Oak Ridge National Laboratory
# REVIEW
• MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY •

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# Of Scale and Science

Since the construction of the pyramids some five thousand years ago, humankind has marveled at projects of extraordinary scale. America's reputation as an emerging world power was enhanced enormously by the Panama Canal and the Transcontinental Railroad, less because of their function than the unprecedented level of political and operational discipline required to build them. Barely three years since the first neutrons were produced, one often senses that the image of the Spallation Neutron Source remains more a "Modern Marvel" of engineering scale and complexity than a facility that is now turning out some of the world's most advanced materials research.

The reputation is understandable. Boldly conceived as a neutron source that would surpass the performance of European and Asian competitors by a factor of ten, the SNS was a design challenge beyond the capabilities of a single national laboratory. The ability to marshal the collective talents of six diverse labs, to sustain congressional support for large appropriations in a period of fiscal restraint—followed by the delivery of a $1.4 billion project on time, on budget and on scope—is one of the truly great success stories of the Department of Energy. Ironically, the political and operational discipline that made possible one of the world's largest science projects is a success story that often overshadows the remarkable research being generated today at the SNS.

This issue of the ORNL *Review* provides a snapshot of the initial research produced by an international collection of scientific talent working with an unmatched array of instruments at the SNS. Some 200 papers have already been submitted for publication in fields ranging from biological sciences to polymers. As the volume of data and publications expands, the SNS is on a path to redefine the scope and potential of materials research. Such a lofty goal is not unreasonable for one of the world's largest and most modern research facilities. The delivery of groundbreaking science is viewed as an expectation of the Department of Energy, an obligation owed to the American people and a self-imposed responsibility by an SNS research staff aware of their unique moment in history.

The SNS, unlike the launching of a ship or the dedication of a bridge, remains a work in progress. Having achieved a beam power of 870 kilowatts, the SNS has smashed the previous world record of 150 kilowatts and is ahead of schedule to reach the goal of 1.4 megawatts. Roughly one-half of the eventual total of 25 enormous instruments have been installed, and the number of researchers seeking to use the instruments is oversubscribed.

Perhaps because the march toward an unprecedented magnitude of power and instruments is ongoing, public fascination with the scale of the SNS appears undiminished. As proud as they are of what they have built, the SNS research team is now focused on finding solutions to some of humankind's most important scientific challenges. If successful, the science they hope to produce, and the applications of that science to the international community, will reshape the image of the SNS for generations to come.

Billy Stair

Billy Stair
*Director, Communications and External Relations*

# News & Notes

## NOAA-Oak Ridge Expand Climate Modeling

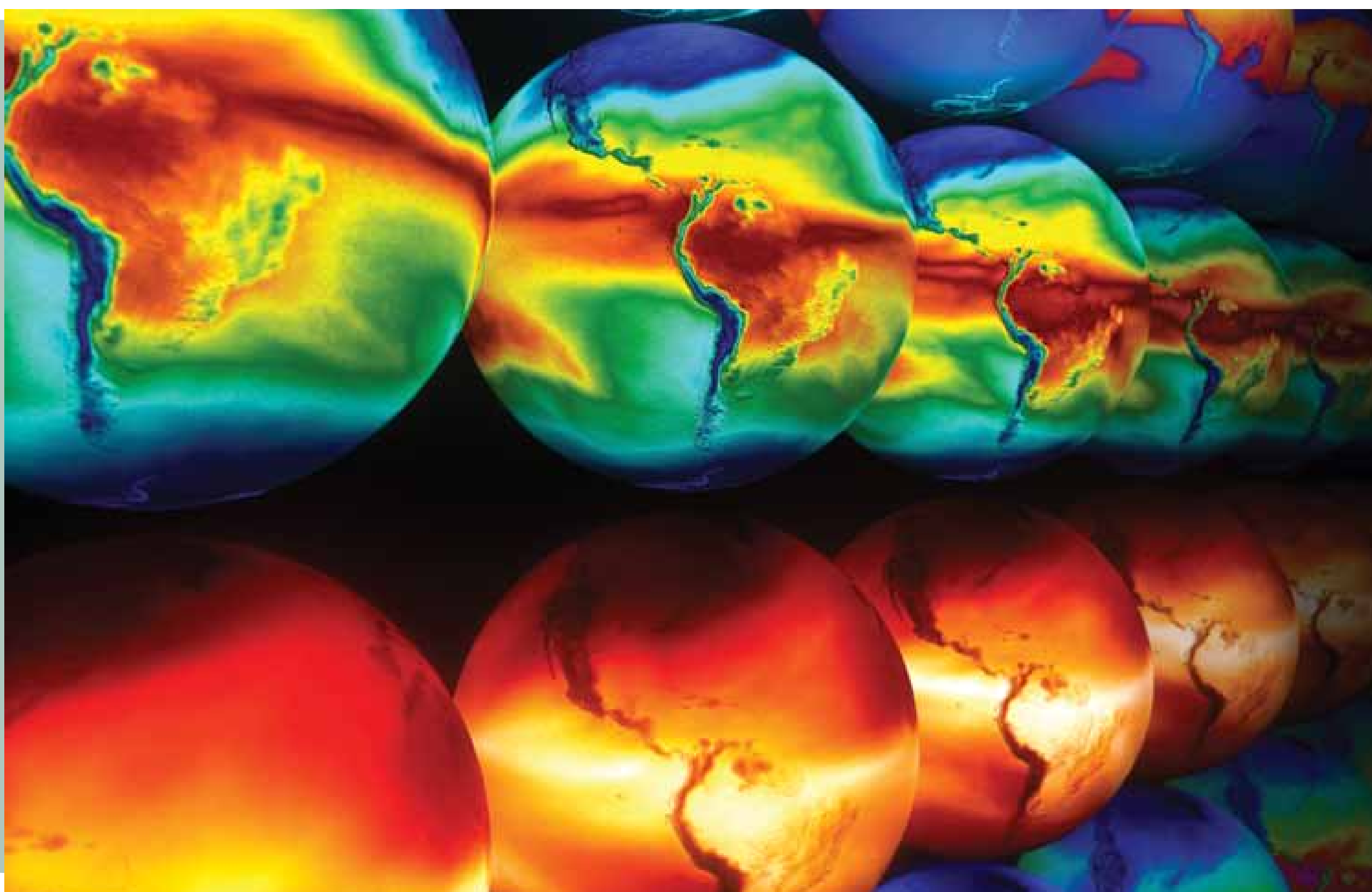
The National Oceanic and Atmospheric Administration will provide $215 million to Oak Ridge National Laboratory over the next five years to support climate research, further bolstering ORNL's role as a U.S. hub for broad-based work on global climate change.

