Oak Ridge Researchers Develop Technique for Direct Probing of Grain-Boundary Structure

S.J. Pennycook of the U.S. Department of Energy's Oak Ridge National Laboratory (ORNL) and his associates have developed a technique for deducing the atomic structure of defects and interfaces in materials. This method may ultimately allow scientists to tailor or "change the recipe" of metal alloys, ceramics, and superconducting materials and, consequently, to detect, alter, and remove flaws and impurities, opening the door for industry to create the materials best suited to the application at hand. Pennycook and his group began the project with a study of $SrTiO_3$ bicrystals. This study limits the number of degrees of freedom associated with the interface and provides a realistic opportunity to probe the structure-property relation for single isolated boundaries. Determining the atomic and electronic structure of the grain boundary on an atomic scale requires a technique that probes both composition and chemical bonding with atomic resolution. By combining high-resolution Z-contrast imaging to locate the cation columns at the boundary, with simultaneous electron energy loss spectroscopy to examine light-element coordination at atomic resolution, the researchers produced a detailed atomic structure model for an undoped grain boundary in $SrTiO_3$.

High-resolution Z-contrast imaging in the scanning transmission electron microscope (STEM) provides an incoherent image, in which changes in atomic structure and composition across an interface can be interpreted directly, without the need for preconceived atomic structure models. Parallel detection electron energy loss spectroscopy (PEELS) can be used simultaneously to provide complementary chemical information on an atomic scale.

The researchers showed that by combining the cation coordinates (Sr and Ti-O column positions) obtained from the Z-contrast image with the Ti-O coordination from PEELS, it is possible to propose a model for the grain-boundary structure directly from experimental data.

In Pennycook's experimental model structure, the positions of the O atoms were then refined with bond-valence sum calculations. The half-occupied Sr columns represent attractive sites for large dopants that substitute for Sr, whereas the Ti and O vacancies are likely sites for smaller dopant atoms. Because the surrounding atoms are seen to relax to accommodate the presence or absence of the Ti-O columns, these sites could accommodate dopants of different valences.

This model, said the researchers, could form the basis for a detailed theoretical investigation of such possibilities, upon which the role of dopants and processing in the development of the grain-boundary potential barriers could then be examined. They believe that further structural studies in conjunction with electrical characterization could finally elucidate the structure-property relationships for grain boundaries in electronic ceramics.

These studies were described in the article, "Direct Determination of Grain Boundary Atomic Structure in $SrTiO_3$," in the Friday, October 7 issue of *Science*, page 102.

Celler Appointed Fellow of The Electrochemical Society

George K. Celler of AT&T Bell Laboratories has been appointed Fellow of The Electrochemical Society for his contributions to processing of electronic materials, including silicon on insulator formation, rapid thermal processing (RTP), and laser annealing, and for leadership in x-ray lithography. Celler implemented the first RTP system with large-area high-intensity tungsten halogen lamps. He was honored at the Society's 186th International Meeting on October 11, 1994.

Celler received his MS degree in physics from the University of Warsaw in 1969. He was a research scientist at the University of Vienna and at the International Atomic Energy Agency, later moving to Purdue University to pursue a PhD degree in solid-state physics, which he received in 1976. He then joined the Western Electric Engineering Research Center and, in 1979, moved to AT&T Bell Labs.

Celler is also a Fellow of the APS and a member of IEEE, and has organized several symposia for MRS.

Rice Receives ASME Award

James R. Rice, Gordon McKay Professor of Engineering Sciences and Geophysics at Harvard University, has received the Timoshenko Medal of the American Society of Mechanical Engineers. The award is conferred annually in recognition of distinguished contributions to the field of applied mechanics.

Rice received the medal "for seminal contributions to the understanding of plasticity and fracture of engineering materials and applications in the development of computational and experimental methods of broad significance in mechanical engineering practice."

He completed studies in engineering and applied mechanics at Lehigh University, receiving a PhD degree in 1964, then moved to Brown University's Division of Engineering prior to assuming his present position.

