STM Shows Atomic Buckling of Gold Surface Layer

Researchers at IBM's Almaden Research Center, San Jose, California, announced they have made the first direct observation of the buckling of the surface layer of gold atoms—a phenomenon important in studying crystal growth. The team obtained detailed atomic-resolution images using an ultrahigh vacuum scanning tunneling microscope (STM).

Their observations confirm the features of a surface distortion called "reconstruction," first inferred 15 years ago by another (indirect) technique. Reconstruction is common in many metals, but gold is unusual because it is the only metal with a face-centered-cubic structure whose close-packed (111) surface reconstructs. The results also agree with reconstruction models proposed by Japanese and German scientists in 1983 and 1985.

The high-resolution images produced at IBM Almaden show two indicators of the gold surface buckling:

- Twenty-four gold atoms lie along lines that should contain 23; the extra atoms cause a bend in the regular atomic rows (see diagram).
- The extra atoms also pucker the surface vertically, creating a network of paired long, straight humps. The humps rise only about 0.15 A above the surface, about one-tenth an atomic radius.

The research also demonstrates that the STM can be used to study surface structures and defects with atomic-level resolution. The STM was invented and developed in 1979-1982.

Working on the project were S. Chiang, R.J. Wilson, H. Ohtani, C. Mathew Mate, C Woll, and M.D. Miller of the IBM Almaden Research Center, and P.H. Lippel of the University of Texas-Arlington. Their work will be published in the April issue of *Physical Review B*.

Epitaxx to Develop Long-Wavelength Avalanche Photodiode

Under a Phase II Small Business Innovation Research contract from the U.S. National Science Foundation, Epitaxx, Inc. will develop a simple high-performance avalanche photodiode (APD) for long wavelength optical communications.

According to Epitaxx president Greg Olsen, "the device has application wherever a highly sensitive photodetector for the 1.0 to 1.7 micron spectral region is needed; this includes high-speed (above 1 gigabit/s) fiber optic communications, eyesafe range finding and LIDAR."

APDs are light detectors that have built-in gain or multiplication of the detected signal. An ordinary detector converts one photon into, at most, one electron. APDs can multiply the photo-induced electrons by "smashing" them into the device's crystal structure, freeing additional electrons. The company is considering multiplication factors of 10-30 times for its APD, which is composed of crystalline layers of indium gallium arsenide and indium phosphide. The structure was pioneered by S.R. Forrest of the University of Southern California, who consulted on the project.

Los Alamos Dedicates Electron Microscopy Facility

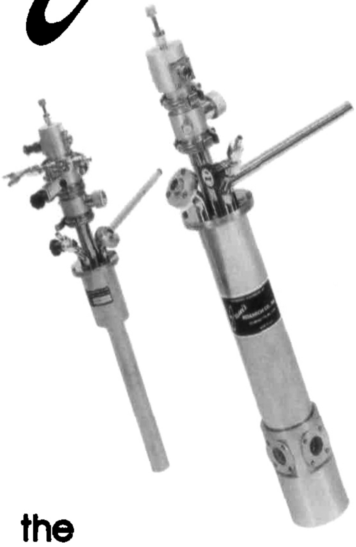
Colloquium Features Sir Peter Hirsch, Other Experts

Two new electron microscopes installed at Los Alamos National Laboratory's Center for Materials Science were dedicated recently during a one-day colloquium on electron microscopy. The instruments can magnify objects more than 10 million times, allowing researchers to directly examine atomic structures and determine the chemistry of metal alloys, polymers, ceramics, and other materials.

Prof. Sir Peter Hirsch of the Department of Metallurgy and Science of Materials, University of Oxford, opened the Los Alamos colloquium with a lecture on "Materials Under the Microscope." "Microscopy," he said, "is an essential tool for the materials scientist, for elucidating basic mechanisms, and for the development of materials." He gave examples of how microstructural and compositional studies have been used to advance the knowledge and understanding of defects in crystals, of materials such as diamond, metals and alloys, and of semiconductors.

Five experts in microscopy continued with lectures on their areas of expertise:

- R. Gronsky, University of California, Berkeley, considered "High Resolution Electron Microscopy";
- H.L. Fraser, University of Illinois, explained "Microdiffraction in the Study of Materials";
- J.I. Goldstein, Lehigh University, discussed "X-Ray Energy Dispersive Spectroscopy";
- P.E. Batson, IBM Yorktown Heights, focused on "Spatially Resolved Electron Energy Loss Spectroscopy: Binding and



Sir Peter Hirsch of Oxford University (center) discusses the capabilities of the two new electron microscopes at Los Alamos' Center for Materials Science with Don Parkin (left), director of the Center, and James F. Smith (right), technician in charge of the electron microscope facility.

