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Oak Ridge National Laboratory REVIEW

• MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY •

Recreating the Strength of Diamonds

The World's Most Water-repellent Surfaces

Simulating the Universe's Origins

Oak Ridge National Laboratory
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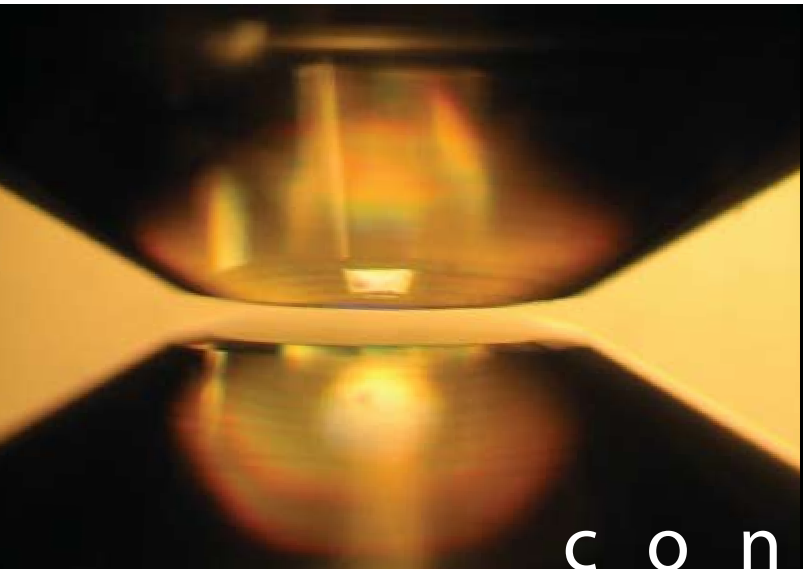


contents

EXTREME SCIENCE

On December 14, 1911, a team of five men and 16 dogs arrived at 90°00'S, the first time in recorded history that humans stood at the South Pole. Led by Norwegian Roald Amundsen, one of the most significant scientific endeavors of his era was accomplished under some of the most extreme conditions found on Earth. Unlike the tragic expedition of Robert Scott that followed weeks later, Amundsen succeeded because he had an appreciation for the extreme conditions, and because he prepared carefully.

Nearly a century later, the scientific community confronts challenges in some respects as daunting as those faced by the Polar expedition. Today policymakers ask for assurance that containers storing spent nuclear fuel can resist corrosion for thousands of years. An automotive industry engaged in a ferocious international competition demands new materials that are lighter and stronger but at the same time cheaper than steel or aluminum. Meanwhile, scientists must respond to the growing demand for electricity with rapidly accelerated efforts to harness the sun's energy for generating electricity for transportation, industrial and residential applications while addressing concurrent challenges in electrical storage and grid infrastructure.

For researchers at Oak Ridge National Laboratory, each of these challenges requires entering a new dimension of discovery where exploration is undertaken at the extreme borders of science with tools unimaginable only a decade ago. In ORNL's nanoscience center, researchers control the structure of materials over a distance one million times smaller than a human hair. Next door, the Spallation Neutron Source is uniquely suited for the study of materials under extreme conditions, including pressures approaching those found at the center of the Earth. In ORNL's Center for Computational Sciences, a supercomputer conducts classical simulations of three million atoms at 270 trillion calculations per second. Data used by scientists attempting to understand the mysteries of the universe are measured, not in centuries, but in billions of years.

This issue of the ORNL *Review* features a sampling of research that could be defined as "extreme science." The research topics represent a broad variety of unique scientific challenges that can be understood only in the context of extreme conditions of pressure, temperature, magnetic fields, radiation and intense light. These extreme conditions, in turn, can be studied only with some of the world's most sophisticated scientific instruments. One of the most exciting aspects of conducting research "on the edge" is the discovery that many materials under extreme conditions behave in new and unexpected ways. The ability to realign atoms under extreme conditions, for example, holds the potential for some materials to be as much as 100 times stronger than previously thought possible.

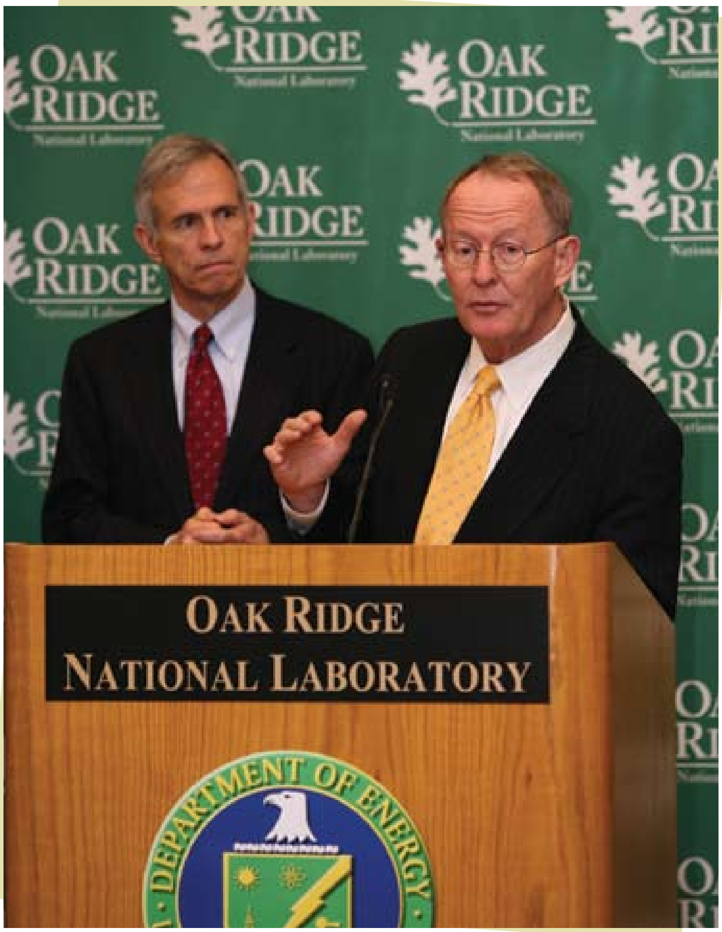
Working with the Department of Energy, ORNL is rethinking both the strategies and potential made possible by the ability to explore the extreme edge of science. The process requires that we abandon a host of assumptions that for decades have shaped our instincts about the limits of scientific inquiry. We are proving capable of this change, and are preparing for a journey that will lead us into new realms of discovery. Borrowing from Roald Amundsen a century ago, "Victory awaits him who has everything in order—luck, people call it."

Michelle Buchanan

Associate Laboratory Director
for Physical Sciences

News & Notes

Manhattan Project for clean energy independence



U.S. Sen. Lamar Alexander, with Congressman Bart Gordon, lists seven grand challenges to make America less dependent on foreign oil.

U.S. Sen. Lamar Alexander of Tennessee proposed a new five-year Manhattan Project for Clean Energy Independence during his May 9, 2008, visit to Oak Ridge National Laboratory. He was accompanied by two Tennessee members of Congress—U.S. Rep. Bart Gordon, chairman of the House Science and Technology Committee, and U.S. Rep. Zach Wamp, who represents ORNL in the Third Congressional District and is a senior member of the House Appropriations Committee.

At the forum hosted by ORNL Director Thom Mason, Laboratory scientists offered ideas on research needed to achieve what Alexander called "clean energy independence." ORNL Corporate Fellow David Greene discussed the new generation of batteries, combined with peak-load pricing of electricity, required to transition to an electric fleet of automobiles. He said that one of the national goals should be to double automotive fuel economy by 2030.

Dana Christensen, ORNL's associate laboratory director for energy and engineering sciences, emphasized the importance of closing the fuel cycle to enable the expansion of carbon-free nuclear energy in the United States.

"By independence I do not mean that the United States would never buy oil from Mexico or Canada or Saudi Arabia," Alexander said. "By independence I do mean that the United States could never be held hostage by any country for our energy supplies."

During the discussion that led to the passage of the America COMPETES Act of 2007, the senator noted several participants suggested that "focusing on energy independence would force the kind of investments in the physical sciences and research that the United States needs to maintain its competitiveness."

The growing demand for oil worldwide and corn-fed ethanol in the United States is driving up gasoline and food prices, motivating the public to address the availability and cost of energy with a greater sense of urgency. This challenge comes as Americans are increasingly aware that burning more coal for electricity is contributing to sustained global warming.

Alexander noted that characteristics of the Manhattan Project 65 years ago could be applied to the current initiative for clean energy independence. Foremost is the urgent need to proceed quickly along several tracks toward a common goal. Alexander added that long-term success would also require Presidential leadership and bipartisan support from Congress.

Alexander said a contemporary Manhattan Project for energy should undertake "seven grand challenges" that would put America on the path toward clean energy independence within a generation. Alexander's seven grand challenges are:

1. Make plug-in hybrid vehicles commonplace
2. Make carbon capture and storage a reality for coal-burning power plants
3. Make solar power cost competitive with power from fossil fuels
4. Safely reprocess and store nuclear waste
5. Make advanced biofuels cost-competitive with gasoline
6. Make new buildings green buildings by using known

technologies to reduce energy waste

7. Provide energy from fusion

"Despite 'the gathering storm' of concern about American competitiveness, no other country approaches our brainpower advantage—the collection of research universities, national laboratories and private-sector companies we have," Alexander said. "And this is still the only country where people say with a straight face that anything is possible—and really believe it."

Alexander's comments were echoed by Congressman Wamp, who asserted that nuclear power—if managed safely and efficiently—holds a key to the region's ability to provide adequate energy in a way that does not contribute to carbon emissions. Wamp stressed his belief that Oak Ridge, as it did once before, will play a key role in developing new technologies to increase America's security.

Congressman Gordon stressed the need to fund the Advanced Research Projects Agency–Energy (ARPA-E), an agency modeled after the Department of Defense's DARPA that will provide aggressive funding for innovative research projects carried out by science and technology experts from industry, universities and federal laboratories. Gordon believes the program will give researchers unprecedented flexibility and resources to develop new technologies through high-risk, high-return research that can provide breakthroughs to meet the nation's most pressing energy challenges.

ORNL Director Mason said the original Manhattan Project, which spent 60% of its $2 billion in Oak Ridge, illustrated the importance of parallel paths of research to determine which approaches work best and which simply do not work.

University of Tennessee lands NSF supercomputer

Tennessee Governor Phil Bredesen helped mark the official launch of the latest supercomputing project at Oak Ridge National Laboratory, a partnership among ORNL, the University of Tennessee and the National Science Foundation.

The NSF has awarded a $65 million grant to the University of Tennessee for construction of a second petascale supercomputer at ORNL. The new computer, dubbed Kraken, will be used to tackle some of science's largest problems. The University of Tennessee team will study the intricacies of climate change, planetary evolution and materials design.

The funding includes $30 million for computer hardware and $35 million for operation of the system over the next five years. The new supercomputer, which will be built by Cray and AMD, will be capable of nearly a thousand trillion calculations per second, or 1 petaflops.

University of Tennessee President John Petersen and Tennessee Governor Phil Bredesen, at the official launch of the NSF petascale supercomputer project at ORNL

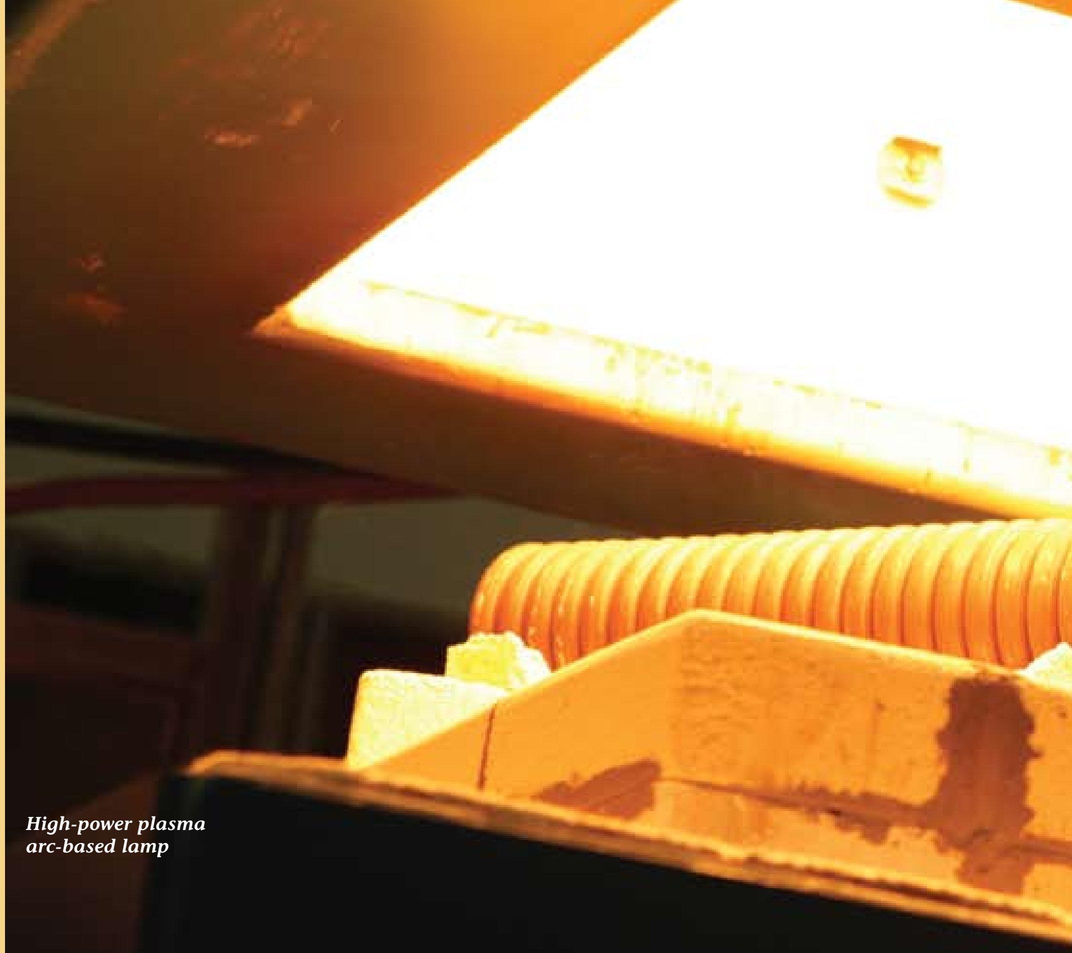
Global Venture Challenge marks second-year success

An event combining a venture capital forum and a business competition for university students attracted participants worldwide who shared business ideas to help solve global energy problems. The event, in its second year, is a unique educational and business forum that brings together at a national laboratory students from educational institutions, employees of government contractors and of industrial firms and venture capitalists.

Teams in the business competition included the University of California at Berkeley, Cornell, Yale, the University of Texas, the University of Tennessee, and Imperial College of London.

SNS in Guinness Book of World Records

The Department of Energy's Spallation Neutron Source at ORNL has been officially confirmed by the Guinness Book of World Records as the world's most powerful pulsed neutron spallation source. The accelerator-based SNS recently ramped up beam power to more than 300 kilowatts, producing 4.8×10^{16} neutrons per second. The SNS is currently sending neutrons to five instruments of an eventual 24. The first scientific paper based upon research from an SNS experiment has been accepted by Physical Review Letters. Each time the SNS ramps up toward an eventual beam power of 1.4 megawatts, this incredible tool for "seeing" the positions and motions of atoms and molecules in materials will set a new neutron production standard.



High-power plasma arc-based lamp

Miraculous

Novel surface treatments are greatly increasing the durability of industrial tools.