Thomas Zacharia, ORNL's deputy lab director for science and technology, says Oak Ridge is becoming increasingly attractive for agencies engaged in climate studies that wish to leverage their assets and get the most out of their resources. Zacharia says the National Science Foundation and NASA, two other federal institutions involved in climate research, already have a strong presence at ORNL. "The investments by DOE, NSF, NOAA and NASA are really bringing together an integrated capability, making Oak Ridge a place of choice for inter-agency projects."

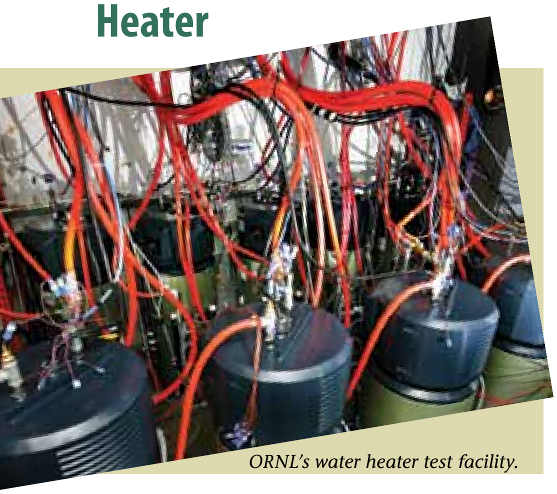
"NOAA's investment is huge," Zacharia says, noting that the Department of Commerce is one of the major players in climate change with "tremendous research capabilities."

"The new agreement between NOAA and the DOE has already provided $73.5 million in Recovery Act funds to ORNL, with similar amounts to follow over the next four years," he says. "The lab expects to hire 25 to 50 additional climate researchers as part of the expanded effort."

One of the key Oak Ridge attractions is the lab's stable of supercomputers, headed by the Cray XT5 "Jaguar"—the world's fastest computer for open science, which is frequently called upon to run the most difficult climate-simulation models. ORNL also is home to observational experiments, including outdoor studies that evaluate and measure the impact of climate-related factors—such as carbon dioxide—on ecosystems.



## ORNL, GE Collaborate on High-Efficiency Water Heater



*ORNL's water heater test facility.*

A collaboration between ORNL and General Electric will result in the manufacturing of a "hybrid" electric water heater that consumes half the energy of standard models while providing hot water in the quantities homeowners demand. The product will be the first water heater from a major manufacturer that meets the new 2009 DOE Energy Star standards for electric storage water heaters.

"The typical electric storage water heater raises the temperature of the water in the storage tank using only electrical heating elements," says Patrick Hughes, the Director of ORNL's Building Technologies Research and Integration Center. "The new heat pump water heater moves heat from the surrounding air into the water tank, thus requiring much less electricity from a power plant to heat the water."

GE initially was attracted to the partnership by ORNL's reputation as a leader in the field of energy efficiency. "ORNL has been doing research on heat pump, or 'hybrid,' water heaters for at least a decade," says Hughes. "GE periodically scans the horizon for new technologies to use in their appliances. They read our research and visited Oak Ridge to meet our team and tour our facilities."

As a result of subsequent collaboration, one of the world's leading companies was able to take advantage of ORNL's unique testing facilities. "We have a lab capable of performing accelerated durability testing on a fleet of water heaters," Hughes says. "About 10 months of operation in our facility is the same as 10 years of service life. GE made a number of design changes related to the appliance's durability, performance and controls as a result of this testing."

Hughes is optimistic that hybrid water heaters will catch on with consumers. "GE is one of the strongest brands in the world," he says. "High volume enables affordable pricing, which in turn gives GE the ability to shift a large share of the electric storage water heater market to hybrid electric water heaters."