Rice is a Fellow of the American Academy of Arts and Sciences, ASME, AAAS, and AGU. He is a member of the American Academy of Mechanics, the American Society of Civil Engineers, and MRS. He was elected Honorary Fellow of the International Congress on Fracture and is a member of the National Academy of Engineering and the National Academy of Sciences. Rice was a member of the NRC Solid State Science Committee and National Materials Advisory Board.

Ti-Coated Zeolite Process Aids Radioactive Cleanup

A newly patented process is successfully removing most of the radioactive elements from nuclear waste at West Valley, New York, the site of a former commercial nuclear fuel reprocessing plant. Approximately 450,000 gallons of waste at the site have been separated, using an ion exchange process developed in 1991 and patented in 1994 by researchers at the U.S. Department of Energy's Pacific Northwest Laboratory (PNL) in Richland, Washington.

The process employs a titanium-coated zeolite (a mineral used in ion exchange and commercial water treatment plants) to separate radioactive elements from the chemical contents of the waste tanks. PNL scientists used a form of zeolite ion exchanger that is known to remove radioactive cesium. By adding titanium in the form of sodium titanate, they caused the exchanger to remove plutonium and strontium as well. This material, known as Ti-zeolite, recovers small quantities of plutonium from highly alkaline radioactive wastes.

Developed by PNL scientists Lane Bray and Leland Burger, the approach removes most of the radioactive material from the liquid or acqueous waste. After separation, the liquid waste—which then contains very low levels of radioactivity—is treated by mixing it with concrete for low-level waste disposal. The small volume of ion exchange material, containing the bulk of the radioactive plutonium, cesium, and strontium, eventually will be vitrified or melted into glass logs, preventing the radioactivity from leaking into the environment.

The Ti-zeolite process has been transferred to private industry for commercialization. UOP of Des Plaines, Illinois, a joint venture of Allied Signal, Inc. and Union Carbide Corporation, has developed an optimized commercial manufacturing process for the titanium-loaded zeolite.

Growth Chamber to Help with Environmental Cleanup

Using interim facilities at the Pacific Northwest Laboratory (PNL), U.S. Department of Energy (DOE) scientists recently designed and constructed, and are now using, a prototype chamber to grow crystalline films of oxide materials. The researchers, of the DOE Environmental Molecular Sciences Laboratory (EMSL), scheduled to open in 1997, will use the films to develop methods for separating and destroying contaminants or stopping their movement in the environment. EMSL materials scientists will grow the oxide materials, while physical chemists will expose the oxide films to contaminants, such as carbon tetrachloride, to understand how chemical pollutants interact with oxide surfaces.

Scott A. Chambers (an EMSL materials scientist who led the effort to build the growth chamber) and his colleagues are using the low-pressure chamber to grow two types of oxides—ones representative of those found in minerals in the natural environment, and oxides that could be used to separate and destroy contaminants. Regarding the latter, Chambers points to silicotitanates, a class of materials known to selectively separate radioactive cesium from only certain kinds of solutions. He hopes that insight into chemical molecular workings will help scientists manipulate materials such as silicotitanates for the purpose of separating cesium from a wider variety of solutions, leading to improved separation and treatment efficiency for radioactive wastes.

EMSL researchers are also growing oxides that represent minerals found in the natural environment, to study interactions between natural substances and pollutants. To gain an in-depth understanding, says Chambers, the scientists cannot simply scoop up soil or use industrial oxide powders, which generally contain many kinds of contaminants and defects. Rather, his group must grow model oxide films, using the chamber. Chamber-grown oxide films, he says, "are carefully prepared so that the composition, crystal structure, and impurities of the oxide are known and can be controlled. We need to understand specific defects in the absence of others if we are to understand the surface chemistry in any level of detail."

Understanding oxide surface chemistry, says Chambers, may lead to advances beyond the area of environmental cleanup—to research that could improve various steps in chemical processing, aid in the development of hydrocarbon traps for automobile exhaust systems, lead to improved ion exchangers for the removal of radionuclides from tank wastes, and improve thin-film gas sensors that employ oxides.