When Arvid Pasto first heard about an amazing surface treatment in 2001 from a lawyer named Mark Deininger, his first thought was, "This sounds like snake oil." But Pasto, then director of the High Temperature Materials Laboratory at Oak Ridge National Laboratory, changed his mind after talking to a long-time trustworthy friend at the same scientific conference in Pittsburgh where Deininger personally described the innovation. The friend is a consultant to Deininger's company.

Soon thereafter, Pasto arranged for Deininger, president and chief executive officer of C3 International, to come to Oak Ridge to meet with group leaders of materials sciences and technologies.

From 2002 to 2006, the unique surface treatment underwent a variety of tests involving a half dozen researchers. ORNL researchers were amazed that a Russian inventor had found a way to attach rare-earth elements to an organic chain. When the organic compounds leave, the rare earth left behind bonds to the substrate as nanocrystals pin down the element.

The ORNL researchers validated the properties of this remarkable surface treatment that Deininger describes as "an implantation that anchors a nanofilm." Blue and others call it a "molecular infusion, or implantation, surface treatment," or MIST.

The surface treatment contains 3-nanometer crystallites that plug the thin oxide film into the grain boundaries of a bulk material's surface, making the material extremely resistant to wear so it lasts longer. ORNL researchers measured the dimensions of the crystallites that make the ultrathin film adhere extremely tightly to the surface. No other "coating" has particles this small that bind to a surface.

Deininger lists other extremes associated with the special surface treatment. "MIST is extremely easy to apply by dipping or spraying and extremely cost effective and economical," he says. "The coating is extremely green and environmentally friendly. It is also extremely versatile because any one of 97 different elements can be used in MIST on a variety of surfaces, from metals to ceramics to glasses to carbides. The permutations add up to more than 200 million properties."

Today the American company that grew out of a Russian discovery has a research facility on the ORNL campus—the first private company to be housed at a national laboratory. Opened for business under Pasto's leadership on March 19, 2008, C3 International is a tenant of the Oak Ridge Science & Technology Park.

When Deininger came to ORNL in 2002, he gave a presentation on his company's solution-based technique for depositing ultrathin films of rare-earth oxides and other elements. Researchers were attracted by the processing temperature that anchors the nanoscale coating to an underlying substrate—a temperature on the order of 400°C that could be easily achieved by infrared light from a tungsten-halogen lamp in the lab of ORNL's Craig Blue, then leader of the Laboratory's materials processing group.

Pete Angelini, then manager of the Industrial Technologies Program, said

Coatings

to Blue, "Let's see if Mark can pass the aluminum die-casting test. No one has yet proven that a coating can handle the liquid metal attack."

A user agreement was set up, allowing Deininger to work with researchers at the High Temperature Materials Laboratory and in Blue's high bay to evaluate the ultrathin coating. Blue applied Deininger's coatings to steel thermocouple sheaths that were then immersed in aluminum.

To make an aluminum automobile part, for example, hot molten aluminum must be poured into a steel mold to obtain a specific shape. Casting aluminum components in steel dies is a problem because hot aluminum has an affinity for sticking, or soldering, to the steel in these molds. "You have to sandblast the aluminum off the steel die after you open it so the mold can be used again," Pasto says.

Blue dipped a steel thermocouple sheath in Deininger's cerium oxide liquid and then plunged the coated sheath in molten aluminum. He compared the sheath's resistance to attack from the aluminum to that of an uncoated sheath by measuring how much aluminum adhered to the surface. When he dipped the sheath in the coating liquid twice, he found that the sheath lasted twice as long as the uncoated sheath; in other words, the durability increased 100%. When he dipped the coated sheath three times, 200%; 4 times, 300%; eight times, a 700% increase in life extension. Stated differently, Blue observed an almost direct linear correlation between the thickness of the ultrathin coating and the durability of the coated component.

Researchers at HTML used Auger spectroscopy, X-ray diffraction and transmission electron microscopy to evaluate the surface treatment and its ability to increase the wear resistance of coated objects. Studying a zirconium oxide coating, they obtained beautiful TEM images showing that the sizes of the zirconia particles ranged from 3 to 5 nanometers.

Deininger then tried zirconium oxide coatings for the aluminum-and-steel challenge. He used a steel pin normally used to push a molded aluminum part out of the steel die. The molten aluminum tends to stick to both the die and the steel pushout pin.

C3 International President Mark Deininger (right) with Arvid Pasto

"The easiest way to test whether the C3 zirconium oxide film effectively resists aluminum attack on steel is to characterize the coated pushout pin," Pasto explains. "Mark proved that the coated pin resisted aluminum attack and could be used over many times without need to blast the aluminum off the steel pin." C3 International passed the test.

"We made great strides in aluminum die casting and filed patents on this application in 2003," Deininger says. But pressures on the U.S. automotive industry made it difficult for C3 to penetrate a highly competitive market.

"We have a business model at C3 International to look for partners that are strategically located in an industry to scale up our surface treatment technology," Deininger explains. "In late 2007 we signed a license agreement with Magna-Tech Manufacturing in Indiana, which treats aluminum parts coming out of the steel dies and is involved with every major aluminum diecaster in North America. The company does not make the dies.

"We are training Magna-Tech employees how to apply the custom-engineered chemical surface treatment. The coating is designed to extend the life of the die tools from which aluminum components are made as well as the parts themselves."

Under the Bright Lights

Few things attract our attention like a sudden burst of light at night. In Oak Ridge, researchers have the capability not only to produce but also control intense lighting in the lab coming from the world's most powerful plasma arc-based lamp.

For eight years Craig Blue has been demonstrating the potential industrial applications of rapid radiant heating using flashes of infrared light from tungsten-halogen lamps and then shorter flashes of light from a high-power plasma arc-based lamp (see photograph on pp. 4-5). Vortek Industries of Canada manufactured the early arc-based lamps. Mattson Technologies, a California company, purchased Vortek in 2004.

Blue manages industrial technologies and materials processing at Oak Ridge National Laboratory, which owns two high-power plasma arc-based lamps. Blue has advised Mattson on how the lamp can be used as a research tool.

By adjusting lamp-processing parameters such as flash time and power densities, Ron Ott can reach several extremes in a pursuit to achieve advances in flexible electronics.

"We can flash the lamp down to 1 millisecond while discharging 12 megawatts, providing to the surface 20,000 watts per square centimeter and heating the surface on the order of 1 million degrees per second. Only nature can exceed these extremes."

Ott leads a group that explores the potential of the high-power lamp's photons in helping to fabricate more-efficient, lower-cost thin-film batteries, thin-film transistors and photovoltaic cells for converting the energy of sunlight into electricity.

Chaitanya Narula, leader of ORNL's Physical Chemistry of Materials group and a catalyst chemist, has found ways to use engineered C3 surface treatments on particulate exhaust filters for diesel engines. As a result, the traps use less energy to remove carbon and last longer. A similar application of the coating in oil refinery cokers slows carbon buildups, resulting in reduced releases of carbon dioxide to the atmosphere.

"The ORNL coating achieved a 20 to 30% increase in disc cutter lifetime despite the presence of mountain rock such as gneiss and granite."

"The range and scope are extremely small and extremely large at the same time," says Pasto. "We can spray this surface treatment with nanofilm dimensions on extremely large industrial tools in steel and petrochemical plants. Applying a nanofilm onsite to stainless steel tubes and huge rollers is unheard of."

Deininger asserts that MIST is extremely divergent in its applications, based on the number of industries that will likely find uses for the technology: steel and aluminum for the automotive industry, particulate exhaust filters for diesel engines, petrochemicals, fuel cells, microelectronics, solar energy and food processing.

Boring in

Although Georgians experienced a severe drought in 2007, they are not far removed from periods of heavy rain and flooding. One problem plaguing Atlanta had been the inability to store and treat combined sewage and storm-water overflows from major rainfall events. Two tunnels have been built to capture and store the overflows and then convey the polluted water to treatment facilities, preventing sewage from entering and contaminating area rivers.

In 2007 when the tunnels were being completed, an experiment was under way. Normally, a Herrenknecht tunnel boring machine chews through mountain rocks until its steel disc cutter rings are smashed into metallic hexagons too worn to crush rock. When the cutters are no longer performing well, the machine is pulled back out and the disc cutters are replaced—an expensive procedure. During the experiment the disc cutters at the front end had been coated with a material developed by ORNL materials researchers. As hoped, the tunnel boring machine penetrated deeper than usual through the mountain rock.

ORNL's Bill Peter and Craig Blue have developed an iron-based, 200-micrometer-thick, nanocrystalline coating formed by heating amorphous powders with laser light. The coating's specific application is designed to increase the lifetime of the disc cutter rings in tunnel boring machines. Preliminary results indicate that the novel coating extends the lifetime of the disc cutter 20 to 30%.

The researchers put the amorphous powder into a polymer binder and sprayed the powder onto a disc cutter. Blue explains that the extremely high heating and cooling rates of their laser-based technique change the non-crystalline bulk metallic glass powder into a nanocrystalline structure, while creating a metallurgical bond between the coating and the steel cutter substrate. The strength of the bond prevents the coating from spalling, or breaking into chips.

"The laser, in effect, heats the glassy coating and a small layer of the substrate beyond the melting temperature," Peter says. "Convective stirring occurs, changing the chemistry of the coating. An extremely high cooling rate prevents grains from coarsening, producing a

Continued on pg. 8

"Our focus is to do high-temperature processing of non-crystalline silicon over broad areas on low-temperature substrates," Ott says. "Non-crystalline silicon and silicon-germanium layers are cheaper than crystalline silicon layers.

"We have shown that we can initiate solid-phase crystallization, which will introduce a nanocrystalline structure with fewer defects and higher efficiencies. The goal is to optimize the microstructures to improve photon collection efficiencies for solar cells while not altering the underlying substrate."

Furthermore, the lamp's flash of light will heat only the surface layers to extremely high temperatures. The substrate will barely be heated at all. That means the underlying layer, which is usually metal to withstand high-temperature processing, can be replaced with a cheaper plastic substrate capable of bending and conforming to a desired shape, giving rise to the term "flexible electronics."

In 2004 Blue, Queen City Forging in Cincinnati, Ohio, and others received an R&D 100 award for an optimized combination of radiant and convection heating for processing materials. The forging company now uses this technology to make lightweight aluminum forged components to replace more expensive and heavier titanium and other metal parts for aerospace and automotive applications.

In February 2008, producers and cameramen with the cable television program "Modern Marvels" came to ORNL to film the high-power plasma arc-based lamp for a feature on ultrahigh-temperature heating that will likely grab viewers' attention.—*C.K.*

Continued from pg. 7

nanocrystalline composite coating with high wear resistance.

"We heat and cool the coating at thousands of degrees per second. We found that laser fusing these coatings works well on many steel substrate components that see high wear rates, such as drill bits and disc cutters."

The chemical composition of the coating came from a program they worked in that was jointly funded by the Defense Advanced Research Projects Agency and the Department of Energy's Office of Civilian Radioactive Waste Management/ Science and Technology program. The goal was to develop coatings with high corrosion resistance for the steel canisters that will confine high-level radioactive waste at Yucca Mountain in Nevada.

"This is the first time that a coating applied to a disc cutter survived the extreme environment of boring a tunnel," Peter says. "Our coating was first tested at a one-of-a-kind linear cutting machine at the Colorado School of Mines. The machine simulates loads in a tunnel. We used a video camera and still-shot camera to monitor the changes in disc cutter coatings. However, we obtained 'real' laboratory results when we took cross sections of tested disc cutters and analyzed their coatings."

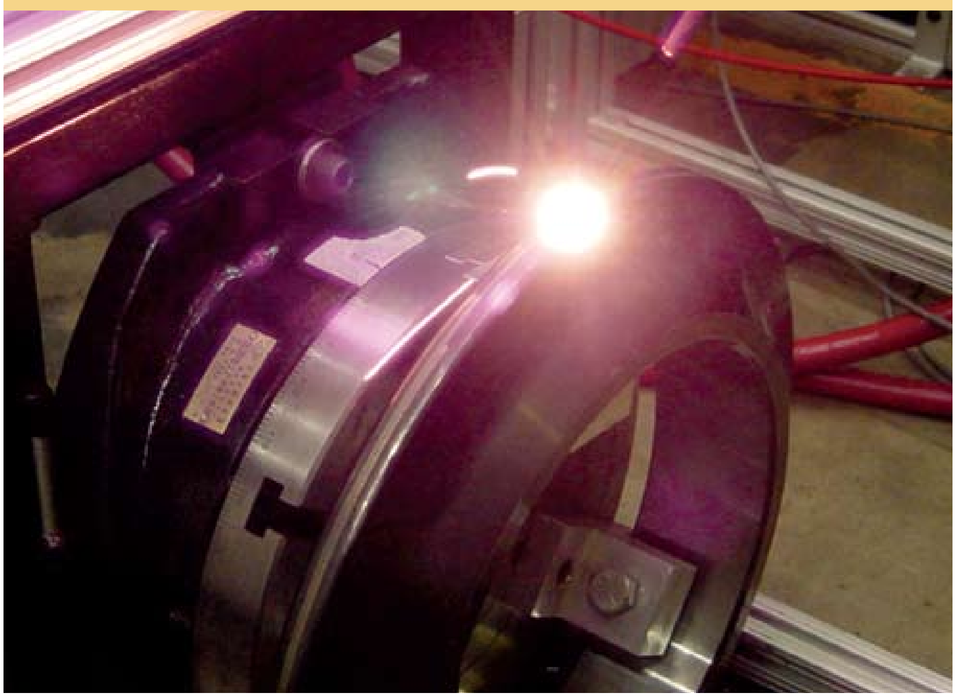
The experiment was also the first time that any coating survived in this machine, and the School of Mines has been testing coatings for 30 years. The benchmark was one the ORNL researchers had to pass before they could test their coated cutters in the field.

Operating a $25 million tunnel boring machine costs $100,000 to $150,000 a day. Peter rode on the machine testing the ORNL coating on four disc cutters.

"This machine is monstrous," he says. "Tunnel boring machines are like small factories traveling underneath the ground. Machines can be as large as 50 feet in diameter and over 100 feet long with more than 50 circular cutters. Each disc cutter measures 17 inches in diameter and weighs 60 pounds.

"The boring machine pulverizes rock directly underneath the disc cutter, causing the rock to crack. After two cracks intersect, a chunk of rock is removed. Hydraulic rams push the machine forward against the rock wall at five-foot intervals. The machine lays down electrical wires and track as it puts up the tunnel. The humidity was so high in this extreme environment that I could not take photos of the disc cutters up front."

"We heat and cool the coating at thousands of degrees per second, which works well on many steel substrate components that see high wear rates, such as drill bits and disc cutters."



About 45% of a tunnel boring machine's downtime is due to changing out disc cutters as a result of wear. Herrenknecht uses a proprietary H-13 steel for their $350 disc cutters. The company is interested in finding a coating that costs no more than 10% of the disc cutter price and increases lifetime by 20 to 30%.

"At the Atlanta job site we showed that four disc cutters with the ORNL coating achieved a 20 to 30% increase in lifetime despite the presence of mountain rock such as gneiss and granite," Peter says. "Some of our coating remained on the disc cutters after they traveled 300,000 linear feet through rock. A competitive coating failed immediately, but our coating was still on the disc cutter after seven five-foot pushes.

"The Atlanta site is considered significant because it has some of the worst conditions that a boring machine could face. The disc cutters with our coating showed slow abrasive wear. Many of the disc cutters without a coating lost significant chunks of metal."

The ORNL team will test coated disc cutters under more typical mountain conditions, such as abrasive slurry, which has the consistency of toothpaste. An even greater improvement in the lifetime of coated disc cutters is expected under these conditions.

"Martin Herrenknecht, founder of Herrenknecht about 30 years ago, visited ORNL recently to look at our coating technology and was impressed by the money-saving potential," Blue says. "Through the Work for Others program here, he funded further testing of our coating and bought 20 disc cutter rings for us to coat and test."