The Department of Energy estimates that if just 10 percent of the nation's 4.8 million annual electric water heater shipments were heat pump water heaters meeting Energy Star standards, the 480,000 units would reduce power consumption by nearly 1.3 billion kilowatt hours and save consumers $130 million in energy costs annually.

An added incentive for consumers comes in the form of federal energy efficiency tax credits that will cover 30 percent of the total installed cost of these water heaters—if they are placed in service between now and 2016. The units will be available to consumers by the end of calendar year 2009. An additional manufacturing plant is scheduled to open in Louisville, Kentucky, in 2011, creating an estimated 400 jobs.

## Electric Vehicles Becoming a Reality

The Department of Energy has selected Tennessee as one of five states participating in what is being described as "the largest deployment of electric vehicles and charging infrastructure ever undertaken."

Tennessee's role in the project is an outgrowth of Governor Phil Bredesen's conversations with Nissan North America, Oak Ridge National Laboratory, the Tennessee Valley Authority, and other public and private partners committed to promoting the use of zero-emission vehicles, including electric vehicles. DOE's announcement of the electric vehicle project involving Nissan and the state of Tennessee is one of 48 new advanced battery and electric drive projects that will receive $2.4 billion in funding under the American Recovery and Reinvestment Act.

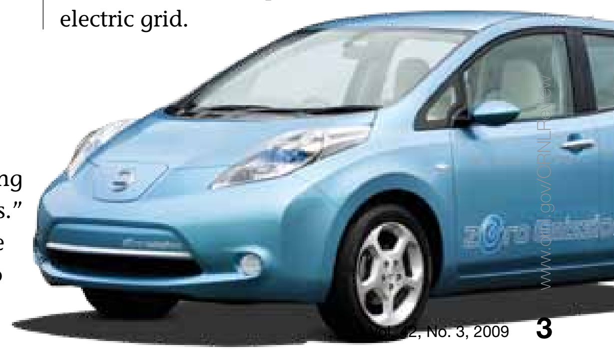
"Our clean-energy future depends on the adoption of new technologies," Bredesen says. "It's gratifying to see Tennessee joining other top clean-energy states at the leading edge of this exciting new project."

The multistate project will be funded through a $99.8 million DOE grant to Electric Transportation Engineering Corp. (eTec), a subsidiary of ECOtality, Inc., a Phoenix, Arizona-based leader in electric transportation and storage technologies. eTec, in partnership with Nissan, will take advantage of the early availability of the Nissan Leaf, a newly unveiled zero-emission electric vehicle, to develop, implement and study techniques for optimizing the effectiveness of charging infrastructure that will support widespread electric vehicle deployment.

In its news release, DOE cited the project as an initiative that will help "establish American leadership in creating the next generation of advanced vehicles."

The project will install electric vehicle charging infrastructure and deploy up to 5,000 Nissan battery electric vehicles in strategic markets in five states: Arizona, California, Oregon, Tennessee and Washington. In the Volunteer State, the initial investments will focus on Chattanooga, Knoxville and Nashville. Approximately 2,500 charging stations will be installed to support as many as 1,000 cars that are expected to be purchased for use in commercial and government fleets and by individual consumers.

Oak Ridge National Laboratory will assist the project by studying the interaction of the charging stations, some of which will be solar powered, with TVA's electric grid.




# NOW, THE SCIENCE

## The SNS seeks to integrate a variety of scientific disciplines.

*The SNS control room. About 250 engineers, physicists, and technicians are required to operate the SNS.*

Just months after a single keystroke produced the research facility's first neutrons in the spring of 2006, the Spallation Neutron Source became the world's most powerful neutron source, a feat achieved while operating at only about 10 percent of its design power. Two years later, the SNS continues to explore new scientific dimensions, measured in the sheer magnitude of neutron flux and in the quality, breadth and vision of some of the most ambitious programs ever contemplated in the materials sciences.


Physics / Diagnostics Station
Physics / Diagnostics Station

*The facility's 1,000-foot linear accelerator delivers hydrogen ions at almost 90 percent of the speed of light.*

## Overpowering

The scientific community has no shortage of superlatives to describe the efforts required to get the massive $1.4 billion project funded, built and in the business of producing groundbreaking research. The efforts, indeed, are ongoing. Researchers hope to increase the power of the SNS proton beam to an unprecedented one megawatt before the close of 2009.

"On the facility development side of the house, we have come a very long way," says SNS director Ian Anderson. "Zero kilowatts to one megawatt is an incredible distance to have covered. We accomplished what we said we would do all the way through, despite considerable challenges along the way."

"Earlier this year we were within reach of the megawatt level," Anderson says. The machine was running reliably at 870 kilowatts when we made a few modifications designed to enable us to reach the megawatt milestone. Suddenly a problem occurred with the stripper foils used to create protons from the accelerator's hydrogen ion beam. Having never encountered that reaction, we reduced the machine's power, providing an opportunity to examine the process while allowing our science programs to continue uninterrupted."

Anderson believes the experience illustrates one of the challenges of running a major user facility like the SNS, where the unique needs of an international science program must be balanced with an expectation to reach operational milestones, like increased power levels, that are part of the project's commitment to the Department of Energy.

Despite these expectations, running reliably and maintaining a high level of scientific output remain the primary goals for the SNS.