Symposium Honors Advances in Materials Research that Made It to Market

Sponsored by the National Association for Science, Technology, and Society (NASTS) in cooperation with the Federation of Materials Societies (FMS), the First National Symposium honoring the most significant "real" advances in materials research—advances that have made it to the marketplace—was held in Washington, DC in September 1994. The Symposium identified, highlighted, and honored materials science contributions which have resulted in technology, and affected society in some way.

Nominations were received from members of the Materials Section of the National Academy of Engineering and the presidents of the member societies of FMS. A committee of materials scientists and engineers selected those projects—and the people responsible in one or another stage in the chain from discovery to marketplace—which represented the most significant advances made by their community in the last decade. Committee members included: G. Dieter, dean of engineering, University of Maryland; J.J. Gilman, professor of materials science, UCLA; A.M. Diness, Institute for Defense Analysis; R.A. Laudise, director, materials, AT&T Bell Labs; J.E. Nottke, Senior Research Fellow, Dupont; and R. Roy, Evan Pugh Professor of the Solid State, Penn State.

The following received recognition for materials science advances:

Gold Ribbon

Philippe Becker, AT&T Bell Laboratories, and **Elias Snitzer** and **David Payne**, representing the development of erbium-doped optical fibers.

Alfred Cho, AT&T Bell Laboratories, for contributions to the research on materials for cascade lasers.

David Claspell, Magnequench, representing the discovery and commercialization of new rare earth boride magnets.

R. Danforth, Carlton Ash, and **I. Drent**, Shell Development Company, for the discovery and development of polyketone thermoplastics.

Joseph Davidovits and J. Sawyer, Lonestar Cement Co., for the development of new very early high-strength cement.

Edith Flanigen, U.O.P., for the synthesis of zeolites based on $AlPO_4$.

L.J. Gauckler, Swiss Federal Institute of Technology, for the development of a biological process of enzyme catalysis of ceramic forming.

Raymond Hemphill and **David Wert**, Carpenter Technology, for the development of Aermet 100, high-strength, high-toughness steel.

David Hoffman, R.J. Riedner, C. Greskovich, and **D. Cusano**, GE R/D and Medical Systems, the team creating HiLight ceramic for improving medical x-ray practice.

K. Inomata, Toshiba Research Center, Kawasaki, Japan, for the development of new metallic glasses for high-frequency applications.

Sheldon Kavesh and **Dusan Pervorsek**, Allied Signal Corporation, for Spectro polyethylene fiber.

S. Matsumoto, M. Kamo, Y. Sato, and **N. Setaka** of NIRIM, Tsukuba, Japan, for the development of methods to produce diamond at one atmosphere by CVD.

Marc Newkirk, Lanxide Corporation, for the discovery of a radically new materials processing technology protected by 3,000 patents.

R.E. Newnham, L.E. Cross, and **D. Skinner**, Penn State, for the conception and development of a family of new composite transducers.

A.W. Sleight, Oregon State University, representing the field of perovskite-based high T_c superconductors.

Edward Steigerwald, PCC Airfoils, Inc., for a key role in the successive, successful developments leading to today's single-crystal aircraft turbine blades.

Blue Ribbon

D.K. Agrawal and colleagues, Penn State, for the discovery of new zero-expansion ceramic family NZP-CTP.

R.M. Beasley (retired), Lockheed Missiles and Space Company, for development of rigidized structural ceramic insulation.

H.S. Ghandhi, J.S. Hepburn, K.S. Patel, and **M.G. Meneghel**, Ford Motor Company, for the development of the rhodium-free automotive three-way catalytic converter.

Pierre-Gilles de Gennes, Ecole Supr. de Phys. et de Chem., for theoretical advances which have affected liquid crystal technologies.

J.B. Goodenough, University of Texas, representing contributions to the development of lithium battery electrodes.

Shimshon Gottesfeld, Los Alamos National Laboratory, for the development of fuel cells for transportation.

S. Komarneni and colleagues, Penn State, for the development of ceramic nanocomposites via the sol-gel route.

K.M. Prewo and colleagues, United Technologies Corporation, for the development of glass-ceramic structural composites.

Maurice Ward, for the unorthodox discovery and development of the high-performance insulating material, Starlite.