Peter will coat 20 rings and test them on Herrenknecht tunnel boring machines as they bore the Gotthard Tunnel underneath the Swiss Alps.

The 11-mile-long Gotthard tunnel will be the longest running tunnel in the world. Preliminary tests suggest that, in the extreme environment of the Swiss Alps, the ORNL coating is likely to pass another benchmark test and is even less likely to be passed off as snake oil.—*Carolyn Krause*

Under Extreme Pressure

Achieving the pressure at Earth's core-mantle boundary is now plausible.

The pressure and temperature conditions that humans commonly experience on Earth are but a small subset of the conditions to which most materials in the universe are subjected. These conditions include very low pressures in outer space ranging up to very high pressures at the centers of neutron stars, as well as temperatures ranging from nearly absolute zero to many thousands of degrees kelvin.

Throughout the universe pressure is expected to span more than 60 orders of magnitude. At very high pressures the electronic structure of atoms is altered as positions of electrons orbiting nuclei are changed, leading to unexpected chemical interactions.

Scientists' current understanding of the electronic structure of atoms in elements on Earth forms the basis of modern chemistry's set of rules. Under extreme pressures and temperatures, the electronic structure of chemical bonds would likely change as electrons are squeezed between atoms, leading to different "rules" of chemical interaction.

Knowing the new rules might allow researchers to more easily synthesize new materials and engineer materials to meet ever-increasing demands. Scientists have created extreme conditions in the laboratory for many decades. A particularly difficult task has been to probe the properties of materials subjected to extreme conditions.

The Spallation Neutrons and Pressure (SNAP) Beamline instrument at the Spallation Neutron Source, which first opened its neutron beam shutter on Jan. 24, 2008, has the potential of exerting pressures near those at the boundary between Earth's mantle and iron core (~100 gigapascals) on a wide range of materials and simultaneously performing neutron scattering studies of these materials under extreme conditions. Collecting neutron scattering data under these extreme pressure conditions would be another world record for Oak Ridge National Laboratory.

Chris Tulk, a condensed matter physicist who oversaw the construction of the SNAP instrument, is eager to do scientific experiments in which neutrons are used to determine changes in a material's structure after a sample is placed under high pressure over a wide range of temperatures. He says that SNAP's suite of pressure-generating devices can easily cause changes in a material's molecular bonding, crystallographic structure and interactions of atoms.

The increased neutron flux of SNS, combined with SNAP's large-volume, gem anvil and gas pressure cells, will enable researchers to conduct neutron diffraction experiments over a large range of pressures and temperatures never before available in the United States.

At the SNS, diamond anvil cells will squeeze tiny samples to generate pressures nearing those at the Earth's core, enabling scientists to investigate atomic-level changes in material structure and properties using neutron scattering.

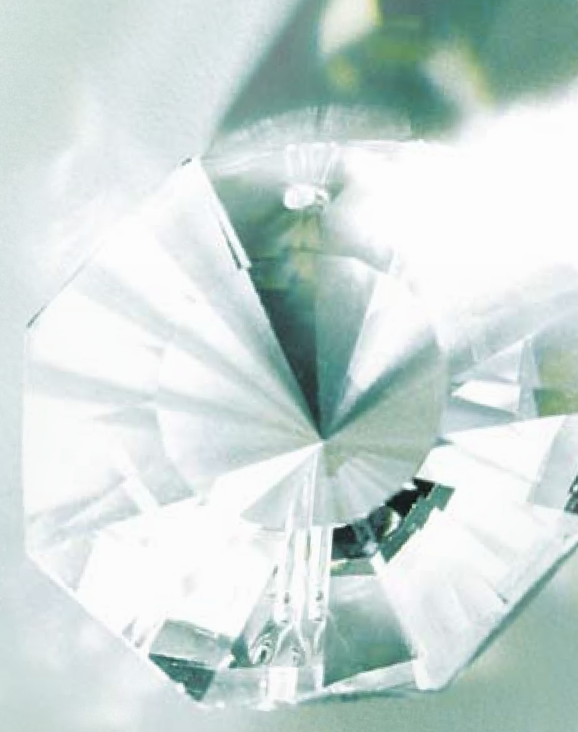
"At high pressure, a sample's crystal structure, or the spatial distribution and bonding of the elements, could transform from one set of symmetry operations to another," says Tulk. "Simply to accommodate the decrease in volume resulting from the increase in pressure, the sample thus transforms from one crystallographic structure to another.

"Changes in electrons' ranges of energies can cause a material to go from electrically insulating to conducting to even superconducting. Scientists still struggle to understand these changes."

Using neutron scattering, Tulk expects to observe atomic-level changes as hydrogen gas is compressed enough to become a crystal, as water is pressurized along with natural gases to simulate methane hydrates deep in the ocean, and as protein samples are subjected to the same temperatures and pressures as extremophile microbes found in thermal vents deep in the ocean. Magnetic properties of molten iron under pressure might help researchers better understand Earth's core and magnetic field.

"SNAP was conceived and built to be a user facility," Tulk says. "We are eager to engage with other research groups at ORNL and throughout the world to enhance their scientific programs." —*C.K.*

EXTREMELY Strong



Scientists seek to recreate the strength of diamonds in artificial materials.

In a strongman contest among Earth's natural materials, nothing competes with the diamond. With a hardness of 96 gigapascals, diamonds demonstrate more than twice the hardness of second-place finisher boron nitride and nearly 100 times the hardness of stainless steel.

Theoretical physicists Chong Long Fu, the late Gayle Painter and postdoctoral researcher Xing-Oiu Chen have been trying to unlock the secret of diamond's strength. They are among a number of theorists, experimentalists and engineers at Oak Ridge National Laboratory, working to understand, develop and test new breeds of materials that mimic the strength and toughness found in nature—without having to recreate the forces that formed them.

Diamonds are, of course, made of carbon. But, Painter pointed out, so is graphite, diamond's near polar opposite on the hardness and toughness scale. Thus, the answer lies not simply in the atoms themselves but in their structure, alignment and the bonds among them.

"The big difference between carbon in graphite and carbon in diamond is that in diamond a large linking structure exists that goes all the way through, and each of those links is a strong bond," he said. "In graphite, the structure is similar to a honeycomb with very weak forces between the rows. The explanation lies not just in how the electrons move but also in which directions they move." In other words, diamonds feature a three-dimensional lattice with very strong bonds that makes the material virtually impenetrable—and the choice for products such as cutting tools and precious jewelry. Other elements, such as metals, have less sturdy structures, with weaker bonds that are easier to break apart.

The theorists have been working on the idea that carbon and boron, elements used to create diamonds and boron nitride in nature, could be incorporated into metals to create materials that could vie for diamond's strength. They also look for materials that can be made at zero pressure or high pressure, producing different properties.

"We are looking at the transition metals that have "holes" boron and carbon can easily fill and form strong bonds with," Fu says. "Ultimately, we are looking for a material that has high strength and high hardness and is easy to make."

Using supercomputing capabilities at the National Energy Research Scientific Computing Center in Berkeley, California, Fu and his colleagues have predicted the enhanced mechanical strength and hardness of the metals tungsten, hafnium, tantalum, rhenium, osmium and iridium when reinforced with boron atoms. Combining these elements could produce alloys that feature the same strong covalent bonds and lattice structures found in diamonds, boron nitride and other super-strong natural materials.

Fu shows a diagram of the network of atoms and bonds, arrayed in tinker-toy-like fashion, that forms when boron is incorporated into a theoretical sample of the metal tungsten. The resulting tungsten boride has the incompressibility of a diamond, at 1,000 gigapascals, and the hardness of its runner-up, boron nitride, at about 45 gigapascals. Tungsten, by itself, although one of the hardest metals, measures just 10 gigapascals in that category and 520 gigapascals in incompressibility.

The next step is to discover how to synthesize the new tungsten boride alloy under ambient conditions in a laboratory. Potential applications could include highly wear-resistant cutting blades for tools, bearings and bearing sleeves and a variety of other components for use in industries from aviation to the military. The work also fits in neatly with the Department of Energy's larger research objectives.

"This research ties in wonderfully with energy," Painter said. "The goal is simple. If things do not wear out, energy is not expended to make their replacements nor are processes shut down to replace parts."

Future efforts are being made to explore the potential of marrying transition metals with carbon and nitrogen both in zero pressure and high-pressure scenarios.

"Under high pressure the bonds become shorter, and when the bonds become shorter they become stronger," Fu says. "We will add pressure and see what happens."—*Larisa Brass*

Note: *Gayle Painter died March 26, 2008, following a brief illness. He was a senior member of the Materials Theory group in ORNL's Materials Science & Technology Division. He worked at ORNL for 39 years.*

Maximum Strength

Studying the theoretical strength of materials takes researchers down a new path.

Biting a gold ring is an age-old test of authenticity, but, in fact, extended line defects or dislocations within the atomic structure are what render this precious element so malleable. Using dislocation-free gold, workers could, at least in theory, build skyscrapers.

For years, scientists have been studying the theoretical strength of metals, which can be 1,000 times greater than their typical strength because of defects and dislocations that prevent atoms from occupying their perfect positions. The smaller a sample, the closer the material comes to achieving maximum theoretical strength as the defects are, in effect, eliminated until all that remains is a very tiny, defect-free sample.

Researchers have been intrigued, however, by the difficulty in demonstrating this theoretical strength using a recently developed method that employs a focused ion beam to hew micrometer-sized pillars, which are then compressed to test for strength. While the theoretical strength of metal whiskers was reached decades ago using a tensile test to pull each whisker apart , researchers have found that in compression testing many of the recently made pillars did not respond as expected.

Easo George, an ORNL materials scientist with a part-time appointment at the University of Tennessee, says he and colleagues thought the focused ion beam technique might also introduce dislocations, thereby weakening the micro-pillars. While doing work on a "completely unrelated" project, the researchers stumbled upon an entirely new way of forming these tiny metallic shapes.

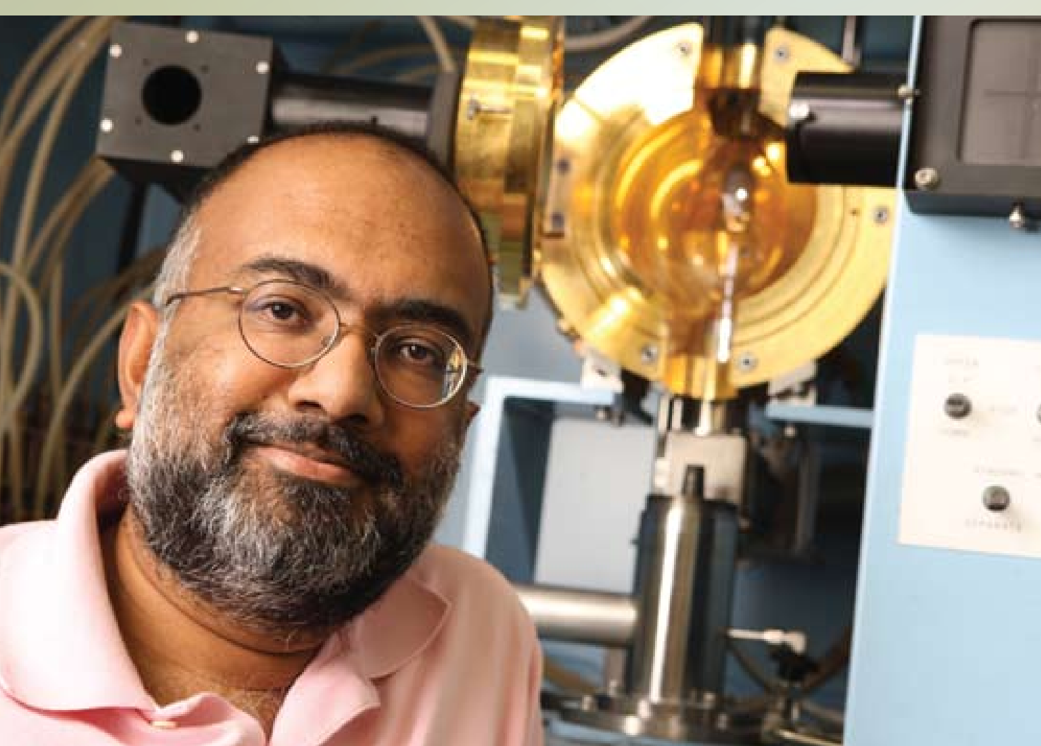
Using the new method, the researchers produced micro-pillars using a xenon arc lamp to grow an in situ composite of nickel aluminide and molybdenum fibers through a process known as floating zone directional solidification. An acid wash then etches away the nickel aluminide matrix, leaving behind thousands of free-standing monocrystalline molybdenum pillars.

"Now that we have these naturally made pillars , we do not need to do any additional work," says George. "We can change their size by altering the rate at which we grow them—a much cleaner process." ORNL researchers used an instrument called a nano-indenter to conduct compression tests on the new pillars and found that all the tested pillars yielded at the theoretical strength.

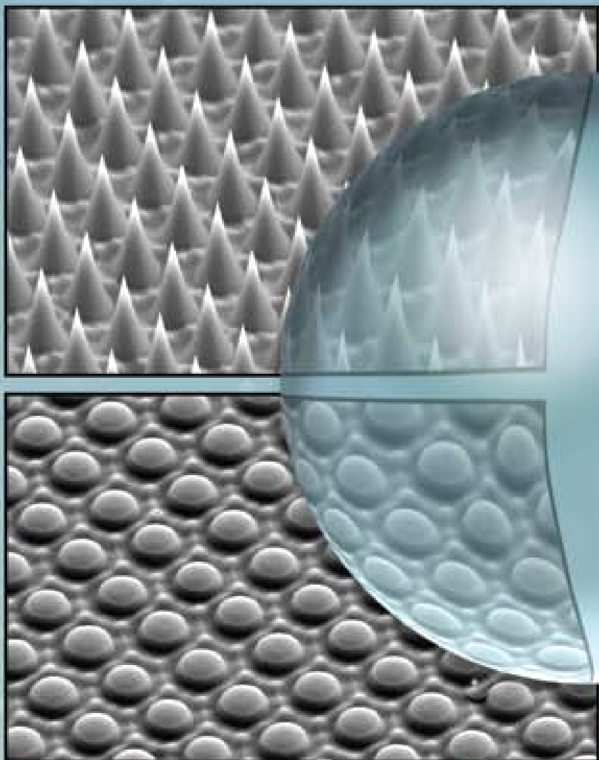
"When we demonstrated this result, many of the people who were testing the pillars made by the ion beams took notice," George says. "This discovery now allows us to compare experimental results and theoretical predictions in a much better way and to carefully introduce dislocations into each pillar in order to study their effects in a well-controlled manner."

While interesting at a basic discovery level, the research also has potential applications. As electronic devices, sensors and other technologies become tinier, predicting and testing the behavior of materials in very small amounts become increasingly important, George says. In addition, because nano-scale features are needed to strengthen even bulk materials, a growing need exists to isolate and characterize such features.

"We cannot simply push toward the theoretical strength limit," George says. "We also must make materials tougher and more ductile. But with at least a factor of 100 between what is feasible theoretically and what is typical, we have a lot of room for improvement. Understanding the nature and behavior of dislocations will be important in pushing us toward the goal of dramatically improved properties of materials." —*L.B.*



Easo George with the high-temperature optical floating zone furnace used to produce monocrystalline molybdenum alloy micro-pillars



By varying the chemistry of the etching process and the glass composition, researchers produce different surface microstructures and aspect ratios that range from flat tops to cones with long needlelike structures.

Extremely Waterproof

Making some of the world's most water-repellent surfaces has become an ORNL niche.

In July 2003 when Brian D'Urso and his wife Vicky arrived at Oak Ridge National Laboratory as Eugene P. Wigner Fellows, Brian learned he had to find a new project quickly. The project he was supposed to join had fallen apart.