Electronic Structure from Subnanometer-Size Areas"; and

- J.C.H. Spence, Arizona State University, highlighted "Novel Microscopies and Spectroscopies."

Laser Spectroscopy Reveals Polymer Structure

Many details of polymer structure can now be determined by a spectroscopic technique co-developed by researchers at IBM's Almaden Research Center, San Jose, California, and the E.I. duPont de Nemours Research Laboratory, Wilmington, Delaware. The technique, called Fourier Transform Raman spectroscopy (FT-Raman), couples the FTIR interferometer and a recently available continuous-wave infrared laser (Nd:YAG) with Raman spectroscopy.

IBM physicist John Rabolt described the first scientific applications of FT-Raman in two invited papers presented at the "Pittsburgh Conference," held March 6-10 in Atlanta, Georgia.

Rabolt's first paper described the role of FT-Raman in finding how silicon- and germanium-based polymers change their ultraviolet absorption reversibly when heated. When the polymers are heated above a specific temperature (12 C for Ge-based polymers, 42 C for Si-based materials), their planar zigzag backbone chains change into helix-like shapes. This rearrangement is responsible for the polymer's shift in ultraviolet absorption. When cooled, the molecules return to the planar structure.

Visible light used in conventional Raman studies had been ineffective because the light resonates with the Si-Si and Ge-Ge bonds along their backbones. The strong resonance usually overwhelmed the faint Raman signals from structurally important side groups. No unwanted resonance occurs with FT-Raman, says Rabolt, and the resulting spectrum clearly indicates the bond concentrations of both the backbone and side chain groups.

Rabolt's second paper described a modification of FT-Raman spectroscopy to determine the detailed structure of colored thin films. These materials include nonlinear optical materials used to change the color of laser light. The coloring agents absorb visible laser light, normally used in Raman studies, and the absorption heats the film, damaging it or changing its composition. FT-Raman avoids this problem, according to Rabolt, because the sample does not absorb infrared light. But, to make the technique work, the researchers had to devise a new system incorporating integrated optics and optical fibers tailored to infrared light. The laser light is directed lengthwise through the 2-micron-thick film, which acts as a waveguide to contain the light.

The researchers examined the structure of a yellow dye (2-nitro-5-decylaminobenzoic acid) dispersed throughout a cellulose acetate polymer film. They found, surprisingly, that rather than coalescing by the hundreds into tiny crystalline enclaves as expected, the dye molecules are clearly isolated from each other—dispersed singly throughout the polymer.

"It is significant," Rabolt says, "that this powerful analytical technique uses the same infrared light frequency used in nonlinear frequency doubling experiments. We may soon be able to observe the detailed structure of the dye molecules while they are converting infrared light to green."

Working with Rabolt were V.M. Hallmark and C.G. Zimba. The polymers were made by R.D. Miller, and the yellow dye was made by R. Twieg.

A. Schriesheim Appointed to National Commission on Superconductivity

Alan Schriesheim, director of Argonne National Laboratory, has been named by the White House to the new National Commission on Superconductivity.

The 21-member commission will review major policies regarding U.S. applications of research advances in superconductors as well as help Congress develop a strategy to assure U.S. leadership in superconductivity developments and applications.

Schriesheim has extensive experience in the field, heading the largest publicly funded U.S. research and development effort on high superconductors at Argonne. In addition, he is a member of the board of directors of the Council on Superconductivity for American Competitiveness, the NASA Space Systems and Technology Advisory Committee, and the Illinois Governor's Commission on Science and Technology.

Lake Shore Acquires Rights to Superconductor Technology

Los Alamos National Laboratory has signed an agreement giving Lake Shore Cryotronics, Inc. exclusive rights to both market a more efficient technique for measuring the quality of new high temperature superconductors and to the pending patent on the technology invented by James D. Doss, an electrical engineer in the Medium Energy Physics Division at Los Alamos.

This marks the first license granted by the laboratory in the high temperature superconductivity field. It is additionally significant because this agreement represents the first royalty-bearing license granted by the Los Alamos since Energy Secretary John Herrington urged U.S. laboratories to share new technology with private industry last June.

The technology, "eddy current superconductor characterization," relies on introducing radio-frequency electromagnetic fields into untested materials. This allows the relative energy loss to be measured in superconductive ceramics.

