Cray, Los Alamos Sign CRADA Based on Computer Industry Model

Based on a model agreement for cost-shared ventures between Department of Energy (DOE) laboratories and the computer industry,* Cray Research, Inc. and Los Alamos National Laboratory (LANL) signed three cooperative research and development agreements (CRADAs) for (1) developing a more accurate oceanic-atmospheric model for studying global climate change, (2) reducing the cost of designing and developing advanced computer chips by developing advanced software to simulate electromagnetic wave effects in ultrahigh-speed electronic devices, and (3) improving computational chemistry capabilities required to meet industrial needs to model large protein molecules containing more than 1,000 atoms. (Today's modeling systems limit studies of molecular dynamics to molecules of a few hundred atoms.)

This CRADA signing comes a week after President Bush announced the model agreed to by DOE and the computer firms as part of his agenda to promote sustained economic growth and new jobs. The terms of the Cray-LANL CRADAs provide for approximately $1 million in support of the three projects by Cray and about $650,000 by DOE over a two-year period.

**Editor's Note*: See "DOE, Computer Firms Agree on Model CRADA" in this month's From Washington.*

Advanced Materials Speed America's Cup Yachts

For the first time, all competing yachts in the 28th Defense of the America's Cup are composed of composite materials. Borrowed from the aerospace industry because of their strength and light weight, the composites are graphite fibers embedded in a resinous matrix that solidifies when heated. With them, yachts can be 10 feet longer and 33% lighter using 50% more sail area than former 12-meter class yachts competing from 1958 to 1987. Composites allow inexpensive and efficient construction of complex shapes, and a composite boat can be built in 90 days and can make yachts sail 25% faster.

At Stanford University and the Massachusetts Institute of Technology, aeronautics and astronautics researchers are studying various combinations of yacht shapes, weight distributions, and concepts with the composites. Such physical properties as stiffness, strength, and density help researchers choose composite materials to form hulls, decks, masts, and keels. Keel design is critical. When the rest of the boat is lighter, more weight can be put in the lead bulb attached to the keel, stabilizing the vessel and allowing bigger sails. The hull is composed of a lightweight man-made honeycomb core sandwiched between two composite skins. The honeycomb minimizes the boat's weight while providing stiffness.

Even sails may soon be made of composites. An Italian builder fit a yacht with a carbon-fiber-on-polyester fabric that may be faster than the Kevlar sails currently used in the America's Cup race. The new material stretches only 1% of its length compared with 2.5-4.0% for Kevlar. The added stiffness helps sails keep their optimum shape. The fabric of woven carbon fibers is laminated with a polyester film to control brittleness.

Within America's Cup rules, engineers test thousands of design options via computer, testing boats slammed through simulated winds and waters. Another machine is used to stress the limits of a scale-model keel, and yacht models are subjected to tanks and wind tunnels.

"Ceraming" Creates Harder Wood

Researchers at the University of Washington have developed a process that yields harder, stronger wood by modifying cellulose fiber in wood with ceramic material. "Ceraming" is similar to petrifying wood but can be completed in days.

Six tree species have been tested—Douglas fir, hemlock, Southern pine, red alder, red oak, and cottonwood—and shown to be 50-90% harder than wood and 20-120% stronger, depending on the species.

The research is headed by Ilhan Aksay, professor of materials science and engineering and director of the Advanced Materials Technology Center at the Washington Technology Center. He believes the ceraming process has applications beyond flooring, furniture, doors, and structural timber to far wider potential in electronics and advanced composites.

University of Washington researchers also have been able to completely replace the cellulose in wood with ceramic materials by heating treated wood samples to 500°C. The resulting ceramic is a copy of the original cellulose structure, complete with openings or voids. These voids then could be filled with other ceramic polymeric or metallic materials, Aksay said, to create new composite materials. Some of these composites could be designed as electronic structures to function as piezoelectric devices. Another possibility would be the creation of cellulose-ceramic composites with magnetic storage properties that could perhaps lead to magnetic paper. The researchers have also begun to test the acoustical properties of the new wood-ceramic composite to see if it might be useful for making such musical instruments as violins and guitars.