Two recollections from his days as an undergraduate at the California Institute of Technology and as a graduate student at Harvard University merged into a project idea. At Caltech, where he met his future wife, Brian heard a talk by Naval Research Laboratory scientists about a technique for making nano-channel glass. He found the technique fascinating. A few years later at Harvard, he heard a talk about superhydrophobic materials—waterproof surfaces that repel water almost as well as the water lily and young poplar tree leaves in East Tennessee.

"Unfortunately, honeysuckle vine leaves are also superhydrophobic," D'Urso says with a twinkle in his eye. "If you spray these leaves with Roundup, the herbicide beads up and rolls off to the ground. It's hard to get Roundup to stick. I don't think honey-suckle evolved to defeat Roundup but it works that way."

D'Urso shared his idea with his mentor, John Simpson, who suggested that the two write a proposal for seed money to cover the cost of Simpson's time on the project and the necessary research equipment. The seed money was granted by ORNL's internal funding program.

Over the next few years D'Urso, a physicist, and Simpson, an optical scientist, evolved into a team that can produce the world's most water-repellent surfaces over increasingly large areas by making either sheets or powder-based coatings.

During that time they worked with Mark Reeves of ORNL's technology transfer office to prepare patent applications. Today they hold several patents on a variety of new water-repellent materials that conceivably could be licensed to industrial firms or companies that have military contracts.

The possibilities are virtually limitless. Water sticking to windshields and rain-soaked clothing can be annoying. Cars hydroplaning over slightly wet road surfaces can be dangerous. Well-soaked building materials can morph into moldy health hazards.

The friction felt by water swishing against the hulls of ships causes drag, slowing the transport of commercial products between countries. A surface treatment with spikes might discourage algae from sticking to a ship's hull. One solution might be to coat these items with highly water-repellent powder-based paint. Another could be to cover them with highly waterproof sheets.

"Over the past five years, we have been focused on making extremely superhydrophobic materials and optimizing other properties," D'Urso says. "The purpose of the seed money project was to demonstrate that we could make a superhydrophobic material. Winning the seed money was a critical starting point that launched what turned out to be an interesting project."

In late 2003, the ORNL team contacted Naval Research Lab experts on nanochanneling to find out which glasses they should use for various applications.

The ORNL physicists decided to use an outside company rather than the Naval Research Lab to make a desired material by glass drawing without disclosing the property they were trying to achieve.

"The company's glass experts said, 'This approach using glass drawing won't give you a material with nanoscale or micron-sized channels,'" D'Urso says. "We replied, 'That's OK, we'll worry about what it turns into after that.' We were not trying to make a channeled structure. Rather, we were attempting to produce spikes in an ordered pattern on the surface. We got the material back, etched it with hydrofluoric acid, then processed and coated it to make a superhydrophobic material.

"The first time we made a glass product, it was extremely superhydrophobic. In fact, this first material is probably the most superhydrophobic we ever made because our first scanning electron microscope images showed that the spikes are really ordered and extremely sharp."

The researchers observed very little contact between water and the solid spiky surface. Air flowed through the pockets between the spikes.

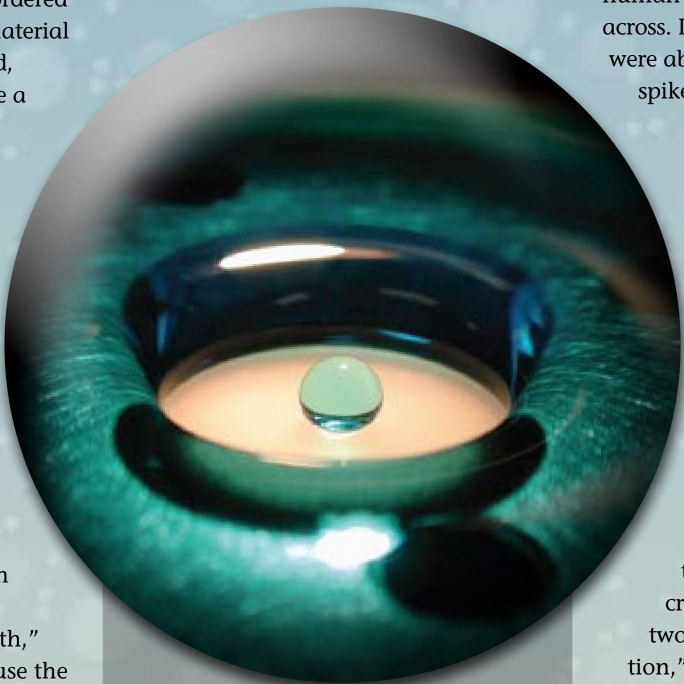
"It was a great model to start with," D'Urso says. "We were excited because the behavior of the material was fantastic."

The spikes have a good aspect ratio—they are very tall compared with their average width and are highly protruding from the surface. The material cannot be made using standard lithography or etching processes.

At the end of summer 2005, D'Urso's financial support from his Wigner Fellowship and seed money was expended, so he and Simpson applied for and received Laboratory Directed Research and Development funding for Oct. 1, 2005 through Sept. 30, 2007.

The purpose of the LDRD project was to expand the range of superhydrophobic materials that could be made in the ORNL lab. Because they had demonstrated the value of the selected fabrication technique in making the first material, they received technology maturation funding to purchase a glass drawing tower so they could fabricate superhydrophobic glasses themselves.

For the LDRD project, D'Urso and Simpson continued to develop differential etching techniques to create spikes in materials drawn from the tower. Think of a pencil that consists of a "core" of graphite surrounded by wooden pencil "cladding." Sharpening the pencil is similar to etching the glass surface to get a spike.



When water strikes the superhydrophobic disk, each drop is repelled to the water on one side. John Simpson calls this phenomenon the "Moses effect," after the Biblical leader who parted the Red Sea.

In the first drawn-glass structure made at ORNL, the core glass was Pyrex, brand name for heat- and chemical-resistant glassware used for cooking. The cladding glass, which has a different composition, was the amorphous material used by the ORNL glass shop to make glass-to-metal seals.

"In differential etching, we immerse the core glass and cladding glass in hydrofluoric acid solution, which attacks both glasses made by glass drawing," D'Urso says. "The cladding glass is etched faster than the core glass. We first get an array of cores inside the cladding glass. The core glass starts to protrude because the cladding glass is etched back faster than the core glass."

The cores are etched from the sides and the top. They become sharpened because the tip of each protruding core is exposed to the acid for a longer time than the base of the core. Eventually the cores are sharpened like a pencil; any further etching removes more material but the tip remains sharp.

The first materials they made had spikes 7 microns apart—smaller than human hair, which averages 50 microns across. In the LDRD project, the researchers were able to shrink the spacing between spikes to 1 micron and even smaller.

"We could make one material and then vary the chemistry of the etching process to get different microstructures and aspect ratios varying from flat tops to long needlelike structures," D'Urso says. "To vary the aspect ratio, we used glasses of different composition or simply changed the etching process."

They also made glasses that spontaneously separated into two different structures, or phases, when heat treated. The two phases penetrated each other, creating a "spinodal" structure. "The two phases have a different composition," D'Urso says. "By using differential etching, we could get one phase to protrude, creating surface roughness."

The scientists also found that, by controlling the size of the protruding surface features, they could make superhydrophobic glasses that are transparent. Such glasses might be useful for windshields.

In 2006 the researchers experimented with different polymers and discovered they could make some polymers superhydrophobic. Simpson concentrated on making superhydrophobic powders by crushing and milling spinodal glass to create nanotextured particles that bond to glass surfaces. D'Urso focused on producing superhydrophobic polymer sheets.

For D'Urso, the collapse of his first ORNL project opened the door to another with tremendous potential.—*C.K.*

Molecules In Jail

Confining catalysts in a particle's nanopores changes their behavior.

When a person is imprisoned, the loss of freedom can be life changing. In a similar way, when atoms or molecules are confined in a pore as small as a few billionths of a meter, the confinement can affect their reactivity and ability to catalyze chemical reactions by speeding up one reaction path relative to another to better control the yield of reaction products.

A. C. Buchanan III, leader of a physical organic chemistry group at Oak Ridge National Laboratory, group member Michelle Kidder and their colleagues have been studying the effect on the chemistry of organic molecules confined in porous media.

"Our focus is to use solid nanoporous materials, such as silicon dioxide, to confine organic molecules of interest to the Department of Energy," Buchanan says. "We were the first to show that confinement in tiny pores of silica can increase the molecules' conventional reaction rate in a gaseous or liquid environment." Silicon dioxide, or silica, is the chemical compound present in sand, quartz and glass.

For many years in the laboratory, organic chemists have run chemical reactions in a fluid inside a glass flask or beaker. "What we are trying to do, under extreme conditions, is observe an organic chemical reaction in pores in a solid silica particle," says Buchanan. "The pores are only two to three times the length of each trapped organic molecule. We chemically attach the molecules inside pores that range in diameter from almost 2 nanometers to under 3 nanometers and can be 1000 nanometers in length."

Porous silica surfaces end in silanol groups, which readily bind with an organic molecule called an aromatic phenol. The chemists attach the maximum number of molecules to the pore walls, achieving monolayer coverage. As the cylindrical pores become smaller, fewer molecules can be squeezed inside.

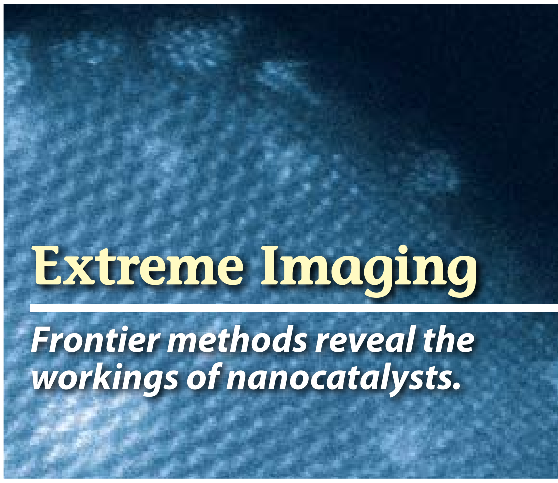
In several experiments, the chemists compared the reaction rates of the organic molecules in the gas phase, on the outside of a nonporous silica particle and inside the pores of mesoporous silica particles where pore sizes vary between 2 and 6 nanometers across.

"We found that, if the molecules are inside the pores, the effect of confinement is to increase the speed of the reaction," Buchanan says. "The molecules are closer together and bang into each other more frequently, increasing the probability of reactions."

Because each pore has a curved surface, the confined molecules tend to be more pointed to each other. If the reaction involves, say, a transfer of one hydrogen atom to another molecule, the desired result will happen more effectively on the inside surface of a pore than on the particle's exterior where the reactants can flop around. In some cases, the reaction rate for confined molecules is 400% to 500% faster than that of the same reactants on the outside particle surface.

One goal of the Department of Energy is to find ways to produce ethanol fuel and other products more economically from cellulosic biomass, such as fast-growing switchgrass and hybrid poplar trees. To make biorefineries profitable, chemists are seeking ways to generate useful products from lignin after separation from cellulose.

Buchanan's group is experimenting with a major structural unit of lignin based on phenethyl phenyl ether (PPE)



Aberration-corrected scanning transmission electron microscopy reveals details of nanoparticles 1-2 nanometers wide, which appear as bright blobs adhered to a titania support, shown in gray. Sample courtesy Gabriel Veith.

Image courtesy Andrew Lupini.

molecules. "We are interested in gaining a fundamental understanding of functional groups in lignin, such as ether oxygen groups," Buchanan says.

When PPE molecules are heated to 375°C in the gas phase, the resulting reaction generates products from two competing pathways. The product yield in one path is three times the yield in the second parallel path.

"If we run the same reaction of PPE molecules confined inside the pores of a mesoporous silica particle, we can increase the chemical selectivity to as high as 45 to 1 versus 3 to 1 for the gas phase," Buchanan says. "We get a 15-fold change in the way the products of pore-confined PPE molecules come out by slowing down one reaction path relative to the other."

The relative product amounts depend upon the pore size, concentration of molecules in the pores and the rigidity of added inert molecules, which can serve as a "surface-confined solvent." If crowding occurs in a pore, the reaction along one pathway can be hindered relative to the other for PPE molecules. By adding rigid inert molecules to a pore, chemists can nearly eliminate a physical rearrangement of PPE molecules, dramatically changing the chemical selectivity of the reaction.

In these ways, chemists may be able to manipulate molecules and their reactions in confinement in mesoporous silica, thus controlling reaction rates and relative yields of reaction products. "Molecules in jail" (a phrase coined by Buchanan) could provide chemists with opportunities to produce larger amounts of desired products from lignin—thus turning a waste by-product of ethanol production into a valuable resource.

Buchanan credits Sheng Dai, leader of the Nanomaterials Chemistry group and staff scientist at ORNL's nanoscience center, who taught him and his colleagues how to synthesize silica particles dotted with pores of different sizes. They learned how to tailor the silica surface to control the chemistry of confined particles. Dai's group produces unique mesoporous carbon materials for various applications.

Mesoporous carbon and silica are made using a detergent-like surfactant whose molecules self assemble into spherical or cylindrical bubbles. A precursor of the carbon or silica particles is condensed around the cylindrical bubbles, which act as a template. The bubbles are burned off or removed in some other way, leaving a mesoporous material containing pores with diameters ranging from 1 to 10 nanometers.

One of Dai's interests is studying the confinement of platinum nanoparticles in the pores of mesoporous carbon to improve carbon cathodes in the fuel cell. Fuel cells supplied with hydrogen are used to produce electricity for electric vehicles.

ORNL researchers have developed a carbon cathode that contains pores 6 to 7 nanometers in width. Platinum nanoparticles 2 nm across can be entrapped inside these mesopores. "Platinum particles are separated by entrapment in cages," Dai says. "Only the external surfaces of the platinum particles serve as an electrocatalyst."

"If the particles come together, they expand and are less reactive," Buchanan explains. "If chemists can keep them separated using pores of the right size, the platinum particles are stable, and all the intrinsic reactivity of the metal particles is available. The reactivity of metal catalysts increases as the particle size decreases."

Dai's material is dominated by internal surface area because of the presence of so many tiny pores. The carbon cathode has 800 square meters of surface per gram of material.

For a fuel cell cathode a platinum catalyst can stimulate the oxygen reduction reaction. "Each oxygen molecule is taken up and chemically bound to a platinum nanoparticle surface," Dai says. "Each oxygen grabs four electrons and combines with a proton to form water—a key reaction in a fuel cell. By increasing stable platinum's effective surface area and the cathode's efficiency, we increase the fuel cell's lifetime."

Similar in some respects to successful prison rehabilitation, confined atoms and molecules can indeed exhibit beneficial changes in behavior.—*C.K.*

Instruments with extraordinary capabilities enable scientists at Oak Ridge National Laboratory to capture images of catalysts only a billionth of a meter wide. Their efforts may lead to a better understanding of the relationship between nanocatalyst structures and functions. This knowledge in turn could spawn improvements in catalysts that make the development and manufacture of thousands of industrial products—including fuels, pharmaceuticals and polymers—both possible and profitable.

At ORNL's nanoscience center, chemist Zili Wu bombards samples with photon beams to monitor catalysts at work. Wu's process combines optical imaging—infrared, Raman and X-ray diffraction spectroscopy—with mass spectroscopy. The technique, operando imaging, makes it possible for scientists to watch catalysts while they operate. The technology also enables researchers to determine which chemical species are generated, and in what quantities, at a reactive surface.

Using operando spectroscopy, the researchers study gold nanocatalysts that turn carbon monoxide into carbon dioxide. The work may aid fuel cell research because the industrial process that generates hydrogen to power proton exchange membranes also produces carbon monoxide, which even in trace amounts can poison electrode catalysts in fuel cells.