"Running at lower power, the machine is stable and the majority of users are able to conduct their experiments," Anderson says. "If we were to try to increase power to one megawatt today, we would have to weigh the likelihood of success against the risk of burning out a few foils and stopping the progress of the science program. We may go for one megawatt at the end of this experiment cycle, just after we shut down for maintenance, when an unexpected problem would not cancel scheduled experiments.

## Producing the Science

The SNS has long been expected to have a major influence in areas traditionally associated with neutron science. As the capabilities of the SNS become increasingly apparent, scientists are realizing that this influence will also extend to fields such as biological sciences and soft matter, where using neutrons as research tools is a relative novelty. The facility's expanding significance is a result of both a quantum leap in beam power and the diversity of experimental instruments deployed or planned for the target station's 24 beam lines.

"Neutron science is a technique that can be used to study a virtually unlimited variety of materials," Anderson says. "We encourage our scientists to engage with their colleagues in other fields at ORNL and in the user community. This familiarity helps direct improvements in instrumentation and capabilities toward the needs of a broader range of science programs and keeps the SNS at the forefront of research."

Even as the SNS matures, its scientific highlights are already numerous. One such highlight is the experimental results related to the newly discovered iron arsenide family of superconductors. Novel research at the facility's ARCS spectrometer has advanced understanding of so called "unconventional" superconductivity, a precursor to a similar understanding of the basic mechanisms that give rise to superconductivity.

Unlocking the door to superconductive materials holds the long-term potential for developing a suite of technologies that could significantly reduce energy consumption. ORNL is in the unusual position of having both the facilities to synthesize these materials and the neutron scattering capabilities needed to study their structure and how they work.

Enhanced fuel cell technology is among the areas of focus for new materials. The Backscattering Spectrometer at the SNS is being used to explore ionic liquids used as membranes in proton fuel cells. The liquids have demonstrated the ability to function at relatively high temperatures, conditions under which standard "Nafion" membranes would have become completely dry.

Recent work on the SNS Magnetism Reflectometer has demonstrated that thin films of metal oxides can become magnetic when combined with paramagnetic films. This development has implications for the enhancement of data storage devices such as memory chips in phones and computers.

New polymers are yet another goal of SNS researchers. The facility's Liquids Reflectometer examines the structure and movement of individual molecules in "self-healing polymers." When these polymer mixtures are damaged, one polymer moves quickly to the surface—"healing" the damage—while the remaining polymers keep the structure stable. Understanding how these materials function and controlling their behavior have wide-ranging applications in the development of lubricants and biomaterials, such as medical implants and antimicrobial agents.

Other polymer–related research employs the SNS's Liquids Reflectometer to focus on the shifting structure of pH-dependent polymer films. These films go through a series of changes related to the acidity of their environment, leading toward the day when they may be used by pharmaceutical companies to encapsulate drugs. When the films migrate to a point where the acidity is different, such as the stomach, they would break down and release the drug.

To the surprise of some, biology is one of the areas in which the SNS is expected to have the greatest impact. The facility's high-intensity neutron flux enables researchers to understand the structure and function of protein crystals and biological membranes in much more detail than was previously possible.

Anderson points out that SNS researchers are also working with bio-inspired polymer membranes using the Liquids Reflectometer. "They are attempting to mimic the function of biological membranes by attaching polymers to substrates and making them functional. The ability to design and build instrumentation that can peer into the structure of membranes and see how they interact with proteins will have a major impact on the field."

Still another discipline being reshaped by the SNS is the study of materials under extreme conditions, including high pressure, extreme temperatures and intense magnetic fields. Anderson observes that, "Most of the time, scientists are not interested in whether materials function at room temperature. They would prefer to understand their properties under conditions in the real world."

Bolstered by unprecedented beam power, the SNS instruments can simulate real world conditions inside an automobile engine, deep in the earth's crust, or in the structure of an aircraft wing.

## Burden of Expectations

In some respects, the SNS has already exceeded expectations. Against the backdrop of cost overruns and unmet schedules that have plagued similar projects, the ability to build one of the world's largest and most complex science facilities on time, on budget and on scope was, in many respects, a historic achievement. The rapid pace with which researchers ramped up the beam power toward the one megawatt threshold intensified further the sense that the SNS would fulfill its scientific promise.

Yet even as scientists pass these milestones, they are aware that their significance is short-lived. The true value of the SNS will lie in its ability to answer fundamental questions that cannot be answered anywhere else in the world. In particular, the SNS must be viewed as a center for neutron science, with capabilities that open up new horizons in disciplines across the physical and biological sciences.

Ian Anderson and his team are fully aware of both their potential and the burden of expectations. Having delivered a facility of unmatched quality, the SNS team is now committed to nothing less than producing the science that can literally reshape the world. R