Introducing ceramics into the cellular structure of wood to improve its strength originated with Ferhan Kayihan, a corporate research and development engineer at the Weyerhaeuser Company in Tacoma, Washington. Weyerhaeuser funded the early research at the University of Washington, beginning in 1990 with a ceramic materials called tetraethoxysilane (TEOS), a silicon compound used for making glass. Wood is soaked in TEOS, a liquid, to impregnate the cells. The sample is then placed in a curing oven where heat and water in the wood cells convert the TEOS into a ceramic. Other ceramic materials were also successfully tried. Aksay said the wood-ceramic composite created looks like wood, although it sometimes has a different color. It retains the grain pattern of the wood, seems to accept stain well, and is easy to work.

The ceraming project is part of a broad University of Washington engineering research program into biomimicking, or the creation of high-performance materials based on biological models such as seashells, bone, and wood. Ceraming duplicates a natural process used by bamboo and some Asian hardwood trees including teak to incorporate minerals in their cellular structure, according to Aksay. Teak trees absorb silicic acid as they take up water and the material precipitates into the wood. As a result, teak will corrode stainless steel and wears out tools faster.

Ion Implantation Strengthens Aluminum Alloy

Implanting aluminum with oxygen ions produces an alloy five times stronger than today's high-strength aerospace aluminum alloys, and with greater resistance to friction and wear, say Sandia National Laboratories researchers. Existing aluminum alloys are usually not as strong as steel alloys and soften significantly at relatively low temperatures (200°C). They are also susceptible to high friction and wear.

The researchers found that oxygen concentrations as low as 5 at.% implanted in the surface of aluminum made it five times more resistant to wear than pure aluminum. For 20 at.% oxygen, strengths as high as 2.9 GPa were measured, exceeding those of high-strength aerospace alloy 7075-T6. For 5 at.% oxygen, a strength of 1.4 GPa was measured. Finite-element computer codes were used to extract the strength of the implanted layer from indentation test results.

Pure aluminum disks 1.87 cm in diameter were bombarded at room temperature with $O+$ ions at energies between 25 and 200 keV, eventually producing a uniformly implanted layer to a depth of 0.5 μm.

A high density of nanometer-size precipitates is produced, which is directly responsible for the high strengths. This agrees with conventional theories of strengthening. Even when heated 1 h at 550°C (about 88% of aluminum's melting point), the alloy remained three times stronger than the aerospace alloy and nearly as hard as 440C steel.

Although ion implantation is currently the only way to produce this strong alloy, researchers hope that eventually it could be made by other, less expensive methods. However, the present method is suitable for direct application to the surfaces of critical components to improve durability.

Awards Announced by APS

Among the 42 recipients of prizes and awards presented by the American Physical Society between July 1991 and June 1992, the following were involved with materials research:

Barbara H. Cooper, Cornell University, received the Maria Goeppert-Mayer Award "for 1992 for her innovative studies of ion-surface interactions in the hyperthermal energy range. Combining experimental data from a highly versatile ion spectrometer with theoretical modeling, she developed accurate ion-surface interaction potentials and provided detailed information about energy deposition and scattering mechanisms."

Robert F. Curl, Rice University, **Harold W. Kroto,** University of Sussex, and **Richard E. Smalley,** Rice University, received the International Prize for New Materials "for the discovery of C_{60}, a new form of carbon."

Glenn H. Fredrickson, University of California at Santa Barbara, received the John H. Dillon Medal for Research in Polymer Physics "for outstanding contributions to the theory of phase transitions, structure, and dynamics of polymers, most notably block copolymers."

Philip A. Pincus, University of California at Santa Barbara, received the High Polymer Physics Prize "for insightful contributions to the theory of complex polymer fluids."