Fred Wudl, University of California-Santa Barbara, **R.H. Friend**, and **A. Holmes**, for contributions to research on light-emitting polymers.

Three Firms Collaborate on Program for Ultralow-Emission Gas-Turbine Combustion Technology

Catalytica, Inc. (Mountain View, California) and Tanaka Kikinzoku Kogyo K.K. (Tokyo) have contracted with General Electric Company to conduct a Phase II large-scale testing program for further developing the Catalytica-Tanaka ultralow-emission catalytic combustion technology for natural-gas-fueled turbines used to generate electricity.

General Electric will fund the Catalytica-Tanaka technology program for its potential application to GE gas turbines, then design a catalytic combustion system utilizing the Catalytica-Tanaka technology. Subscale tests on the new GE system will be performed at GE's Corporate Research and Development Center, with full-scale testing to take place at the GE Power Generation laboratories in Schenectady, New York.

A catalytic combustion system causes fuel to react with oxygen in the air on a catalyst surface to form hot combustion gases that can be used to power a turbine. Unlike normal flame combustion, which produces high nitrogen oxide (NO_x) emissions, catalytic combustion virtually eliminates the formation of this pollutant, which is regulated in many localities worldwide.

Industry/Government Project Aims to Develop Prototype High T_c Superconducting Cable

A prototype high-temperature superconducting (HTS) underground transmission cable will be built and tested under a collaborative project funded by industry and government. A team comprising the Electric Power Research Institute (EPRI, the research and development arm of the U.S. electric utility industry), Pirelli Cable Corporation of Italy (Pirelli), American Superconducting Corporation (ASC), and the U.S. Department of Energy (DOE) National Laboratories at Los Alamos, Oak Ridge, and Ames will pool $5.8 million for the program, announced by the DOE in October at the Applied Superconductivity Conference in Boston.

With Pirelli as the main contractor, the participants plan to build and operate a 30-m, 115-kV length of liquid-nitrogen-cooled cable, designed along the lines of ASC's HTS superconducting ceramic materials. The cable itself will be manufactured at Pirelli's South Carolina plant, with ASC to provide HTS wires for the fabrication of the flexible conductor assembly. The cable design will be hollow at its core, providing a channel for pumping liquid-nitrogen coolant to the superconducting wires surrounding the core.

The prototype cable, along with a splice and terminations, will be delivered to EPRI for qualifications testing under actual utility operating conditions. High-voltage testing is expected to be completed by EPRI in 1998, followed by a field demonstration at either a utility site or at the firm's Waltz Mill Test Center. Pirelli will have final responsibility for the projected four-year program, including completion of the cable, its accessories, preliminary testing, and installation.

The prototype HTS cable system is expected to have a load-carrying capacity of around 2,500 A, as compared to typical copper underground cables, which can handle a maximum load of 1,000 A.

Utilities could increase power transmission capacity of their systems 50–500% by retrofitting outdated systems with HTS cable, according to Don Von Dollen, EPRI's underground transmission manager. Moreover, the HTS cable, with more than twice the power of comparable conventional cables, would require a smaller right-of-way, thereby lowering the excavation and installation costs which can account for up to 70% of the total costs of installing new underground cable.

The $5.8 million HTS cable project includes a $1.2 million Superconductivity Partnership Initiative (SPI) Award from the DOE, a $2.16 million contract from EPRI, and $0.3 million in Cooperative Research and Development Agreements (CRADAs) with the National Labs, with the balance to come from strategic partners ASC and Pirelli. The Department of Energy created the SPI to offer financial assistance to industry-led teams developing HTS components and equipment for electric power systems. HTS has been identified by the federal government as a critical technology for sustainable energy development in the United States.

NCMS Develops Compatibility System to Aid Solvent Users

The National Center for Manufacturing Sciences (NCMS), in collaboration with its member companies, has developed a Material Compatibility System (MATCOMPAT™) to help solvent users wade through the array of non-ozone-depleting alternatives. With ozone levels dropping an estimated 40 percent over the past decade, and chlorine levels continuing to rise as ozone-depleting chemicals in the lower atmosphere drift upward, many nations have banned the manufacture of CFC-based solvents, placing a burden on solvent users.