In another case of extreme imaging, the Department of Energy's Transmission Electron Aberration-Corrected Microscope project aims to meet a challenge posed in 1959 by physicist Richard Feynman, who lamented the lack of a powerful electron microscope. In 2009, scientists hope to deliver an instrument for imaging atomic-scale order, electronic structure and dynamics of individual nanostructures.

"We can resolve two objects separated by a distance about one million times smaller than the diameter of a human hair," says materials scientist Andrew Lupini, whose aberration-corrected scanning transmission electron microscopes rectify the unavoidable imperfections of round lenses. "We can 'see' individual atoms and obtain spectra from single nanoparticles." Such fine detail may guide industrial engineers in optimizing catalyst support structures and preparation methods.—*Dawn Levy*

Defying Traditional Behavior

Understanding how electrons behave may lead to room-temperature superconductors.

When Elbio Dagotto is asked to explain the intricacies of strongly correlated electron systems, he grasps for an analogy. "This is very complicated," he says, stating the obvious about what is considered one of the most important problems in condensed matter physics. Correlated electrons have the best minds searching for needles in a haystack of quantum mechanics in the hope of discovering materials that have fantastic new properties such as superconductivity at room temperature and colossal magnetoresistance.

In some metals, electrons flow without difficulty, largely because the distances between electrons are small enough to enable the metal to conduct electricity. As a result, the so-called "one electron approximation" in these metals is valid because the total is obtained from the properties of individual electrons.

In materials that are strongly correlated, electrons do not serve as freely operating agents. Instead, these negatively charged particles interact with each other, forming collective states that defy the traditional behavior of their singular counterparts. The result, says Dagotto, a theoretical physicist and distinguished scientist at ORNL and the University of Tennessee, is "all kinds of exotic properties."

To explain collective behavior, Dagotto cites a popular analogy to illustrate strongly correlated systems in low-temperature superconductors. "Imagine you are part of a gigantic army of people holding hands," he says. "When the army moves forward, you collide with a rock. The fact that you are attached to a large number of people moving forward will keep you in motion. If you were on your own and collided with a rock, you would stay there. But in a collective state you are pushed forward around the rock. Once the current starts moving in a superconductor, stopping the current is extremely difficult because individual collisions do not affect the collective effect."

Dutch physicist Heike Kamerlingh Onnes discovered this extraordinary behavior in 1911 when he observed that mercury, when cooled to -452°F (about 7 degrees above absolute zero), dispelled electrical resistance, rendering the element a superconductor. A theory to explain low-temperature superconductivity was developed in 1957, but the theory does not apply to the two families of high-temperature superconductors discovered in 1986 and recently.

A collection of outstanding theoretical and experimental physicists has been drawn to ORNL by the presence of the Department of Energy's Spallation Neutron Source, the supercomputing power available through the Center for Computational Sciences and the potential collaborations with fellow researchers at ORNL and the University of Tennessee. The unique combination of resources makes the Laboratory one of the premier U.S. institutions for research on superconductors and other strongly correlated systems.

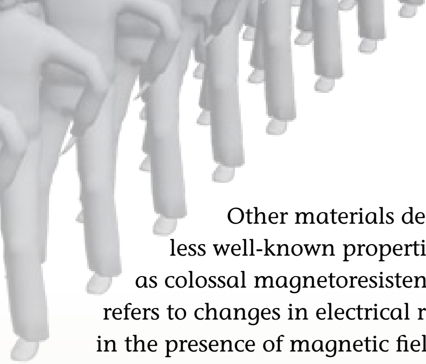
ORNL is home to groups of theorists that develop computer simulations of model Hamiltonian systems— simpler expressions of complex physical interactions; perform first-principles calculations for real materials; explore magnetism and predict the effect interfaces will have on the properties of materials featuring strongly correlated systems. Another group of researchers studies interfaces and surfaces of strongly correlated electron materials experimentally, synthesizes new crystals and thin films and analyzes these samples using neutron sources such as the SNS and ORNL's High Flux Isotope Reactor, as well as electron and scanning tunnel microscopy.

"Oak Ridge is very strong in correlated electron research," says David Mandrus, who leads experimental work in ORNL's correlated electron materials group. Noted theorists in the field at ORNL include Dagotto and David Singh, a world-renowned expert in band structure, which describes rules governing the range of energy an electron is allowed to have within a solid.

For example, ORNL researchers are the first U.S. group and the fourth in the world to publish a paper on the recently discovered second family of high-temperature superconductors, based on iron and arsenic (the first family is based on copper and oxygen).

On the experimental side, the group led by Mandrus grows crystals of materials known or suspected to have an aptitude for correlated electron behavior, which can then be tested using instruments at the SNS, HFIR or other ORNL user facilities. Another experimental group closely associated with the Laboratory's nanoscience center and Materials Science and Technology Division is studying the interfaces and surfaces of strongly correlated systems through laser deposition of thin films. These "superlattices" with atomically abrupt interfaces allow scientists to study the influence of strain and local asymmetry, as well as coupling at the nanoscale, on ferroelectric, transport and magnetic properties.

Superconductors, the poster child of correlated electron systems, demonstrate the extraordinary nature of these materials. In superconductivity, electric current flows without resistance below a certain temperature, effectively creating the closest thing to perpetual motion found in nature.



Other materials demonstrate less well-known properties such as colossal magnetoresistence, which refers to changes in electrical resistance in the presence of magnetic fields. Today's computers store information using very small magnetic regions that, by pointing in one direction or the opposite, define the well-known bits "1" and "0." In the case of some correlated systems, the resistance changes by several orders of magnitude, making them potentially useful for the detection of the small magnetic fields of those bits, as computer processors and memory continue to shrink.

"Imagine you are part of a gigantic army of people holding hands"

"We need a material with a resistance that changes a lot in the presence of a tiny magnetic field," Dagotto says. "Some of these strongly correlated systems possess that property with the caveat that, like superconductivity, these materials are chilled to low temperatures. One goal is to be able to trigger these phenomena at room temperature, a breakthrough that would make them much more useful for practical application."

Achieving this goal requires a much better understanding of why correlated electrons behave the way they do, a question at the heart of research by Dagotto and others at ORNL. The field of strongly correlated systems is divided into several paths of attack, with some scientists focused on superconducting materials and others looking at ways to add functionality to semiconductor devices using these new materials, primarily transition metal oxides, in a path of research known as oxide electronics.

Other researchers are theoretically or experimentally probing the interfaces between layers of material that exhibit exciting new properties. Still others are growing crystals of materials that have shown promise as superconductors and then are characterizing them using neutron diffraction or electron microscopy.

Hans Christen, leader of ORNL's Thin Films and Nanostructures group, is experimenting with microscopic layers of materials that show promise as strongly correlated systems to learn how these films interact with each other to give the superlattice interesting properties.

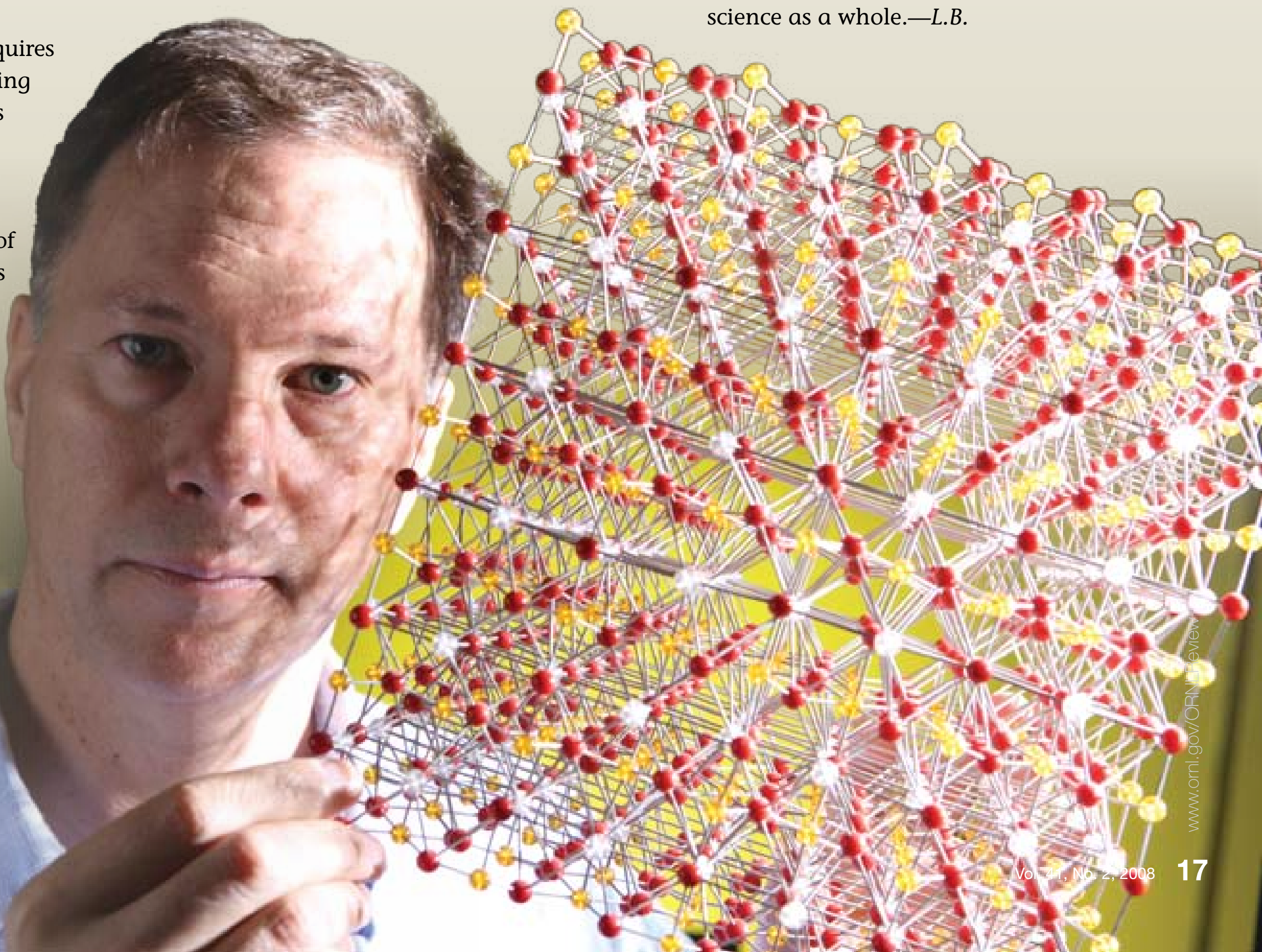
"We start with a well-prepared crystalline surface and then use pulsed laser ablation to create a highly energetic vapor that condenses onto a substrate and grows a thin layer," Christen says. "We repeatedly grow layers of magnetic materials where electron correlations are important."

Electron correlations operate on a certain length scale, but Christen and his colleagues can layer the materials they are studying on a shorter length scale to disrupt some interactions and create new ones. They can get self-organized pockets of competing states, such as conducting and insulating phases.

This ability to manage correlated electron behavior in which a very small input triggers a big response shows promise for applications such as sensors. Similarly, researchers in the Low-Dimensional Materials Physics group have been patterning complex oxides into extremely narrow "channels" to see the effect of self-organization on current flow.

In Mandrus's lab, scientists grow bulk samples of interest in correlated systems research, with a focus on transition metal oxides. The work also includes doping promising new materials with electrons to test their potential as superconductors.

ORNL's work with strongly correlated systems represents the forefront of research not only in physics but also in the future of science as a whole.—*L.B.*



David Mandrus shows a model of the perovskite crystal structure, a fundamental building block of interesting complex oxides.

WHERE It All Began

Researchers seek answers to universal questions.

More than 13 billion years ago, some scientists theorize, the cosmos underwent a super-fast expansion, in effect growing from the size of an atom to that of a grapefruit in a fraction of a second. Initially, according to the Big Bang model, our universe was a hot soup of quarks, electrons and other particles. But, before the split-second expansion ended, the cosmos cooled enough for quarks to clump into protons and neutrons.

According to this theory, some 300,000 years later electrons combined with protons and neutrons to form atoms, mostly the hydrogen and helium that formed stars. Most of these "first-generation" stars subsequently exploded, giving rise to all the chemical elements that formed planets and made possible life on Earth. Today the cosmos—which includes ordinary matter (4.6%), dark matter (23.3%) and dark energy (72.1%)—is expanding at an ever-increasing rate.

Theorists postulated that the matter existing in the first ten-millionth of a second after the Big Bang consisted of free quarks, anti-quarks and gluons that collectively behaved like a gas, a "quark-gluon plasma," or QGP. A large international team of physicists set out to recreate this state of matter, under laboratory conditions, at the Relativistic Heavy Ion Collider, or RHIC, at the Department of Energy's Brookhaven National Laboratory. At RHIC nuclei collide at nearly the speed of light, resulting in extremes of temperature and density that have not existed since shortly after the Big Bang.

Strong evidence suggests that the extreme conditions created in RHIC collisions briefly free quarks and gluons from their prisons inside protons and neutrons. The results also suggest, however, that the QGP behaves more like a liquid than a gas.

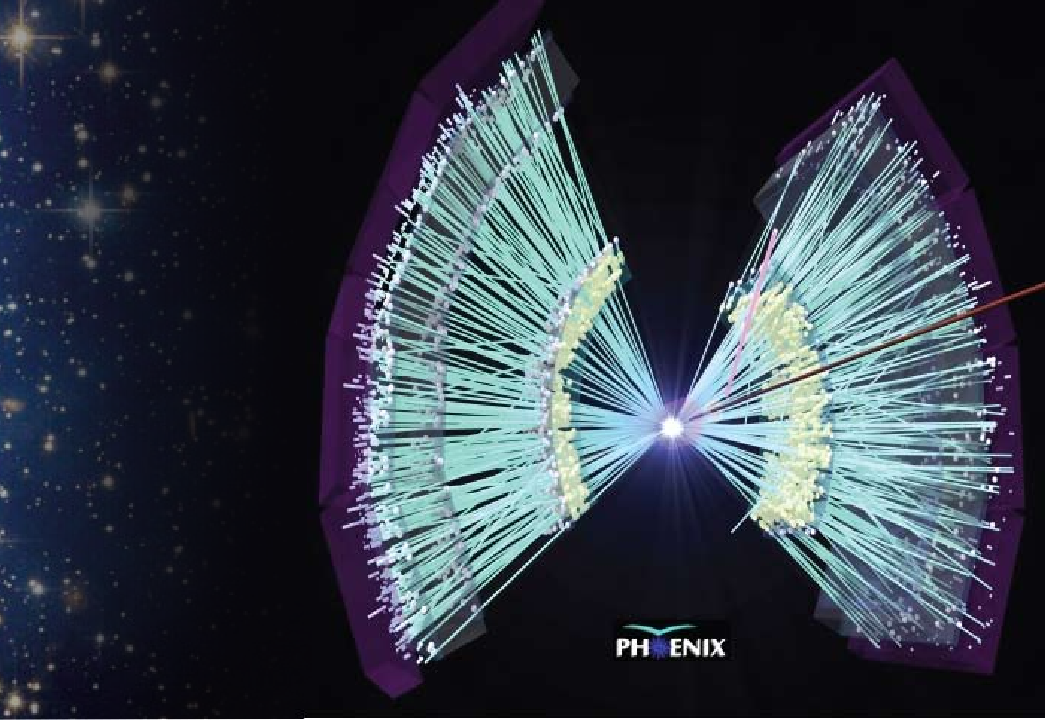
Oak Ridge National Laboratory researchers are part of the international team that has been conducting QGP experiments in the 1980s and 1990s at CERN in Switzerland and, since June 2000, at Brookhaven National Laboratory's RHIC facility in New York. Vince Cianciolo, an ORNL physicist who helped develop one of RHIC's particle detector arrays called PHENIX, recalls that the measurements at the collider showed that the recreated QGP was almost a "perfect liquid" because its viscosity was measured to be close to zero. "The QGP flowed better than water," he notes.