Robert A. Street, Xerox Corporation, received the David Adler Lectureship Award in the Field of Materials Physics "for outstanding contributions to the materials physics and technology of amorphous semiconductors. In particular, his experimental discoveries and theoretical models of defect and dopant interactions in hydrogenated amorphous Si have been crucial in advancing the field."

Direct Observation of High-Temperature Superconductor Oxygen Atoms

Using an ultrahigh voltage electron microscope, a research team at Japan's National Institute for Research in Inorganic Materials (NIRIM) of the Science and Technology Agency (STA) has directly observed and photographed the oxygen atoms of a high-temperature superconductor. The ultrahigh-resolution high-voltage electron microscope (UHR-HVEM) was developed at NIRIM by Shigeo Horiuchi, Yoshio Matsui, and Bin Okai. Its point-to-point resolving power is 1.04 Å at an accelerating voltage of 1,300 kV, 1.25 Å at 100 kV and 1.4 Å at 800 kV. Computer simulation techniques enhance its image.

One of the first direct observations using the UHR-HVEM was the column sites of oxygen atoms in a ZrO_2 crystal. The most recent, as reported in the *Japan Journal of Applied Physics* (Vol. 31) is the tetragonal $YBa_2Cu_3O_{7.7}$ crystal. It was observed for the [001] as well as [100] orientations at an accelerating voltage of 800 volts. This voltage was used in order to minimize damage by the irradiated electrons. Dark spots from the oxygen were directly detected in additional to those of Y, Ba, and Cu atoms (see

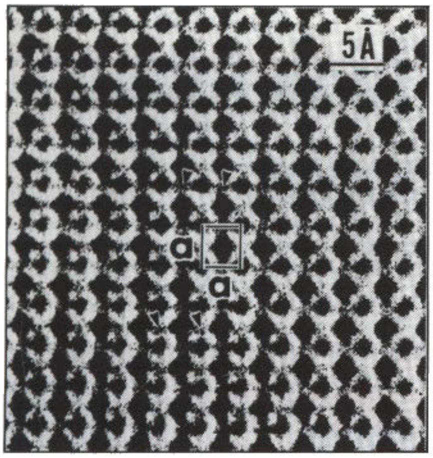

Photo of UHR-HVEM image of $YBa_2Cu_3O_{7.7}$ fragment examined at 800 keV. The large black spots are barium atoms and the black spots in the four corners surrounding the barium atoms are copper atoms. The small black dots (indicated by the arrows) between the copper are oxygen atoms.

photo). As a result, the crystal structure was confirmed to be similar to that of the tetragonal $YBa_2Cu_3O_{7-x}$ ($x > 0.5$) crystal. Excess oxygens are considered to be accommodated in the otherwise vacant sites.

Since oxygen is considered to play an important role in high-temperature superconductor phenomena, this observation will hopefully contribute to a greater understanding of the high-temperature superconductive mechanism, which is still unclear at many points.

F.S. Myers

Carbon/Carbon Turbine Rotor Powers High-Temperature Turbojet

A turbine rotor made of carbon/carbon composite materials, designed and fabricated by the LTV Corporation, has been successfully tested in a turbojet engine operating in excess of 1650°C at the Allied-Signal Aerospace Company's Garrett Engine Division in Phoenix, Arizona. This demonstration of the use of carbon/carbon for rotating components in a turbojet engine exceeded previous temperatures by more than 500°C.

This engine does not need a cooling system due to its increased material strength retention at very high temperatures (conventional engine technology must maintain metal component temperatures of less than 1000°C). It also is capable of twice the thrust at which it was tested and, fully optimized, would provide even more thrust and a lower fuel consumption, say LTV representatives. Test results showed that uncooled carbon/carbon engine components work well at hypersonic temperatures and speeds (Mach 6 +).

A tough, lightweight material, carbon/carbon can be fabricated into intricate shapes. Fabrication begins with a resin-impregnated graphite cloth formed in multiple laminates. The material then undergoes curing and high-temperature pyrolyzation. A high-density coating is applied to resist oxidation.