# Where None Have Gone Before

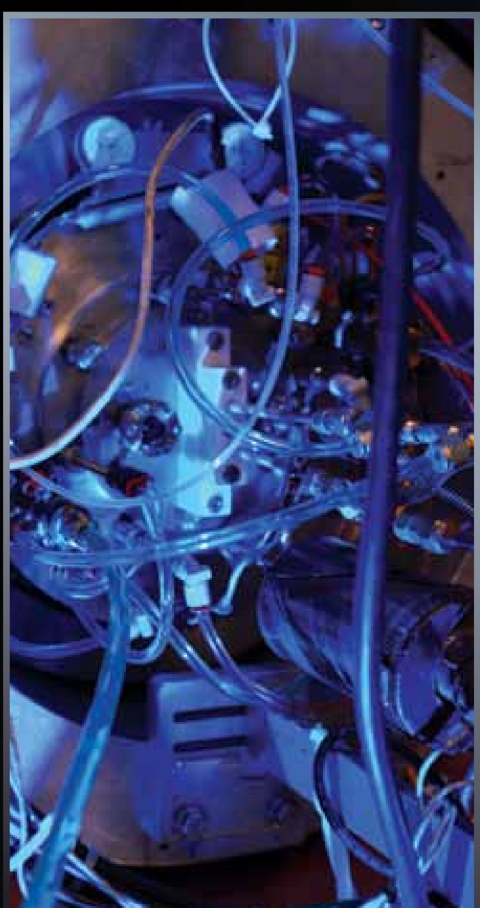
## *The SNS seeks to break the world record by ten-fold.*

As the Spallation Neutron Source nears the one-megawatt milestone, one of the world's largest scientific facilities is restoring America's leadership in the field of neutron science. This success is made all the more impressive by the fact that, while the design and start-up of the facility have drawn on the experiences of its predecessors, the path to one megawatt has been an exploration of uncharted scientific territory.

"The SNS story begins more than two decades ago when the Department of Energy gathered a variety of scientific groups to think about the research tools that would be needed in the future," says Stuart Henderson, who heads the project's accelerator program. "One of the conclusions they reached was that a megawatt-class pulsed neutron source would be critical to closing the gap between neutron research capabilities in the U.S. and those in the rest of the world."

Henderson says that reaching one megawatt is significant on several different levels.

"For researchers, the one-megawatt mark means delivering on a decades-old dream," he says. "In a more formal sense, reaching this threshold will fulfill the commitment we made when DOE agreed to undertake the SNS project."



*Hydrogen ions are generated and pre-accelerated in the SNS's front end before entering the linear accelerator.*

One-megawatt also represents a significant milestone on the way to the goal of a near ten-fold increase in power over international facilities that were state of the art when the SNS was proposed. When the SNS came online, the world's most powerful neutron source was the ISIS facility in the United Kingdom—running at a beam power of about 150 kilowatts. The SNS is designed for peak performance at 1.4 megawatts.

"A quantum leap in performance is the kind of improvement funding agencies want to see with a proposed new facility," Henderson says. "They understandably don't want something that already exists. Agencies prefer to be at the clear forefront of science, which often means performing at a factor of 10 better than your predecessors."

Since the first neutrons were generated in 2006, SNS scientists have been involved in a long and complex process of slowly increasing the facility's beam power.

"Our initial goal was a modest 60 kilowatts," Henderson says. "That sounds low, but at the time it was a third of the power of the world's biggest pulsed neutron source."

By August of the following year, the SNS was producing a 180-kilowatt neutron beam, surpassing the power of ISIS and entering the *Guiness Book of World Records* as the world's most powerful neutron source. Breaking the world record was one of several occasions when the excitement generated by reaching a milestone was tempered by the size of the task ahead. SNS scientists who thought getting to 180 kilowatts had been hard wondered aloud about the challenge of going all the way to 1.4 megawatts.

The anxiety was well-founded. As the SNS runs at increasingly higher beam power, scientists have encountered phenomena never before seen and not entirely understood. As a result, a graph of the SNS's beam power since 2006 trends upward, but the upward slope is punctuated by dozens of peaks and valleys.

"In the valleys we would be flummoxed by problems that kept us from making any progress," Henderson says. "Sometimes we would increase power and decide something wasn't quite right, so we would have to take a step back to address the problem. Each jump in the graph represents a point at which we reached an understanding of a limitation we were encountering well enough to fix it and move forward."

As an example of this process, Henderson recalls that, in early to mid-2008, beam power was limited because beam particles were being "lost" on the walls of the accelerator in the area where the beam is injected into the accumulator ring. After diagnosing the problem, new hardware was designed, built and installed to provide more space and enable better steering of the beam. After this change, beam power nearly doubled in the following four-month period.

The accelerator team's goal for the near term is to achieve one megawatt of beam power. Having achieved 870 megawatts by the scheduled maintenance shutdown in August, Henderson thinks that SNS has a good chance of passing that milestone before the end of the year, following the summer maintenance shutdown of the facility.

To achieve this jump in beam power—a jump equal to the previous world record—one of the tactics Henderson's group will use is to increase the length of the accelerator's pulse—or burst of particles—from 600 microseconds to the design level of 1000 microseconds. The result would send 40 percent more particles to the target with every pulse. If successful, the new strategy should push the SNS past the megawatt level, within sight of the 1.4 megawatt beam the facility was designed to produce.

As the SNS operates at increasingly high beam power, the accelerator complex must deliver reliable and stable beams for the user program. Henderson views the process as a balancing act. "We must deliver reliable beams for users while simultaneously exploring new ways to increase the beam power. When these two goals conflict, reliable operation takes precedence."

Since its inception, the SNS has been defined by long-term plans. With approximately one-half of the instruments in place in the target building, planning is already under way for both a power upgrade and a second target station that would double the facility's potential research output.