Recreating an extreme form of matter, like that existing in the first ten-millionth of a second after the Big Bang, requires a collider, extreme in both size and capabilities. RHIC uses 15 megawatts of electricity and 1600 miles of superconducting wires to create magnetic fields that steer two beams of gold nuclei in opposite directions in a giant ring more than two miles in length. RHIC's accelerators boost the energies of these beams to 100 billion electron volts per proton or neutron in the beam, bringing them to 99.995% of the speed of light. Some constituent particles in the gold nuclei collide head-on, causing protons and neutrons to melt together to form a quark-gluon plasma similar to that formed at the beginning of time.

For an average collision of two gold nuclei, 6,000 particles are emitted. The particles are detected and analyzed by PHENIX using nearly 500,000 individual particle detector channels. ORNL researchers designed and built the PHENIX muon identifiers and lead-glass electromagnetic calorimeter. They also developed electronic components for other PHENIX particle detectors.

Some findings at RHIC did not agree with theoretical predictions. Two such findings involve a heavy quark known as the charm quark, a particle that has a mass about 2,900 times that of an electron. The charm quark is one of six elementary particles having electric charges of one-third or two-thirds that of the electron. This particular quark is not found in everyday matter.

Measurements in gold-on-gold collisions show that particles made of light quarks lose a substantial amount of energy as they pass through the QGP. This



For an average collision of two gold nuclei traveling in opposite directions at the Relativistic Heavy Ion Collider, 6,000 particles are emitted. Many are detected and identified by an array of particle detectors called PHENIX.

result was expected. However, according to Cianciolo, "When we looked at charm quarks, we found that they lose just as much energy as light quarks. That result was surprising because of the difference in mass. Theorists are developing models for the energy loss to explain that finding."

"The charm quark was also observed to participate in the collective flow of the QGP medium. Using an analogy, if we throw a short stick (representing a light quark) on top of a flowing stream, we would expect the stick to be carried along with the water's motion. But if we push a boulder (representing a heavy quark) into the stream, we would be amazed to see the boulder flow as readily as the stick. Theorists must try to explain this surprising result."

Other theorists pose questions about the universe that may be answered by studying the neutron using two instruments at DOE's Spallation Neutron Source at ORNL. Most SNS instruments use neutrons to decipher the structure and molecular motions of various physical and biological materials. In contrast, experimenters from 30 collaborating institutions at the SNS Fundamental Neutron Physics Beam Line will focus on the neutron itself.

"For us the neutron is a rich complex object," says Geoffrey Greene, professor of physics at the University of Tennessee and leader of ORNL's fundamental neutron physics project. "We will study neutron properties. We know the neutron has a mass, a magnetic moment and a lifetime, which we hope to measure. It is unstable and decays by emitting an electron. Although the neutron is electrically neutral, theorists conjecture that it may have an electric dipole moment in which the positive and negative charges at the neutron's poles are slightly displaced. We hope to measure this little asymmetry in the neutron's charge distribution."

If the researchers can determine whether the electric dipole moment is zero or another value, the measurement could shed light on "spontaneous symmetry breaking," which in physics describes a phenomenon in which tiny fluctuations act on a system at a critical point, determining the system's fate.

"For example, no law of nature states that every person driving in America must drive in the right lane," Greene says. "In most countries people drive in the right lane because of tradition, practicality and police officers. However, in a few nations, people must drive on the left, breaking the symmetry."

Theorists believe the universe once had equal amounts of matter and antimatter, reflecting symmetry between matter and antimatter. Early in the Big Bang, matter and antimatter annihilated each other. Astronomical observations indicate that the universe is, for all practical purposes, made entirely of matter. The matter we see is the result of some interaction that led to an extremely small excess of matter. Remarkably, the amount of matter left in the universe is only one part in 10 billion parts of the original amount.

"But why such a tiny amount of matter?" Greene asks. "We suspect that initial symmetry between matter and antimatter were broken some way and that the same interaction that broke this symmetry could also create a neutron electric dipole moment."

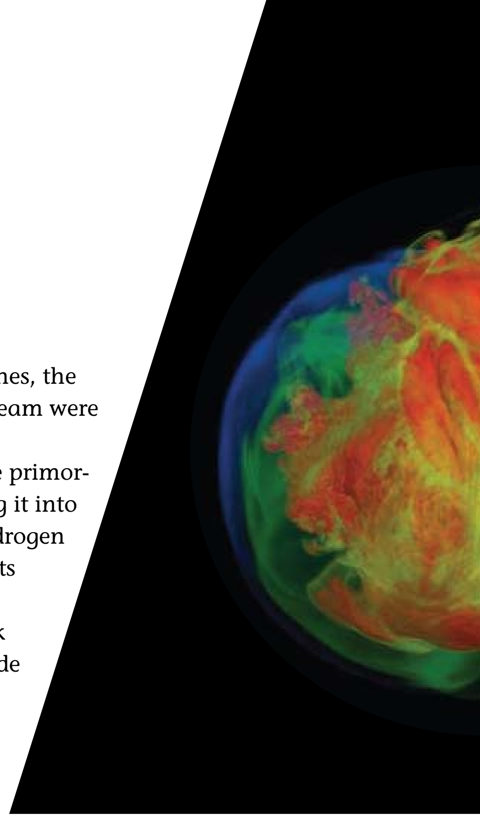
Scientists have been searching unsuccessfully for the electric dipole moment for more than 50 years. Interestingly, the first electric dipole moment search occurred in 1950 at ORNL. Greene says that the effect is so small that, if the neutron was blown up to the size of the Earth, the electric dipole moment would correspond to one electron being displaced a few microns from the North Pole.

"If we see this tiny effect at the SNS, we would have very strong support for the notion that the matter-antimatter asymmetry is the result of a spontaneous symmetry breaking," Greene explains. "If we do not see the effect, that would imply that theorists' version of matter-antimatter asymmetry is wrong or unlikely."

In 2009 the electron dipole moment and the neutron lifetime experiment will be performed on separate instruments at the Fundamental Neutron Physics Beam Line. Because the SNS will provide 10 times more neutrons per pulse than any previous machine, Greene and his colleagues will more precisely measure a neutron's half-life by detecting the energetic electron emitted by a decaying neutron. Nuclear radioactivity—also called beta emission or the "weak force"—is the emission of electrons by decaying neutrons. A free neutron has a half-life of about 10 minutes, according to previous experiments elsewhere by the international team.

Measurements of neutron lifetime and details of decay will shed light on basic scientific questions: Why does the universe at a particle level show a preference toward left-handedness, an effect known as parity violation? Does a typical neutron decay in a preferred direction, ejecting a lone electron from the south pole rather than the north pole? Or, is a little right-handedness left over? Experimenters at the SNS hope to make extremely precise measurements, providing tiny but important clues to help answer large questions that are, quite literally, universal.—*C.K.*

THE Universe Is Us



You may be a homebody, but your atoms have been around. The calcium in your bones, the oxygen that keeps you alive, and the iron that ferries oxygen through your bloodstream were produced at billions of degrees in stars that self-destructed billions of years ago.

Stars do not just light the night sky; they also act as element factories, taking the primordial hydrogen produced by the Big Bang more than 13 billion years ago and turning it into the building blocks of worlds. The lightest nuclei fuse to become progressively heavier elements; hydrogen becomes helium, which becomes carbon and oxygen, which become silicon, on up the line. Elements heavier than iron take different paths, but they still take them inside stars.

"The Big Bang left the universe with hydrogen, helium, and a little bit of lithium," explains Oak Ridge National Laboratory astrophysicist Raphael Hix. "Everything heavier than that has been made since then through a stellar process."

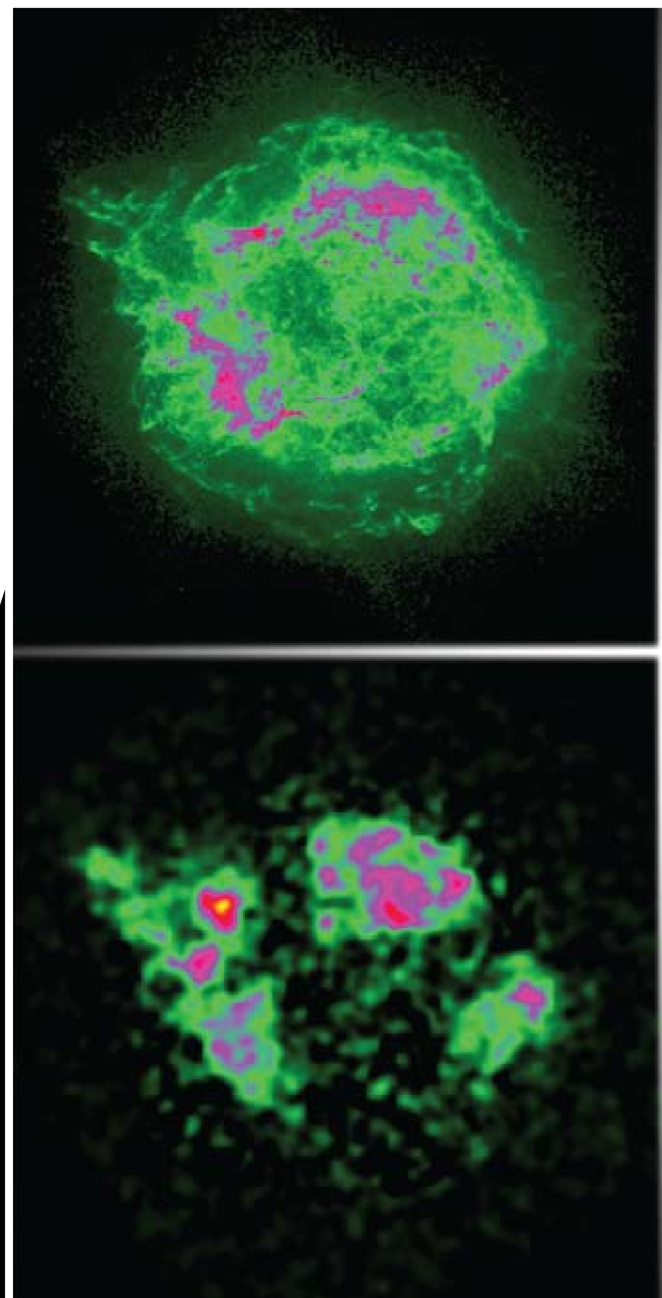
Hix has made a specialty of understanding these processes, known as nucleosynthesis. The study must answer two critical questions: How were the elements produced, and how did they get distributed? Our own sun, for example, also produces new elements, but they will not be available for new worlds. Instead, the sun will end its existence drifting through space as a slowly cooling mass of carbon and oxygen. To seed new worlds, a star must blow up.

Hix pursues his investigations through simulation, using computers as modest as an office work station and as grand as ORNL's Jaguar supercomputer, the world's most powerful open science machine. He is active in a variety of collaborations and is a co-principal investigator of the project "Multidimensional Simulations of Core Collapse Supernovae."

The project—awarded 16 million processor hours in 2008 through the Department of Energy's Innovative and Novel Computational Impact on Theory and Experiment program—models massive stellar explosions, with Hix's contribution focusing on element creation. By comparing the distribution of elements produced in the model with those observed in supernovas, Hix and his colleagues hope to fine-tune their model, which must accurately simulate the destruction of a star 10 to 20 times the mass of the sun and as large as the Earth's orbit around the sun.

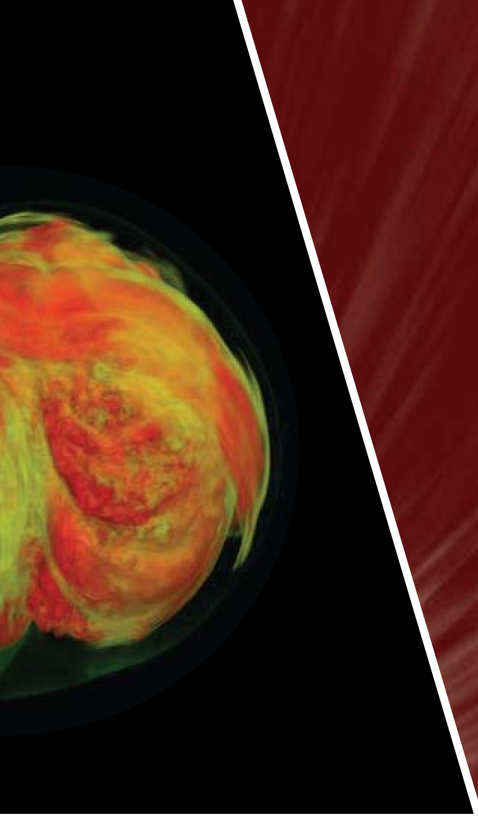
The team eagerly anticipates the arrival in the next year or so of systems able to perform more than 1,000 trillion calculations—known in the field as "petascale" systems. With such systems, Hix said, the collaboration hopes to be able to model all the isotopes created in a supernova and give us a better idea of how we came to be as we are.

"If you say the word 'universe' to somebody, they picture the starry sky at night," Hix says. "But actually, the universe is right here. Our bodies, as individual atoms, have been through extremes of temperatures, billions of degrees. It had to be to get here. Without those processes, we would not be here. And so the universe is here—it's sitting in this room."—*Leo Williams*



Computer simulation (top) of a massive star early in a core-collapse supernova. An ORNL group generated data for this image produced at the University of California at Davis.

The Chandra X-Ray Observatory provided this observation of the supernova remnant Cassiopeia A, giving the best map yet of heavy elements ejected in a supernova. At upper left is a broadband X-ray image, while the other three images show X-rays produced by ions of silicon (upper right), calcium (lower left), and iron (lower right).



EXTREME LIGHT SOURCES

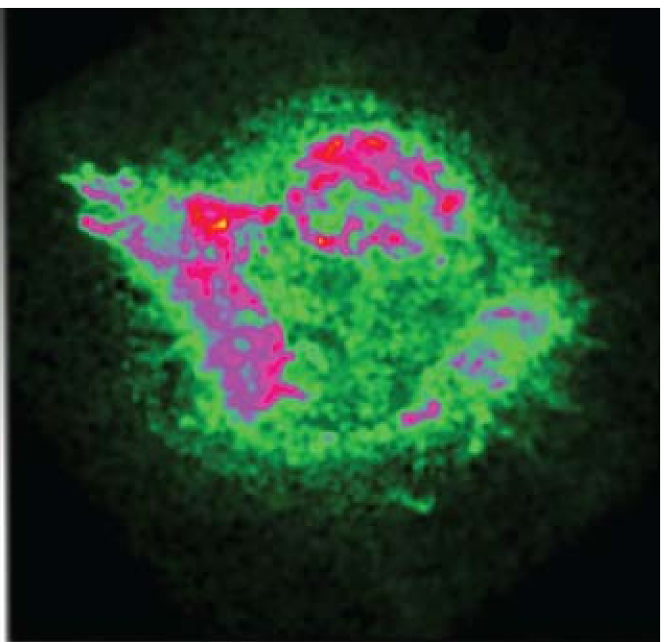
In research that could evolve into a new light-source niche for ORNL, atomic physicists led by Dave Schultz are using laser pulses to create conditions found in stars and planets. The work involves extremes of time and energy in increments imperceptibly small and unfathomably large.

The research described by Schultz involves zapping a solid or gas target inside a 10-micron focal spot with an incredibly energetic burst of light and then monitoring the resulting debris.

