on both sides with palladium. The palladium is laid down with a specific crystallographic orientation that allows hydrogen to move easily through the membrane.

The hydrogen molecule binds to the palladium surface, breaks into individual atoms, migrates through the metal layers, and recombines into a hydrogen molecule, resulting in pure hydrogen that can be produced in high volume. The hybrid metal structure overcomes the cracking and oxidation common to previous membranes.

According to the researchers, the membrane will pass hydrogen at a faster rate and with a lower materials cost than standard dense palladium membranes. Researchers are in the initial stages of applying this technology to fuel cells which require pure hydrogen to function correctly.

### Fiber/Matrix Distribution Alters Mechanical Behavior of Ceramic Composites

Scientists at the Naval Research Laboratory (NRL) have established a link between the fiber/matrix distribution and the mechanical behavior of ceramic fiber, ceramic matrix composites (CFCMCs). Todd Jessen of the Mechanics of Materials Branch and principal investigator found that matrix-rich regions, or channels, as fine as 80  $\mu\text{m}$  could alter both the strength and fracture resistance of these composites by more than 25 and 35%, respectively, depending on orientation of the channels. These matrix-rich features, which control the mechanical response, are large enough to be detected using x-ray tomography. Jessen's work has shown that sorting CFCMCs, using the matrix channel orientation as a discriminator, greatly reduces the mechanical property data scatter within a test population and results in consistent failure processes within each subgroup. "This correlation between properties and microstructure and the subsequent ability to predict mechanical response based on microstructural features is a big step toward developing the reliability in CFCMCs required

to see these materials in use in actual devices," said Jessen.

The research team applied this CFCMC microstructure/property concept to develop a series of CFCMCs with significantly enhanced mechanical properties. By controlling the arrangement and placement of the fibers within the microstructure, strength and fracture resistance improvements of more than 40 and 70%, respectively, were achieved as compared with conventional CFCMCs. These enhanced performance composites can be optimized for either maximum strength or toughness by altering the microstructural design. They also reduce the use of expensive BN coatings on the fibers, which are typically required to achieve the desired mechanical response. The researchers showed that selective placement of the coated fibers within the structure can reduce from 100% to 20% the fraction of fibers requiring the coating without adversely affecting performance. Jessen said that their research demonstrates that the controlling failure processes are structurally dependent rather than compositionally dependent, which means their findings can be applied to all CFCMCs.

### Heeger Receives 1995 Balzan Prize

Alan J. Heeger, a pioneer of the new and rapidly expanding field of electrically conducting plastics and director of the Institute for Polymers and Organic Materials at the University of California—Santa Barbara, is the recipient of a 1995 Balzan Prize for the "science of new nonbiological materials." Ceremonies were held November 24, 1995 in Berne Switzerland.

The prestigious prizes, each of which carries an award of 350,000 Swiss francs (about \$300,000), are given annually for achievement in the arts, cultural history, and the sciences by the Milan-based International Balzan Foundation. About every three years, it also gives a major humanitarian award.

The foundation cited Heeger for "his outstanding contributions to materials science and his leadership...in the new and interdisciplinary field of semiconducting and metallic polymers."

In 1976, Heeger and his colleagues, Alan MacDiarmid and Hideki Shirakawa, discovered they could make a polymer with a single free electron that would give it the electrical and optical properties of metals and semiconductors. Until then scientists doubted such polymers could be created.

Lighter, more flexible, and easier to process than metals or silicon-based semi-

conductors, these polymers quickly raised the prospect of a wide range of industrial applications such as transistors, light-emitting diodes, and plastic batteries.

In its statement, the foundation said, "Professor Heeger has been not only a leading personality in the discovery of conducting polymers, but also a pioneer in exploring the basic science underlying their properties and in establishing the conceptual and theoretical framework of the entire field."

In 1990, Heeger and UC—Santa Barbara materials scientist Paul Smith founded the Santa Barbara-based research and development company UNIAx Corp. To commercialize the polymers, some of them under license from the University of California.

One product under development is a light-emitting plastic that could be used to replace rigid semiconductor light sources in electronic devices ranging from clocks to computers to flat television screens. A manufacturing advantage is that it can be applied as a liquid thin film.

### Metallurgist Melvin Jackson Receives Coolidge Fellowship Award

The GE (General Electric) Research and Development Center's Coolidge Fellowship Award was presented in October 1995 to Melvin R. Jackson, a physical metallurgist. Jackson was honored for "major contributions in metallurgy and metallurgical processes that have helped make GE's aircraft engines and land-based gas turbines the world leaders in operating efficiency, reliability, and environmental performance."

The Coolidge Fellowship, granted annually, recognizes outstanding and sustained contributions to science or engineering by a member of the R&D Center's research staff. A Coolidge Fellow receives a special medallion and is granted a one-year leave to follow individual research pursuits at a university or research institution, within GE, or elsewhere, supported by the R&D Center.

Jackson has made important contributions in various areas of metallurgy, including alloy development. He invented several advanced nickel- and niobium-based alloys developed for current and future commercial aircraft engines and land-based gas turbines. He has also developed special repair alloys and processes for use in high-performance military aircraft engines to refurbish single-crystal and directionally solidified high-pressure turbine vanes.

In the late 1970s, Jackson was a key member of the research team that devel-

oped advanced corrosion-resistant coatings for the hot-gas-path components of turbines. Applied in a low-pressure vacuum chamber employing a white-hot plasma torch, these coatings enable the high-temperature components to resist corrosive and erosive elements in fuels and environment.

Jackson was also instrumental, in the 1980s, in demonstrating the feasibility of employing the low-pressure plasma spray process to create freestanding parts. With this approach, the molten metal is sprayed onto a sacrificial form where it solidifies instantly and is built up to achieve the desired size, shape, and thickness of the fabricated part. This technique creates composite structures made of different alloys with different properties in different locations.

In a recent team project, Jackson helped develop materials and fabrication concepts for producing double-walled combustors for large power generation gas turbines. In this construction, cooling air

is used more efficiently, reducing the amount needed for cooling. This produces a significant reduction in nitrogen oxide emissions.

### Sōmiya Receives Purple Ribbon Award

In November 1995, Shigeyuki Sōmiya received the Purple Ribbon Award from the Japanese government. The award recognizes contribution to the academic, cultural, and artistic fields. Sōmiya's area of interest is in inorganic industrial chemistry, especially inorganic hydrothermal reactions. He has developed applications of hydrothermal reactions to inorganic industrious chemistry, especially from fundamental study of hydrothermal fine powders, hydrothermal reaction sintering, hydrothermal synthesis, hydrothermal crystal growth, hydrothermal corrosion, phase relations under hydrothermal conditions, hydrothermal hot isostatic pressing, and hydrothermal decomposition, to produce very fine powders of zirconia.

### AVS Albert Nerken Award Goes to Mattox

Donald M. Mattox is the recipient of the Albert Nerken Award of the American Vacuum Society (AVS) for his invention of the Ion Plating Process and its continued development. This award recognizes outstanding contributions to the solution of technological problems in areas of interest to AVS. Mattox has also been elected as a Fellow of AVS.

Mattox first reported the concept of "ion plating" in 1963 while at Sandia National Laboratories. Ion plating uses controlled concurrent bombardment by energetic ions during deposition to modify film properties. Initially Mattox's work was directed toward improving film adhesion and surface coverage. Later it was shown that the concurrent bombardment could be used to modify other film properties such as residual film stress and density, and to enhance chemical reactivity during reactive deposition processes. □

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