"For the power upgrade, we are proposing to double the SNS beam power," Henderson says. "The promise will be to deliver two megawatts of power. But we are designing a system that should be able to produce three. We hope to start the project next year."

The success of the SNS in achieving its power goals has been a research windfall for scientists, enabling them to run more experiments on a broader variety of materials, gather larger volumes of data and explore more physical and statistical detail than ever before. Henderson is emphatic about the scale of the effort required to make the achievement possible.

"A lot of people appear to view the SNS as a sort of microwave oven with three buttons, for low, medium and high neutrons," Henderson says. "They seem to think we can just set it to high and turn it on."

The reality is far different. Thus far, the SNS has succeeded, not simply because it is well-designed but because it is operated by about 250 highly trained engineers, physicists and technicians who constantly monitor and tune one of the world's most complex scientific instruments. Ⓡ

**As the SNS runs at increasingly higher beam power, scientists have encountered phenomena never before seen and not entirely understood.**

## A Losing Bet

The scientific vortex of the SNS is its target—the focal point where high-energy proton pulses collide with atoms of mercury, creating showers of neutrons. Once focused into a beam, the neutrons enable researchers to study the structure and internal dynamics of materials in unprecedented detail.

The SNS target, unlike its predecessors at other neutron facilities, is filled with a self-cooling flow of liquid mercury that is pumped through the target at high speed. The first-of-its-kind device was designed to remain cool in the face of extraordinary quantities of energy deposited by the proton pulses.

"The target is a unique and amazing thing," Henderson says. "Because the SNS target is so unusual, there were a lot of early concerns about whether such a novel experiment would work at all."

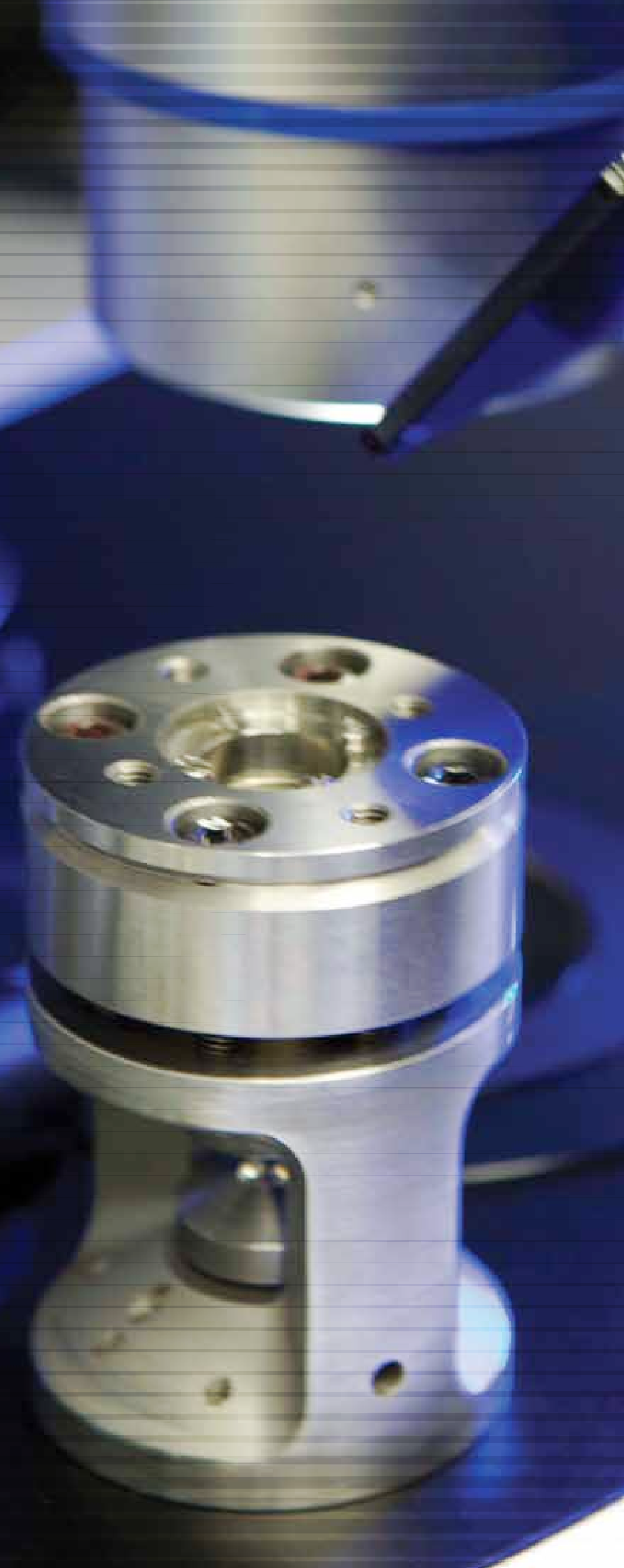
Targets made of solid metals, like tungsten and tantalum, would normally have been used for a pulsed neutron source. As the design of the SNS evolved, scientists became convinced that the energy of the intended beam was going to be so high that a solid target would have trouble dissipating heat quickly enough.

Despite extreme conditions of operation, the SNS mercury target has proved to be remarkably durable and is still in use. SNS staff started a pool in early 2007, predicting when the target would need to be replaced. The entire staff lost.