How extreme is the process? Schultz says the pulses of light, generated by a technology called chirped pulse amplification, range in power from hundreds of terawatts to one petawatt. In comparison, the Tennessee Valley Authority's peak electricity production on the sultriest of summer days is a mere 32 gigawatts. A gigawatt is a billion watts; a terawatt, a trillion watts; and a petawatt, a thousand trillion watts.

How can ORNL's atomic physicists harness more power than a large utility can generate?

"We do it for an extremely short time," Schultz says.



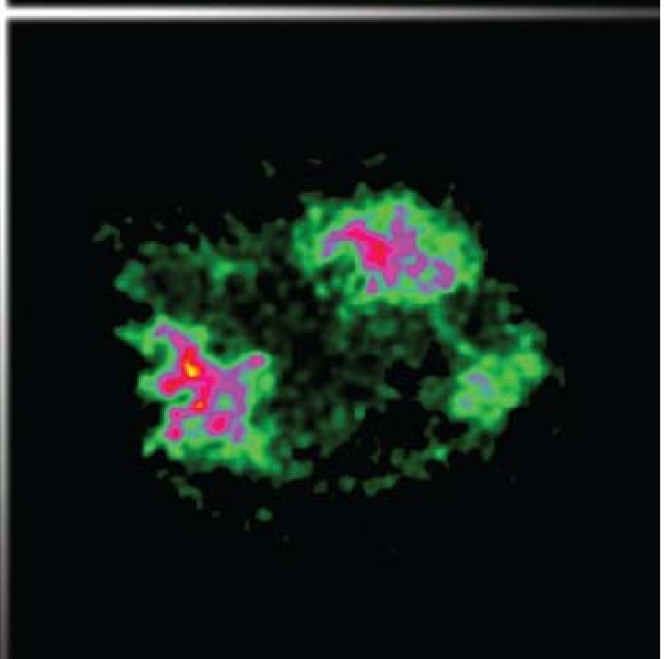
In fact, the duration of the pulses is broken down into femtoseconds, which is 10-15 of one second--well shy of how quick a cat can wink its eye. In fact, light can travel only 15 microns in 50-femtosecond-long bursts.

The work involving these incredibly powerful bursts in incredibly brief intervals is performed at two university-based facilities—the Hercules facility at the University of Michigan and the Diocles facility at the University of Nebraska.

About the only aspects of the ultrafast, ultra-intense laser experiments that are on an earthly scale are the facilities themselves. Both Hercules and Diocles are room-sized, crammed with specialized equipment.

"ORNL researchers work with the laser center staff to fire the 50-femtosecond, hundreds-of-terawatt laser pulses into the targets and then detect and analyze the explosion debris to understand the conditions they have created," Schultz says.

These "conditions" include gigapascal pressures and temperatures in the millions of degrees. The researchers also study the resulting turbulent plasmas that are scaled versions of astrophysical plasmas.



"Light is a unique carrier of energy because photons are not charged, and a lot can be put in one place," Schultz says. "Electrons, which are negatively charged, are impossible to pull together because they repel each other. The number of uncharged photons in each short pulse is enormous."

The researchers may also exploit the laser-produced plasma's ability to accelerate electrons (up to 400 megavolts in recent experiments), generate intense, ultrafast X-ray pulses and produce rare isotopes.

The laser-produced plasma acts as a linear accelerator to generate electron beams that upshift scattered light pulses into high-energy X-rays. The laser linac is a mere few millimeters long, extremely short when compared with the 331-meter-long linac at ORNL's Spallation Neutron Source.

Besides providing grist for the knowledge-of-the-universe mill, the chirped-pulse amplification studies could eventually enjoy a number of spin-offs. Intense, ultrafast X-ray pulses and rare isotopes for medical and basic science applications might become extremely valuable on Earth.—*Bill Cabage*

Predictions at the EXTREME

Researchers seek to predict chemical reactions over thousands of years.

When ordinary steel gets wet, the alloy composed primarily of iron rusts. Less widely understood is what happens at a molecular scale. Scientists have found that oxidation occurs at the interface between water and steel to form oxides and hydroxides making up the rust, often accompanied by loss of solid material into solution, or dissolution.

The processes that contribute to the phenomenon of corrosion involve the transfer of ions and electrons across this interface. In corrosion, charge transfer leads to degradation of the solid. Charge transfer enables the storage of chemical energy in batteries, which are designed to be used as a source of electrical energy when needed.

Indeed, how ions and electrons travel across the interface is of interest to electrochemists working on improving the lifetime and reliability of batteries, especially the lithium ion battery, which will be a critical element of hybrid and plug-in electric vehicles.

An electric double layer resides at the solid-water interface, so insights into the boundary's nature might help researchers increase battery capacity and lifetime. In a battery the charges must be transferred past the double layer, requiring an understanding of how the interface enables the battery to do work or store energy.

Dave Wesolowski, an ORNL geochemist, is leading a multidisciplinary research team trying to understand the structure and dynamics—the relative positions and motions of ions and electrons—of the electric double layer. To obtain this information, the researchers are using both ORNL's supercomputer and Spallation Neutron Source. Wesolowski explains the electric double layer this way:

"When a metal or oxide is exposed to water, the electrical charge distribution in the water phase is not uniform, inducing electrons and atoms to redistribute at the surface. As the surface becomes charged, water dipoles, which have separated positive and negative poles, and metal ions in the solution are attracted to the surface, forming an electric double layer. Away from that interface, the solid and liquid phases are electrically neutral without a net charge."

"Chemical reactions occur easily in bulk water, but at the interface water molecules are rigidly attracted to the surface, resulting in a barrier to reactions there," Wesolowski says. "All reactions that occur between a solid phase and liquid phase must occur in the interfacial region. In the region we call the interface, the structure and dynamics are not like the structure and dynamics of the bulk solid phase or the bulk liquid phase."

In recent years Wesolowski and other scientists have had the opportunity to use both experimental and computational tools to probe the interfacial region. Wesolowski's team has used the powerful X-rays of the Advanced Photon Source at Argonne National Laboratory to conduct surface spectroscopy and scattering. They also probed interfacial dynamics using backscattering neutron spectrometers at the SNS and at the National Institute of Standards and Technology. They coupled these probes with the computational capabilities of the Cray XT3 supercomputer at ORNL.

"By merging experimental and computational capabilities, my collaborators and I better understand the structure and dynamics of mineral-water interfaces," Wesolowski says. "This is an exciting frontier."

ORNL and Penn State University researchers have been using the Cray XT3 supercomputer at the Laboratory to model 48 water molecules on 48 titanium dioxide surface units.

"We have used a million dollars worth of computing time to get one trillionth of a second of interfacial dynamics," he notes. "We can perform classical simulations over much longer time scales with much less computer time. By using high-level calculations and X-ray probes of surface structure to calibrate classical simulations, we can produce dynamics from the calculations."

The plan is to link the dynamics results of the calculations with the results of experimental probes of surface dynamics using incoherent neutron scattering at SNS. Neutrons interacting with the hydrogen atoms in the water molecules will give a significant signal that should be valuable to theorists.

According to ORNL corrosion expert Pete Tortorelli, the science being studied with respect to the electric double layer is also at the core of what controls dissolution of solids in water (one form of corrosion) or when protective (passive) surface films form. Corrosion-resistant metals such as stainless steels rely on the formation and maintenance of protective oxide layers to fend off extremes of chemical and electrochemical reactivity. For example, a protective oxide film in an aggressive water environment must withstand a potential of ~10^7 volts per meter without breaking down.

In a pressurized-water reactor the fuel cladding consists of zirconium alloy, which reacts with water to form zirconium oxide as a passivating layer. If the cooling water temperature rises to 340°C and approaches 374°C, the critical temperature of water, researchers find they no longer can model the reactor's neutron flux. The reason: the dissolved lithium borate introduced into the primary coolant as a thermal neutron moderator adsorbs onto the zirconium oxide on the fuel cladding surface. The high concentration of boron at the fuel surface muddles the prediction of fuel burnup rates—measures of the number of nuclear fission events that have taken place in the fuel.

Wesolowski, along with retired ORNL chemist Don Palmer, received funding from the Electric Power Research Institute to study the high-temperature ion absorption characteristics of zirconium oxide. He has also been supported by the Department of Energy's Office of Civilian Radioactive Waste Management to investigate ion adsorption on spent nuclear fuel surfaces for applications in nuclear waste disposal. The projects are examples of macroscopic phenomena that scientists would like to understand at the molecular level.

Meanwhile, Tortelli studies high-temperature corrosion. "For our studies of metals, 1000°C and above is extreme," he says. He characterizes work with water environments, 300°C and above as extreme, with pressure as high as 85 atmospheres.

One of the important challenges for researchers is predicting with accuracy the changes likely to occur when the environment of radioactive materials stored at a proposed U.S. nuclear waste repository is subjected to anticipated temperatures, pressures and reactivity over an extreme time—a million years. The repository is located at Nevada's Yucca Mountain, which is made of "tuff"—rock consisting of somewhat stratified volcanic ash.

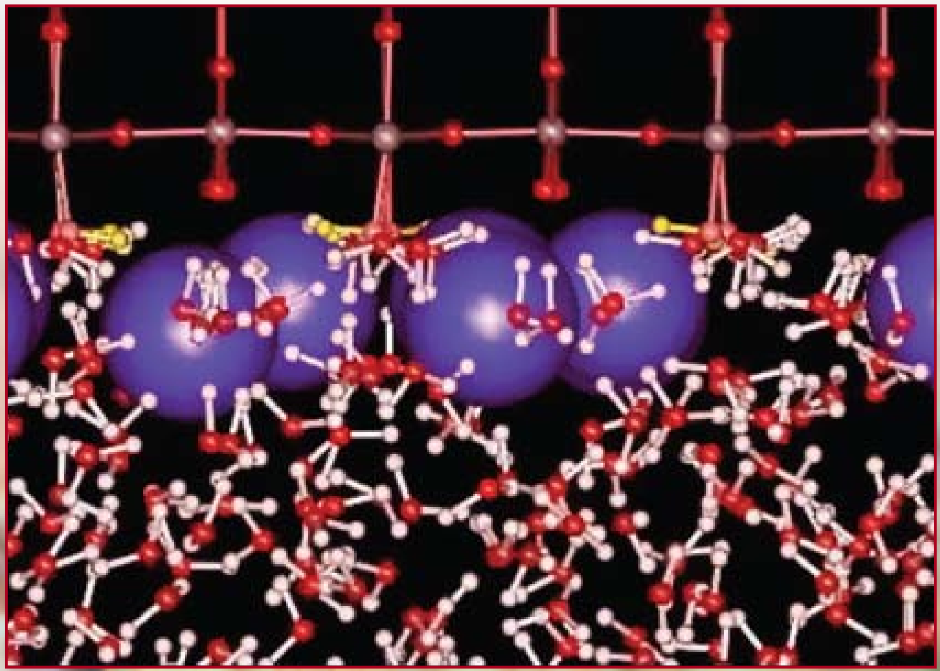
The plan for the Yucca Mountain repository is to accept spent nuclear fuel from the nation's commercial nuclear reactors and to encapsulate high-level defense nuclear waste in glass logs. The materials would be placed inside stainless steel canisters, then enclosed in an outer canister of a highly-corrosion-resistant nickel alloy. A titanium metal "drip" shield would be put in place to keep water or falling rock from damaging the canister surfaces.

"What defines the environment of the Yucca Mountain repository as 'extreme' is not only temperature and reactivity but also time," says Wesolowski. "When scientists consider changes that could occur in glass logs and on spent fuel surfaces for times beyond recorded history, they cannot model every possible reaction with certainty.

"Metals in oxidizing environments and glass containers are, at least in theory, not stable materials. While the metals may survive intact for exceedingly long times, they nevertheless might eventually corrode."

The stakes involved, and the need to understand such extreme possibilities with greater certainty, are ample motivation for researchers. —*C. K.*

Results of computer simulations and X-ray scattering reveal the structure and dynamics of water and positively charged rubidium ions at a negatively charged titanium oxide surface. The near surface fluid structure and dynamics are totally different from those of the bulk solution.



The annual Women in Cable Television leadership conference, held February 2007 in New York City, offered a lunchtime panel discussion billed as "Rarified Air: One of a Kind Leaders." The panel featured the founder of the USA Network, Kay Koplovitz; world-renowned billiard player a.k.a. the "Black Widow," Jeanette Lee; the country's only female master sommelier, Andrea Immer Robinson; and Michelle Buchanan,

Michelle

This issue of the *Review* is devoted to the basic sciences, and in particular the physical sciences, which have lately taken a hit in government funding. What's your elevator speech for explaining the relevance of the research programs you manage?

The physical sciences are at the heart of the Laboratory's endeavors because we do the fundamental science that delivers materials and chemical processes needed in every area of science. In all the workshops I have helped coordinate for the Department of Energy, it soon became obvious that just tweaking today's technologies will not be enough to meet our future energy needs. The entire world is demanding plentiful, cheap and reliable sources of energy, and despite increasing prices, energy demands continue to rise. We cannot maintain this trajectory, especially when you take into account the environmental toll of the world's growing energy demand. There are short-term fixes, such as alternative fuels. But in the long-term we need to transition to a carbon-free energy environment. To do that we must break through the technology bottlenecks we face. The bottom line is that energy is an inextricably linked part of security, environment and the economy. A year ago, people were saying, "Oh , we'll never reach $100 for a barrel of oil," and now the cost has risen to more than $100. We need to act now. We need to invest in technologies that can be deployed immediately, as well as in the long-term fundamental associate laboratory director for physical sciences at Oak Ridge National Laboratory. Buchanan even got to play a little pool on stage.

Buchanan has often found herself in rare company. From being the first woman to graduate from the University of Wisconsin with a doctorate in analytical chemistry to serving as the first female associate lab director at ORNL, she has surpassed her own early career aspirations and helped pave the way for the growing number of women who follow in her footsteps.

Her work has not gotten any easier. Buchanan has faced the challenge of flat dollars for the fundamental and applied research programs she manages, ranging from physics, materials science and chemistry to ORNL's nanoscience center. At the same time, breakthrough developments in the basic sciences are more desperately needed than ever to help meet the energy challenges of the coming decades.

Buchanan serves both as a leader at ORNL and in her field. She has been active in professional societies, as a journal editor and on advisory boards of a number of journals and university and national laboratory programs. She also helped the Department of Energy coordinate a series of workshops on targeted energy issues to identify technology gaps and the fundamental research needed to deliver revolutionary advances in areas such as hydrogen, electrical energy storage and materials in extreme environments.—*L.B.*

Buchanan

In an interview with the *ORNL Review*, Buchanan offered her perspective on the need for next-generation research to solve some of America's grand scientific challenges.

research that will transform our lives over the next 50 years.

ORNL does a range of research, from very basic to applied, and your programs, in particular, encompass that breadth. You hear arguments on what the role of a national lab should be, and often people either say the emphasis should be more basic or more applied. What's your take?

I see this as a cyclic process. Fundamental research drives advances in technology. But needs in the technology area also inspire basic research. To be successful, basic research and applied research must be closely linked. Here at ORNL, our programs are well integrated. We've had some incredible successes in which fundamental science has led to breakthroughs in energy technology.

One example is the development of nickel aluminides here that now are being applied to rollers in steel mills. They have saved industry millions of dollars and many jobs because of what was initially very fundamental research. Another example developed here is a chelator, or separation-type molecule, that will be used to capture cesium ions with a very high degree of efficiency from contaminated underground water at DOE's Savannah River site in South Carolina. In the area of mass spectrometry, concepts developed in the basic energy sciences program are now being applied in biology laboratories and, in particular, at the Bioenergy Science Center at ORNL, where researchers are working to derive biofuel from plants such as poplar trees and switchgrass.

This issue of the *Review* is devoted to "extreme" science. What is your definition of extreme science, and why is Oak Ridge National Laboratory a good place to do this work?