The technique offers several advantages to the researcher. Electrical contacts do not have to be attached to the sample, a practice that can influence test requirements. Because it provides information about the behavior of high-frequency alternating currents in these ceramics, it can also decrease preparation time for testing large numbers of samples. As a result, researchers can save the more expensive and time consuming tests for only the most promising materials.

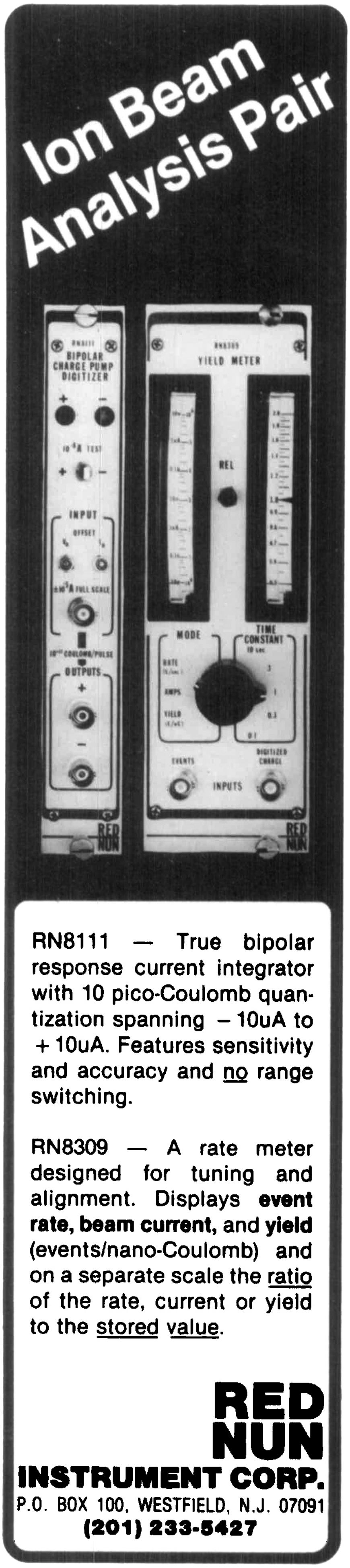
Glass Corrosion Studies Make Fracture Predictions More Reliable

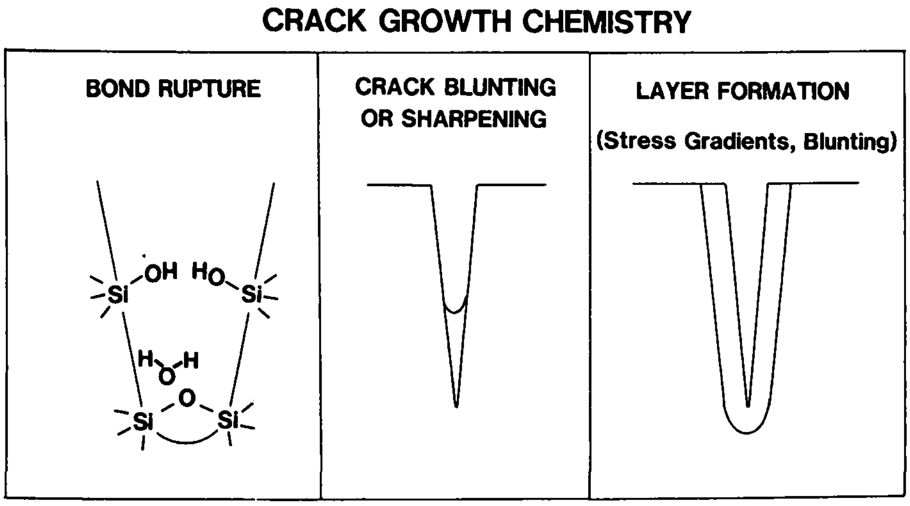
A model that explains how glass cracks and eventually fails has been developed at Sandia National Laboratories. The new model is unique, according to its creators, Terry Michalske and Bruce Bunker, because it explains how chemical reactions that modify the glass surface structure and composition can control the speed with which cracks grow—or whether they grow at all.

The key to the model is its ability to explain the impact of alteration layers on long-term performance of chemically complex, commercially important glasses such as the widely used borosilicate family.

Michalske and Bunker, who are members of the Materials Research Society, won an award for an earlier silica-glass crack-growth model that predicts crack velocities as a function of stress levels and chemical environments, and reliably predicts times-to-failure for design engineers. However, because that model deals with measurements occurring under controlled conditions, it forces researchers to extrapolate from laboratory velocities 100,000 times faster than those occurring under natural conditions. Such extrapolations appear valid for silica glass, but errors associated with chemically complex glasses have long plagued design engineers.