S.I. Raider Receives Callinan Award

Stanley I. Raider, a research staff member at the IBM T.J. Watson Research Center, has received the Thomas D. Callinan Award of the Dielectric Science and Technology Division of The Electrochemical Society. Raider was recognized for his research contributions to thin film interface chemistry and its impact on the processing and properties of semiconducting and superconducting devices.

Raider's x-ray photoelectron spectroscopy studies have probed processes occurring at silicon-silicon dioxide and niobium-niobium oxide interfaces. His research on impurities at silicon-silicon dioxide interfaces has enhanced understanding of time-dependent dielectric breakdown events, of factors affecting silicon oxidation kinetics, and of local interfacial reactions. He invented a reproducible, high-quality niobium-niobium oxide superconducting tunnel junction process that IBM used in its Josephson program. He has originated processes to produce other exploratory superconducting devices and recently used a magneto-optic technique to identify non-uniformities in high-temperature superconducting thin films. Raider has received two IBM Outstanding Contribution Awards and four IBM Invention Awards, and hold five patents and more than 50 technical papers.

Cu-Alkoxide Used for Sol-Gel Synthesis of Cuprate Superconductors

Researchers at the International Superconductivity Technology Center's (ISTEC) Superconductivity Research Laboratory in Tokyo have prepared a new Cu-alkoxide for sol-gel syntheses of cuprate superconductors. It has been identified as a 1-methylpropoxy-hydroxy-copper, a kind of copper butoxide. By using the new Cu-alkoxide for sol-gel syntheses, a couple of cuprate superconductors were found to form even under normal pressure. They were of the low-temperature phases and previously had been obtained only by high-pressure syntheses.

A material such as copper nitrate dissolved in an alcohol has been used so far to supply the Cu component for high-T_c oxide superconductors for synthesizing high-T_c cuprate superconductors by means of a sol-gel technique. But either the hydrolysis reaction has not been uniform or the solubility of Cu in such solutions has been too low. Both problems have been solved by using the new Cu raw material, which has a secondary butoxide group on one side of the Cu atom and a hydroxyl group on the other side.

By using this raw material in sol-gel syntheses, high-quality high-T_c cuprate superconductors such as Ca-doped 124 superconductors ($(Y_{1-x}Ca_x)Ba_2Cu_4O_8$) of $T_c \sim 90$ K and 326 superconductors of ~ 60 K have been successfully obtained under normal pressure. Conventionally, high-pressure synthesis techniques such as hot isostatic pressing were required to prepare these superconductors.

The Cu alkoxide is expected to be useful for sol-gel syntheses of most cuprate superconductors under normal pressure and/or at low temperatures. Sol-gel methods also have advantages over other methods in the controllability of particle size and of sample forming.

CMU Establishes Center for Creating and Processing New Materials

Carnegie Mellon University (CMU) has established a Center for Advanced Deformation Processing Research (CADPR) whose focus will be a hot triaxial compaction device that compacts metal, ceramic, and composite powders at extremely high temperatures, pressures, and shear stresses.

Researchers will investigate the relationship of processing parameters to microstructure and defects. Research will be conducted on a wide range of materials. The device can physically model deformation processes and provide much needed data for computer modeling. CADPR Director Henry R. Piehler said, "By understanding the fundamentals of deformation processing in these areas, we can control and model industrial processes. At this center, we have the technology to process materials that can't be processed in any other way."

During the past two years, Piehler and colleagues have been using the hot triaxial compactor in joint research with Alcoa on consolidating aluminum powders. They have discovered that the most important compaction mechanism of these materials is transient creep, a factor not included in any existing computer models of powder compaction. Another study, conducted with the Metals and Ceramics Division at Wright Patterson Air Force Base, showed that fracture during high-temperature processing of titanium aluminides can be suppressed by using the compactor during processing.