MATCOMPAT uses a Windows™ interface to sort through the material compatibility results developed by an NCMS study. The study evaluates the effects of seven non-ozone-depleting solvents and cleaning solutions, and two common ODC solvents on 13 materials used in electronic assemblies.

MATCOMPAT provides a methodology for choosing between the cleaning alternatives for the majority of materials used in microelectronic parts. Users of the system are involved in the manufacture and/or cleaning of microelectronic parts in industries such as automotive, communications, computer hardware, aerospace, and defense. MATCOMPAT is used as a reference to aid the selection and evaluation of alternative solutions and/or test methods for the users' material- and process-specific compatibility decisions.

MATCOMPAT is being made available for license through William Andrew Inc., a publisher of materials database products. Updates will be provided based on new test results involving six additional cleaning systems. These tests are under way at the Electronics Manufacturing Productivity Facility, an NCMS partner in Indianapolis, Indiana. The entire study, in book form, is available from NCMS.

Dearnaley Named Vice President of Southwest Research Institute

Geoffrey Dearnaley has been promoted to vice president of the Materials Engineering and Technology Division of Southwest Research Institute (SwRI), following the retirement of Ulric S. Lindholm. Prior to this appointment, Dearnaley was an institute scientist and program manager of the Division's Ion Beam Surface Modification Facility. In his new position, he will continue to oversee operation of the facility, and will also direct a staff of more than 80 people involved in all aspects of materials research—engineering, mechanics, applications, and development.

Dearnaley is a Fellow of the Royal Society of London and an internationally recognized leader in research on ion implantation of semiconductors and metals. Before joining SwRI in 1993, he was chief scientist in the Surface Science and Technology Department at the United Kingdom's Atomic Energy Authority Harwell Laboratory, where he initiated development of nuclear particle detectors based on the radiation sensitivity of the reverse-biased semiconductor diode, research that helped revolutionize nuclear particle detection methods.

At SwRI, Dearnaley has been a key participant in the Institute's biomaterials internal research initiative program, working toward development of ion implantation to apply amorphous forms of diamondlike carbon to materials science for biomaterials applications.

Dearnaley is the author or co-author of 290 papers and two books—*Semiconductor Counters for Nuclear Radiation* and *Ion Implantation*—both standard texts in their fields. He holds bachelor's and master's degrees in natural sciences and a doctorate in nuclear physics from Cambridge University.

DOE Announces Sulfur Lamp Lighting Technology

A highly efficient lighting system based on a newly developed, powerful Sulfur Lamp coupled to a large semitransparent light pipe has been unveiled by the U.S. Department of Energy (DOE). DOE has inaugurated use of the system at its Forrestal Headquarters Building and at the Smithsonian's National Air and Space Museum, both in Washington, DC.

The Sulfur Lamp, invented three years ago by Fusion Lighting, a small high-technology firm in Rockville, Maryland, is based on Fusion's discovery that sulfur, stimulated by microwave energy, could be used in place of mercury in their ultraviolet industrial lamps to produce a very bright, near-sunlight-quality light. The high efficiency and small size of the Sulfur Lamp make it ideal for use with the light pipe technology developed recently by A.L. Whitehead of Vancouver, British Columbia. The combination results in long, luminous tubes that can provide high-quality, high-efficiency illumination for large indoor or outdoor spaces.

Light from the new Sulfur Lamp closely simulates sunlight. Light output does not diminish over time, and the life of the sulfur bulb itself is potentially limitless. In the Forrestal installation, energy consumption has been reduced by more than 60%. DOE estimates that the conventional high-intensity discharge and large fluorescent lighting systems typically used to light large areas, use 130 billion kWh per year, for an annual consumer cost of some $8 billion. Moreover, the Sulfur Lamp uses no mercury, a significant environmental advantage over other high-efficiency lamps; disposal of mercury-laden lamps has been an environmental problem.

Fusion Lighting is being sponsored by DOE to develop both high- and low-power versions of the Sulfur Lamp, and DOE is sponsoring further development of light pipe and other optical technologies which can distribute light in more effective ways.