The new model extends crack-growth understanding from pure silica to more complicated glasses. According to Bunker, the key to understanding unusual crack-growth behavior of complex glasses was the realization of two ways in which alteration layers can control crack-growth when it occurs at low velocities. First, glass com-





Cracks can grow when water or other chemicals rupture bonds. Corrosion can change the shape of the crack tip. The key to understanding unusual crack growth in complex glasses was realizing that alteration layers - formed when some elements in the glass dissolve faster than others - can influence crack growth.

position changes that occur during layer formation can cause the layer to expand or contract relative to the unaltered glass below. This creates either compressive or tensile stresses within the alteration layer. Borosilicate crack-growth slows—and can even stop—if alteration layers develop internal compressive stresses when they form. If alteration layers are in internal tension, they literally pull themselves apart. That permits cracks to grow from surface flaws in the absence of external stresses.

Second, glass corrosion processes can change the shape of the crack tip. This can change crack-growth velocities by affecting how external stresses focus on reactive bonds at the crack tip.

To make quantitative predictions of how alteration layers influence crack-growth, Bunker and Michalske conducted experiments to relate glass corrosion processes to crack propagation. The experiments involved the use of binary alkali silicate glasses, soda-lime window glass, and several sodium borosilicate glasses.

First they measured how fast alteration layers form on glass surfaces and determined their compositions in various chemical environments. Next they measured the surface stresses generated in alteration layers as a function of time. Finally they measured crack-growth velocities in the same glasses as a function of applied stress. Results show that deviations in crack-growth behavior seen at low crack velocities can be predicted for complex glasses, provided that the alteration layer properties are understood.

Because of these and other advances, models now exist which offer the promise of accurately predicting long-term performance (20 years into the future, for instance) of glass families whose crack-growth speed isn't governed simply by stress-activated chemical reactions between water and silicon-oxygen bonds. The models also pave the way for techniques to tailor glasses that are more resistant to slow crack-growth, and are more reliable and well-suited for special applications.

Advanced Computing Lab to Open at Los Alamos

Los Alamos National Laboratory is establishing a new computing laboratory that will apply the latest advances in hardware and software to complex scientific problems.

The Advanced Computing Laboratory (ACL) will have three major thrusts, according to Andrew White, deputy leader of Los Alamos' Computing and Communications Division who will direct the new facility. First, it will employ a team concept to problem solving by putting computer scientists and applied mathematicians to work with physicists, chemists, biologists and other scientists.

The ACL will also take advantage of new developments in computer-related fields, such as massively parallel computing, networking and visualization. It will use the latest computing equipment like the 65,000-processor Connection Machine recently installed at Los Alamos.

Finally, the new laboratory will be a "bridge" connecting work performed by researchers at Los Alamos with work by the academic community, federal and industrial research centers, and computer manufacturers.

The ACL is supported by several sources including the Department of Energy's Applied Mathematical Sciences Program, the weapons program at Los Alamos and the Institutional Supporting Research Program at the Lab.

Most recently, it has received support from the National Science Foundation (NSF) as part of a new program in which Los Alamos and other institutions will conduct research on advanced parallel computing. Under that program, Los Alamos is working with Rice University, Argonne National Laboratory and the California Institute of Technology. The ACL will be the interface for the Lab with this new center.

The new NSF Science and Technology Center, called the Center for Research on Parallel Computation, is one of 11 centers recently established by the NSF that will link research institutions, universities and industry in long-term, basic research projects. The Center will be administratively located at Rice.

New Sensors Provide Real-Time Chemical Analysis

Scientists at Los Alamos National Laboratory may revolutionize chemical research by using super-thin films on fiber optics for real-time analysis of chemical reactions.

The process will speed up laboratory chemical analysis dramatically, and will have far-ranging applications in environmental, process-development and biomedical monitoring. Constant, instantaneous analysis of water supplies, monitoring of water migration from hazardous waste sites, process-development monitoring in the building of high-temperature superconductors, and monitoring of a patient's chemical balance are among the potential uses for chemical sensors.

With real-time monitoring, scientists will be able to cut the time frame for their work down from several days to several hours. For example, the team is using real-time analysis of nitric-acid concentrations during the processing of nuclear materials.

The team is trying to develop sensors that are thin fiber optics coated with specially made polymers. In one sensor, for example, a chemically modified polymer interacts with light, setting off a signal of light that travels down the fiber optic to a control point, which can be in a remote area away from where the actual toxic-chemical process is occurring. At the control point, the color and intensity of the light indicates the concentration of the chemical.