In much of the research we do now, we are pushing materials and chemical processes to extremes in energy environments. If you are developing solar cells, you want something that is going to withstand years of the sun's blazing heat and light without having to be replaced. You want new materials that have the strength to withstand extreme stress for a long time. If you look at materials for conducting electricity, the goal is to achieve higher voltages and higher currents without resistive losses or material failure. Now, materials in general can reach only about a tenth of their theoretical strength. We have to understand at the molecular level what causes materials to fail and how we can prevent failure or even develop materials that will self-repair. These are the types of extremes advanced materials must be able to withstand in future energy technologies.

How is the field of science changing for women?

I was the first woman to earn a doctorate in analytical chemistry at Wisconsin. Now, a lot more women are being trained in the physical sciences. Only a very small percentage of women are full professors in chemistry. Out of 200 chemists in the National Academy of Sciences, only a handful are women. Those numbers will increase, I think, as time goes on. I'm encouraged by the fact that increasing numbers of women are going to graduate schools—30 to 40% and maybe more.

Is integrating women into these scientific research areas a natural development at this point or should more be done to open doors for women?

We need to recruit broadly to find the best and brightest staff. We need to mentor young women coming into college and tell them the benefits of a career in research. I think that a lot of times when students are in graduate school the only career possibility they see is to become a research professor. They don't see other opportunities such as conducting research at a national laboratory.

As a recent chemistry graduate from Washington University in St. Louis, your daughter is also taking the scientific route. Nature or nurture?

I think it was her professor at Wash U who convinced her. My husband and I tried to keep out of it. She went to college wanting to be a math major, but she decided she wanted to do research, so she started a second major in chemistry and got hooked. Research is fun. I miss it. When you're doing research and things are working, it is simply exhilarating. That's why you see people working out here all the time, because they just love doing the science.

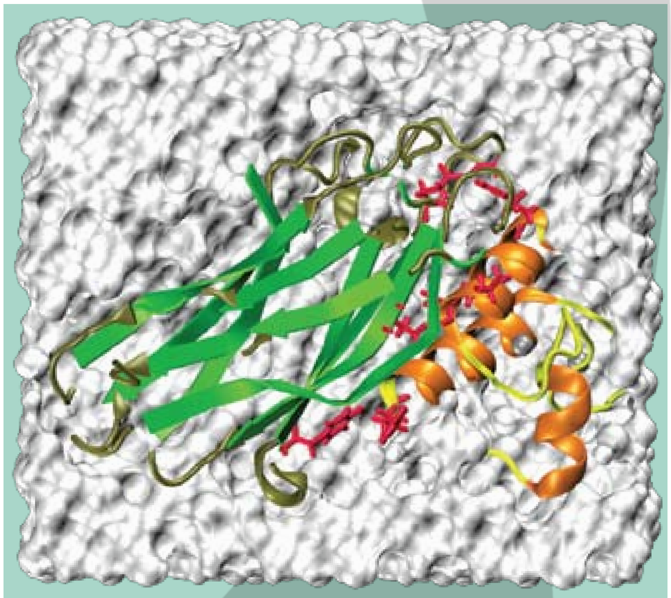
Feeling the Heat

Two interacting proteins move differently as they heat up.

Computer simulations have shown that each pair of proteins bound to each other undergo a profound change in their relative motion as they heat up, a phenomenon that could provide clues to how proteins interact to govern living cells.

The molecular dynamics simulations of protein interactions, product of an international collaboration led by ORNL researcher Jeremy Smith, are being run on the Cray XT4 Jaguar supercomputer in Oak Ridge. The simulations set the stage for neutron scattering experiments to test the theory by measuring the motion of proteins, the worker molecules of life. Smith, who leads the ORNL Center for Molecular Biophysics and holds a University of Tennessee–ORNL Governor's Chair, collaborated with researchers from the University of Heidelberg in Germany. Their study appeared in the April 1, 2008 edition of *Physical Review Letters*.

"The living cell is a network of proteins that talk to each other by interacting, sometimes transiently, sometimes for long periods of time," Smith says. "These interactions are important at every stage of cell function. Understanding the physical nature of these associations will help us comprehend why they form and when."



A visualization of the modeled three-dimensional structure of the potassium-channel protein, performed on ORNL's Jaguar supercomputer.

The simulations performed by his team followed the way a pair of interacting proteins moves relative to each other as temperature increases. Internal motions in proteins and many other materials undergo a rapid softening at a certain temperature, a phenomenon called the "glass-to-liquid," or simply "glass" transition. The new simulations show that a glass transition also is evident in the way proteins in a pair, or "complex," move relative to each other.

At very low temperatures, around -200ºC, protein complexes are frozen stiff in a glassy state. At around -40ºC, they suddenly free themselves up and behave like molecules in a liquid, diffusing randomly relative to each other, while still remaining in touch.

"The effect is a bit like a couple dancing for the first time together at a ball," Smith says. "In the beginning, at low temperatures they just rigidly and uncomfortably hold each other, but after a while, as the temperature rises, they get used to each other and move more fluidly, with more adventurous motions, all while maintaining body and eye contact."

The motion may in the future become measurable using specialized spectrometers at the Spallation Neutron Source, as neutron scattering has historically been a major technique for examining glass transition behavior.

"The importance of neutrons stems from their unique capability of allowing the direct measurement of both where atoms move and how fast they get there—in other words, both the geometries and time scales of motions," he says.

Exactly how protein pairs dance together in a living cell is yet to be determined. Maybe, as in the glass transition behavior, they mimic what happens inside proteins themselves.

In a new theoretical article by Smith, also due to appear in *Physical Review Letters*, he demonstrates that the internal motions in a protein are likely to obey "anomalous subdiffusion" on a "fractal network." In other words, the motion is more complex than usual as it follows a specific geometrical form.

"Possibly the relative motions of proteins in a living cell will follow similar rules," Smith says. "To find out whether this is the case, our team is wasting no time pushing forward with a massive simulation of 3.5 million atoms in a thousand interacting proteins, running on the ORNL Cray XT4 Jaguar supercomputer. This high-performance simulation will stretch the capability of Jaguar but, if successful, will be a rich source of information, helping us to understand the forces between proteins."—*Bill Cabage*

The Next Small Thing

A problem found in one lab is solved in another.

Organic light-emitting diodes increasingly show promise as lighting sources that are more efficient, more cost effective and more flexible than solid-state LED technology. Despite the potential, the technology faces some hurdles.

A University of Tennessee researcher, with the help of colleagues and instruments at Oak Ridge National Laboratory's nanoscience center, has taken steps toward overcoming one of those hurdles by employing two emerging technologies—spintronics and nanotechnology. Spintronics exploits both the quantum spin states and charge states of electrons.

Bin Hu, assistant professor in UT's Materials Science and Engineering department, was one of more than 300 users hosted by ORNL's nanoscience center in 2007 during the center's second year of operation. In his project, Hu worked with researchers at the center and in ORNL's microscopy group to test and analyze the OLED device he had developed at UT.

OLEDs, made up of layers of a polymer and organic compounds, are easy and affordable to make in large quantities using a simple process similar to an inkjet printer. They can also be made with large, flexible sheets, opening the door to a host of potential applications that include portable electronic newspapers, large but inexpensive white lighting panels and big-screen televisions and projectors.

One of the barriers to deploying the technology is the inefficiency that arises when voltage is applied to organic compounds to produce light. The process generates excitons as singlets and triplets with the ratio of 1:3. An exciton is a bound state of a pair of particles that results when a photon kicks an electron out of orbit, leaving a positively charged hole, which binds with the electron when they meet in an organic semiconducting molecule. An exciton has slightly less energy than the unbound electron and hole.

The challenge for Hu is that triplet excitons, at 75% of the population, produce heat that limits the efficiency of OLED devices. Changing the relative ratio between singlet and triplet excitons thus becomes a critical issue in improving OLED efficiency.

The ability to fine-tune electrons— that is, to change the degree to which each electron's spin is aligned with a given direction, or spin polarization—is an important element of spintronics that might offer a way to boost the efficiency of OLEDs. Unfortunately, applying a thin magnetic electrode coating to deliver polarized electrons to these OLED devices has typically produced dismal results.

"For example," Hu says, "if you supply 100 electrons to the OLED, only five electrons have an oriented polarization and 95 electrons are left at random."

After repeated attempts at developing a workable magnetic coating, Hu and UT student Yue Wu tried applying the ferromagnetic element cobalt as the electrode coating to inject charge carriers with spin polarization in both the typical thin film form and also as nanoparticles. The nanoparticles demonstrated a significant improvement of polarization efficiency from 5% to 60%. This improvement of spin polarization efficiency has boosted overall OLED efficiency by 20%.

To understand why the nanoparticles worked better than the cobalt film, Hu turned to ORNL's nanoscience center. There, Hu used ORNL instruments and expertise to characterize the magnetic, spin-dependent transport and structural properties of the OLED devices fabricated in his UT lab. ORNL researchers played a role in helping Hu analyze and better understand the spin-dependent transport across the ferromagnetic nanodot and organic polymer interfaces. Their research results were recently published in *Physical Review B*.

Hu says the spaghetti-like structure of the polymer chains that make up OLEDs create a difficult surface to which a magnetic electrode film can adhere. Nanoparticles, on the other hand, nestle inside the chaotic surface structure, enabling a more uniform response. In addition, although typically a conductivity mismatch exists between the magnetic material and the polymer semiconductor, partial oxidization of the nanodots surfaces helped overcome this barrier, paving the way for more efficient transfer of electrons. The end result: a brighter, more efficient light, as well as a potential host of electronics applications.—*L.B.*

...and the WINNERS are...

Accomplishments of Distinction at Oak Ridge National Laboratory

Gilbert G. Weigand of ORNL's Computing and Computational Sciences Directorate has received the inaugural ***James R. Schlesinger Award*** from ***Secretary of Energy Samuel Bodman*** for his "passion for excellence along with his ability to foster and implement the practices and values that are necessary for the protection of our nation." Weigand is credited with conceiving and implementing DOE's Accelerated Strategic Computing Initiative, which pooled government programs and national laboratories to build the world's best high-performance supercomputers. High-performance computing and simulation at the ASCI level now pervade all areas of science and engineering.

For significant achievements on behalf of the department, Secretary of Energy Bodman selected ORNL's **Dave Felde, Ron Miskell, Jon Kreykes, Jim Sumner, Duane Starr and Alan Parker** to receive the Secretary's Achievement Award.

ORNL's **Office of Intelligence and Counterintelligence** team was recognized for work in DOE's nuclear nonproliferation programs "to mitigate the risk of nuclear proliferation and international terrorism."

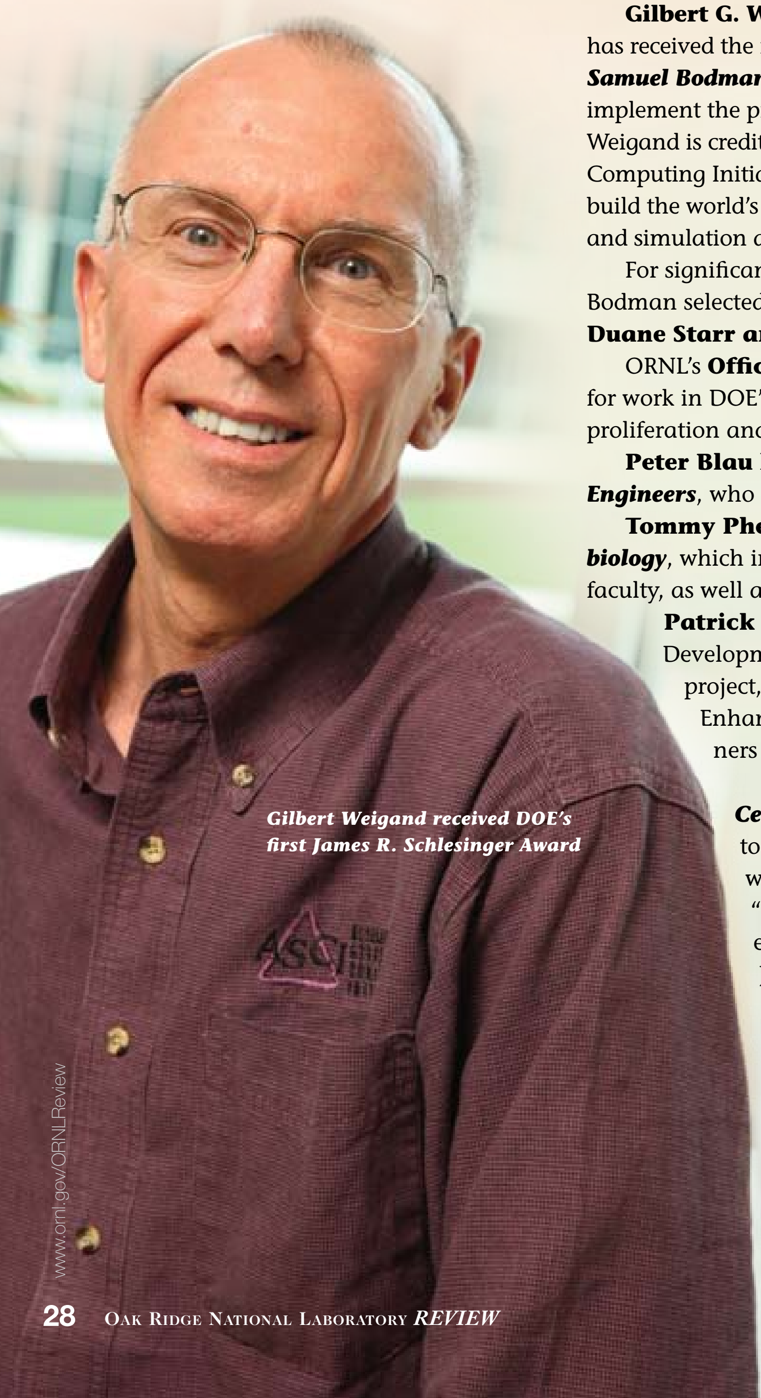
Peter Blau has been elected a ***fellow*** of the ***Society of Tribologists & Lubrication Engineers***, who study friction and wear in materials.

Tommy Phelps has been elected a ***fellow*** of the ***American Academy of Microbiology***, which includes basic researchers, applied researchers, teachers, university faculty, as well as public health, industrial and government service professionals.

Patrick Mulholland received the Strategic Environmental Research and Development Program ***Project of the Year Award*** in Washington, D.C. His project, titled "Riparian Ecosystem Management: Impacts, Restoration and Enhancement Strategies," was cited Dec. 4, 2007, at the 13th annual Partners in Environmental Technology Technical Symposium & Workshop.

Edgar Lara-Curzio has been elected a ***fellow*** of the ***American Ceramic Society***. At the 110th annual meeting of this scientific society to be held Oct. 5-9, 2008, in Pittsburgh, Pa., **Andrew Wereszczak** will receive the 2008 ***Richard M. Fulrath Award***, which recognizes "outstanding academic and industrial ceramic engineers/scientists and efforts to honorably promote technical and personal friendships between Japanese and American professional ceramic engineers/scientists." Also at that meeting ORNL Corporate Fellow **Paul Becher** will be named the recipient of the 2008 ***John Jeppson Award*** of the ***American Ceramic Society***, which recognizes "distinguished scientific, technical, or engineering achievements in ceramics."

The ***Oak Ridge National Laboratory Review***, ORNL's research magazine, received an ***award of excellence*** (second prize) in the magazine category of the International Technical Publications Competition of the ***Society for Technical Communication***.



Gilbert Weigand received DOE's first James R. Schlesinger Award

next issue

Scientific Myths

online extras

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Extremely waterproof materials:
- See video of extremely water-repellent glass.

Catch an exploding star:
- View animated simulation of a core-collapse supernova.

Reference desk:
- Read journal papers on research described in this issue.

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