Princeton, UC-Santa Barbara to Cosponsor "Research in the National Interest"

"Energy-Efficient Vehicles" will be the first in a series of workshops to identify how long-term basic research can contribute to the national interest. Cosponsored by Princeton University and the University of California-Santa Barbara, with funding obtained from the National Science Foundation, the workshops are intended to help realize part of President Clinton's vision, expressed in the recently released U.S. Science Policy, "Science in the National Interest."

The first workshop, "Basic Research Needs for Vehicles of the Future," to be held in January, will bring together scientists and engineers from universities, government laboratories, and industry to stimulate basic research that can contribute to the development of more energy-efficient and environmentally sound vehicles. Cosponsored by the Department of Energy and the NSF, in partnership with Chrysler, Ford Motor Company, and General Motors, the event will focus on six areas: energy storage materials and processes, energy conversion materials and processes, lightweight materials, the impact of emissions on the atmosphere, emission control, and sensors for control, performance, and emissions.

The results of the six individual workshops will be communicated to universities and to government science and engineering communities to solicit contributions for innovations in this area and to help guide future investments in basic science. For more information, contact the workshop coordinator: Alexis Faust, Princeton Materials Institute, Princeton University, Bowen Hall, 70 Prospect Ave., Princeton, NJ 08540-5211; e-mail: afaust@pucc.princeton.edu.

American Superconductor Achieves High Performance in HTS Magnet System

American Superconductor Corporation (ASC) has achieved performance in a high-temperature superconducting (HTS) magnet system that could set the stage for the development of smaller, more efficient electrical equipment. In demonstration, the HTS magnet coil exceeds the threshold of performance required of magnetic coils in commercial motors and generators, representing an advancement toward the commercialization of HTS products.

Developed and manufactured by ASC, the HTS solenoid magnet produces a magnetic field of 2.16 T when cooled to 27°K (410°F) by a mechanical refrigerator. It is anticipated that the first commercial superconducting motors and generators will operate in the 20–40 K range, the goal established by the U.S. Department of Energy's Superconductivity Partnership Initiative Program on HTS motors. Another feature of the magnet is that the bore of the magnet coil is at room temperature, while the magnet itself is chilled to 20 K by an external refrigerator. The magnet is fully superconducting, based on the end-to-end voltage criterion of 1μV/cm, the highest performance yet achieved for an HTS magnet with a room-temperature bore.

"[Our] demonstration proves that HTS materials can create larger magnetic fields than those generated with copper and iron, the traditional materials for motors and generators," says Greg Yurek, ASC president and CEO. The size range for first adoption of HTS technology will be industrial motors with output power of more than 1,000 hp.

ASC presented the results of the magnet system in October at the Applied Superconductivity Conference in Boston.

IBM, Quantum Magnetics Collaborate to Commercialize Superconducting Technology for Magnetic Sensing

Quantum Magnetics (QM) and the IBM Corporation have entered into a joint development and licensing agreement to commercialize superconducting technology for a broad range of magnetic-sensing applications in detection, analysis, and inspection. Over the next decade, this agreement—covering all relevant superconducting technology already developed by IBM and QM, as well as future developments—is expected to result in a new group of advanced and innovative products. The contract was announced in October at the 1994 Applied Superconductivity Conference in Boston.

All relevant superconducting know-how developed at the IBM Research Division's T.J. Watson Research Center is being licensed to QM for exclusive commercial use in magnetic-sensing systems. In addition, QM has access to all IBM superconductivity patents.

Superconductivity, through magnetic effects and superconducting quantum interference devices (SQUIDs), offers unique capabilities for magnetic sensing. Already, IBM has demonstrated practical SQUIDs made from high-temperature superconducting materials, and methods of using them in magnetically unshielded environments, and has discovered specific magnetic signatures for some important substances.

Andrew Hibbs, QM president, and Mark B. Ketchen, senior manager, superconductivity, at IBM Research, will coordinate the collaborative work at QM facilities in San Diego, California and IBM facilities in Yorktown Heights, New York. Initially, QM and IBM will work on commercializing technology that has, partly through government funding, already been developed at both companies. □