The target was replaced during the August 2009 maintenance shutdown. Using a remotely controlled system, researchers will cut the original target into sections to look for signs of degradation.

Henderson says the new target will be essentially the same as the original. "We may spray a proton-activated, light-emitting coating on the surface of the target that is struck by the beam. This coating will enable us to see exactly where the beam strikes the target and how the beam is shaped at that precise point."

Otherwise the "guts" of the target are exactly the same. Why mess with success?



# Cross Pollination

## *The SNS is attracting research beyond conventional physics.*

One of the Spallation Neutron Source's most far-reaching contributions is its ability to bridge research disciplines and to uncover new perspectives on inquiries conducted across the breadth of the scientific spectrum. The real value of the SNS extends beyond providing physicists with an unmatched ability to peer into the structure of materials. Of even greater consequence, the SNS enables scientists from fields as diverse as chemistry, biology and geology to investigate materials, tissues, and processes in ways that might never have been contemplated had the scope of research been limited to conventional physics.

"Many laboratory programs—whether fundamental science, applied science, or working with industry—rely on neutrons to gather data about the materials they use," says Michelle Buchanan, ORNL's Associate Laboratory Director for Physical Sciences. "At Oak Ridge, because we have historic ties with neutron science, a lot of people at the laboratory in a variety of fields are 'fluent' in neutrons."

Buchannan points to two Energy Frontier Research Centers (EFRCs) recently established at ORNL that will further strengthen the synergy between neutron science and these allied fields. "The SNS is pushing several areas of inquiry," Buchanan says. "One is the study of materials under extreme conditions, such as high radiation, strain and stress, temperature, and pressure. Another is investigating interfaces. Both of the EFRCs fall under these umbrellas, so the synergy among disciplines is there as well."

One of the EFRCs, the Center for Fluid Interface Reactions, Structures and Transport, brings together a multidisciplinary research team of laboratories and universities to concentrate on issues related to energy storage and related material properties. The center will have access to the neutron scattering capabilities

***The SNAP diffractometer enables researchers to study samples under conditions of extreme pressure and temperature.***

of the SNS to look at interfacial phenomena, such as how liquids interact with surfaces. Buchanan observes that, "While most people think of a fluid-solid interface as two distinct phases, there are actually incredibly rich chemical and physical processes going on between them."

Understanding how fluids and solid materials interface at a subatomic level will be critical to achieving breakthroughs in key energy technologies, such as improved batteries, solar panels and fuel cells. The new perspectives would also have implications for other energy-related research, such as carbon dioxide sequestration, catalysis and the development of corrosion-resistant materials.

"For example," Buchanan says, "scientists don't understand exactly what makes a battery fail. The liquid-solid interface in batteries is incredibly complex—and with every charge and discharge of a battery, the interface changes. By understanding the changes that happen at that interface, batteries could be designed to be safer and last longer."

ORNL's second EFRC, the Center for Defect Physics in Structural Materials, is also closely aligned with the SNS. This center will bring together researchers from ORNL, six universities and Lawrence Livermore National Laboratory to develop techniques for detecting and correcting microscopic defects in materials and thus develop new materials with unprecedented strength and durability.

A large portion of the center's research will use high-resolution instruments at the SNS to locate and characterize flaws in materials, to determine how they evolve into clusters of defects that eventually become cracks and ultimately lead to failure.

"Whether researchers are working with small solar cells or enormous reactor vessels," Buchanan says, "the goal is the ability to understand these defects and to control them. Knowing what causes a material to fail is critical to preventing future failures. In the case of nuclear reactor vessels, this knowledge can make the difference between vessels with a 30- or 40-year lifetime and vessels with a lifetime of 80 to 100 years."

In scientific terms, research synergy is not a one-way street. The same disciplines that benefit from the analytical abilities of the SNS also exert pressure on the facility to expand its capabilities, sometimes in unexpected directions. "As the SNS instruments are established," Buchanan says, "our scientists sometimes find that they need new capabilities to accommodate a broader range of research than was envisioned when the instruments were originally designed."

One illustration of this influence is a project in which materials science researchers are working with SNS staff to develop new optics that will enable the SNS to focus neutrons beams on smaller areas. This process will enable them to see minute battery components or biological samples in much greater detail than previously possible.

Similarly, polymer scientists are interested in developing experimental chambers that would enable the study of polymers that self-assemble to make unique structures. Buchanan believes understanding how such assembly occurs would be fascinating to scientists. "Because the neutron beam at the SNS is pulsed, instruments can provide time-lapse views of the interactions among these polymers. This would allow us to get a view of how self-assembly happens, rather than just seeing 'before and after' snapshots of the process."

Buchanan credits much of the interdisciplinary appeal of the SNS to the laboratory's concerted effort to reach across research programs and initiate collaboration with neutron scientists. As evidence of the success of this approach, Buchanan notes that one of the first papers published as a result of research conducted at the SNS was led by geochemists. "Now it's not unusual to see papers on neutron scattering authored by people who are not neutron experts."

While the wide applicability of the SNS as a research tool has been a revelation to some, the potential was apparent at the facility's inception. "I remember the first announcement of plans to build the SNS," Buchanan recalls. "Former ORNL Associate Director Bill Appleton surprised a number of people when he said the SNS would be a critical tool for chemistry." She recalls everyone knew the machine would be applicable to all sorts of applied and fundamental materials science research, but few considered the range of areas that would be supported by the SNS.