The Center is funded initially by CMU, its engineering college, the Ben Franklin Technology Center, and eight industrial participants, including Alcoa, Dynamet, Kobe Development, and Richter.

Confocal Resonator Measures Surface Resistance In Situ

A noncontact, quick method for measuring surface resistance in superconductors, thin film and bulk conductors, and chemical reactions, has been developed at Sandia National Laboratories using a device called a "confocal resonator" that can be used *in situ* to map samples to better than 1 mm resolution. Surface resistance is a crucial property of high-temperature superconducting materials, and previous methods for measuring surface resistance were difficult, sometimes requiring trimming or modifying the sample to fit it in a microwave cavity.

The confocal resonator uses a quasi-optical microwave resonance technique, employing a resonant cavity formed between a spherical mirror and the conducting sample. When the structure is in resonance, a standing electromagnetic wave exists, and its properties are strongly affected by the detailed dielectric and conductive properties of the materials in its path. The device can measure the surface resistance of a sample as a function of position and temperature, critical for superconducting material. Measuring the surface resistance of a superconducting wafer before expensive and complicated processing is done is important to determine the film quality and locate any defects.

The technique can be used for any thin-film conductor, potentially affecting such areas as high-energy-density batteries, thin-film growth, corrosion and aging, identification of materials defects, environmental monitoring, high-speed circuits, and microwave applications.

Romig Appointed Director of Sandia's Materials and Process Sciences Center

Alton D. Romig Jr. has been appointed director of the Materials and Process Sciences Center at Sandia National Laboratories effective April 1, 1992. This Center incorporates most of Sandia's research and development in engineering materials, including metals, ceramics and polymers. The Center also teams closely with the Manufacturing Technologies Center to bring materials R&D into production and collaborates with the Microelectronics and Photonics Center on certain electronic materials, especially ceramics. Formerly manager of the Metallurgy Department at Sandia, Romig also holds an adjunct professorship in the Materials Science and Engineering Department at the New Mexico Institute of Technology in Socorro.

Romig joined Sandia in 1979 and has performed research in several areas, including analytical electron microscopy, solid-state diffusion, solution thermodynamics, and phase transformations. Much of his research in these areas has been directed at technological problems, such as those encountered in electronic packaging, soldering, and welding.

Romig is an active member of MRS, serving on the Long Range Planning Committee, the *MRS Bulletin*'s Technical Editorial Board, and the Continuing Education Committee, which he chaired from 1988 to 1989. Also an instructor in the MRS Short Course Program, he has taught courses on transmission and scanning electron microscopy. He co-organized the 1991 MRS Spring Meeting symposium on "Structure - Property Relationships for Metal - Metal Interfaces."

Romig is a past president of the Microbeam Analysis Society (MAS), and a fellow of ASM, International. He also serves on the external advisory boards of various universities. Romig has received two awards for outstanding contributions as a young scientist—the Electron Microscopy Society's Burton Medal and the Heinrich Award from MAS. Romig is the 1992 recipient of ASM's Materials Science Division Award for research excellence. Romig received his education in materials science and engineering at Lehigh University, Bethlehem, Pennsylvania. He is the author or co-author of more than 125 technical articles and has co-authored three textbooks in electron microscopy.

NSSA Established to Provide Voice for Neutron Scattering Community

The Neutron Scattering Society of America was recently established to provide an organized, national voice to more effectively promote and represent the interests of its diverse group of practitioners.

Thermal neutrons, discovered in 1932, provide a low energy probe that is sensitive to magnetic properties and light elements. They possess excellent penetrating power in most materials, yet neutron scattering can be used to explore surfaces and interfaces. Neutron scattering has provided basic information about the atomic and magnetic structure of materials and the physics of neutrons, and it has aided such developments as high-performance magnets for motors and high-temperature superconductors.

Funding, instrumentation, and facilities are key issues for this community. Its broad spectrum of interests spread over several disciplines and its need for major facilities to do "small science" with a brief timeline and small funding can be a disadvantage in the increasing competition for funds and recognition, says Henry Glyde, a member of the NSSA steering committee.

The NSSA aims to identify and communicate needs for facilities and instruments; develop policies; stimulate, promote, and broaden the user base in neutron scattering; and carry out educational activities.

The steering committe is calling for members so that executive board candidates can be nominated and elections held. For information, contact: Jill Trewhella (NSSA-MRSB), Life Sciences Division, Los Alamos National Laboratory, Los Alamos, NM 87545; phone (505) 667-2031; fax (505) 665-3024.

Editor's Note: *For more about the contributions of neutron scattering to materials research, see the November 1990* MRS Bulletin.

Hollow Ceramic Spheres Useful in High-Temperature Insulation

Researchers at the Georgia Institute of Technology have developed tiny hollow ceramic spheres that are strong and endure very high temperature. The invention may provide an alternative to existing industrial and home insulation materials, and could even be used as industrial catalytic supports or timed-release capsules.

Made from a rapid, liquid-forming process, the thin-shelled "Aerospheres" are lightweight, durable, and capable of withstanding temperatures up to 1760°C. Researchers anticipate that these materials will initially be used as insulation for industrial furnaces because other materials currently used, such as kaolin and aluminum oxide fibers, tend to shrink and crack.

Aerospheres may later find use in residential insulation—fiberglass loses insulating properties over time and is only fire-resistant, not fireproof. The ceramic spheres can provide a fire barrier and bear compressive loads as well.

Other anticipated uses lie in pharmaceuticals as Aerospheres with porous shells are developed for slow delivery of drugs into the body, and in catalytic support used as less-expensive, reliable porous "pellets" to absorb catalytic substances to speed chemical reactions.

The first Aerospheres have been made of aluminum oxide. Researchers also worked with mullite, zirconia, and many other ceramic powders. Glass spheres are now being tested because they provide the same degree of thermal conductivity as fiberglass.

Glass Sensor Changes Colors in Response to Chemicals

Researchers from the University of California-Los Angeles (UCLA) have developed a glass that changes colors in response to chemical compounds.

The material, a sol-gel created at room temperature in a table-top laboratory, looks and feels like ordinary window glass. However, the glass is made in a process that entraps enzymes selected for their ability to change color when exposed to specific chemicals. With exposure to glucose, for example, the enzyme, and therefore the glass, turns from clear to red.

Bruce Dunn of UCLA's materials science department said, "The unique aspect of the sol-gel system is the ability to make, from solutions at room temperature, optically transparent glasses that retain proteins or enzymes, yet are still porous enough to allow transport of small substrates into and out of the glass matrix. Because many biomolecules change color in response to other chemicals, and since the glass is transparent, a simple yet reliable organic sensor can be manufactured."

The research, funded by the National Science Foundation, was a cooperative effort between the UCLA's departments of materials science and chemistry and biochemistry.

Advances Reported in Electrically Conducting Plastic

Using a process that allows links to form between the molecular chains in the plastic, researchers from the University of Pennsylvania and Ohio State University have found a way to increase by 10 times the conductivity of a polyaniline plastic.

University of Pennsylvania chemistry professor Alan MacDiarmid and collaborators showed that the links are small crystalline centers in the plastic material. These "junctions" increase conduction by spreading their crystalline organization throughout the plastic when the material is stretched to form a thin foil. The researchers believe that conductivity increases, at least in polyaniline, due to an increase in crystallinity, not simply because of an alignment of molecules which happens when the material is stretched into a foil.

The team found that polyaniline with no junctions increases its conductivity 10 times when stretched into a foil, while the increase for polyaniline with junctions is 100 times. To introduce the junctions, the researchers used a simple gelling process to produce the plastic. X-rays of the gelled, stretched samples show patterns characteristic of crystal organization. The researchers also found that samples with lower levels of crystallinity show similar increases in conductivity while requiring less processing time. The mechanical properties of the stretched junction-containing plastic were also improved compared with stretched polyaniline without junctions. □