"Ten years ago, almost no one thought that chemists would be involved in neutron science. Now I am amazed by the things we can do with neutrons that give us insights into molecular interactions, dynamics and structure. In chemistry and a number of other fields, we are just beginning to see what may be possible."

Buchanan emphasizes that the key to the synergistic relationship between the SNS and research programs across the laboratory is communication and cooperation. "Our problems motivate the folks at the SNS to look for solutions," she says, "and in turn their innovations encourage us to use techniques that we would not have thought about otherwise. We're pushing each other, and the result is new approaches to research." Ⓡ

# Imitating Mother Nature

## *Researchers use two ORNL facilities to develop synthetic cell membranes.*

If imitation is the sincerest form of flattery, then Mother Nature may be blushing at researchers' efforts to emulate the molecular activity that occurs at cell membranes—the boundary between living cells and their environment. Utilizing the combined capabilities of the Spallation Neutron Source and the adjacent Center for Nanophase Materials Sciences, a team of scientists is building bio-inspired, biocompatible synthetic cell membranes to help them understand a range of interactions between synthetic materials and biomolecules.

"Our inspiration comes from Mother Nature," says researcher Brad Lokitz. "In the body and in nature, a number of biological processes occur at interfaces and membranes. We are trying to mimic nature in a very basic way to gain some insight into these processes."

In addition to Lokitz, the research effort includes John Ankner, Jamie Messman and Dean Myles of ORNL; Mike Kilbey and Jimmy Mays, who have joint appointments with ORNL and the University of Tennessee; and Juan Pablo Hinestrosa of Clemson University.

The team's bio-inspired membrane starts with a silicon base, to which polymers are attached more or less evenly across the silicon's surface. The polymer strands provide a framework, or scaffold, for the biomolecules and synthetic cell membrane that are added later.

"The design of the substrate is somewhat similar to a hairbrush," says Lokitz. "If you take a hairbrush and turn it over, the base of the brush would be the silicon substrate, and the bristles that extend out would be the polymer."

While the researchers needed several attempts before identifying a process that resulted in a polymer framework with a uniform thickness evenly distributed across the surface, the results were worth the effort. Lokitz says that in order to use neutrons to study the framework, the process had to be very uniform on the molecular level. "The rougher the surface, the less information can be extracted, so the surfaces must be as molecularly smooth as possible. Considerable time was required before we could consistently produce samples that were sufficiently smooth to take to the SNS and obtain good results."

Having recently perfected the process of creating the substrate and attaching the biomolecules, the team has begun experimenting with attaching a synthetic cell membrane to the substrate. "The membrane was created by team members working at the nanoscience center," says project leader John Ankner. "We developed a synthetic membrane composed of biocompatible synthetic polymers that has some of the physical and chemical properties of a cell membrane." Because the substrate is fairly soft, the attached synthetic cell membrane will be more flexible and more elastic than if attached to a hard surface. Also, by attaching biomolecules to the substrate before applying the membrane, Ankner's team can populate the membrane with structures, such as proteins, that are found in real cell membranes.

Proteins are a particular focus of the team's research because they play key roles in a variety of cellular functions, such as immune response, the operation of ion channels and reaction to toxins. By embedding biomolecules within the membrane, the researchers hope to be able to study the structure-function relationships of the various biomolecules—proteins, peptides, cholesterol—that form the cell's environment.

The team is using the SNS's Liquids Reflectometer to study each phase of this bio-inspired structure, including the polymer scaffold, the attached biomolecules and the synthetic cell membrane. One feature of the reflectometer is its ability to investigate the boundaries between hard and soft matter, an ideal capability for examining the bio-inspired surfaces with which Lokitz and his colleagues are working.

Lokitz notes that having the world's most powerful pulsed neutron source next door to one of America's most modern nanocenters provides a rare opportunity to perform synergistic nanoscience research at co-located, state-of-the-art facilities. "We have the ability to create our samples at the nanocenter, walk next door, and test them at a world-class facility. As we run our tests, the feedback is immediate. If we see that we need to do something differently, we can walk down the hall to the nanocenter, tweak our procedure, and then go back to the SNS and continue the testing."

**"If we see that we need to do something differently, we can walk down the hall to the nanocenter, tweak our procedure, and then go back to the SNS and continue the testing."**

Once a satisfactory scaffold is in place, researchers "functionalize" the process by starting a chemical reaction that allows the biomolecules to bind to the polymers. Researchers then examine the scaffold to understand three things: how the attached biomolecules affect the structure and organization of the polymer scaffold, how being attached to the scaffold affects the stability and structure of the biomolecules and whether the biomolecules can still perform their biological functions when attached to the scaffold.

The Liquids Reflectometer can characterize the thickness, density and orientation of polymers. The instrument is very sensitive to small changes in density or thickness, thus providing researchers with an opportunity to study minute variations in the scaffold, the attached biomolecules or the synthetic cell membrane. "The researcher can observe the surface with just the polymer attached and get an idea of the layer thickness and composition," Lokitz says. He adds that when the team functionalizes the layer by attaching the biomolecules, the instrument is sensitive enough to notice even minute changes.

Anker says the team has reached the point at which they can attempt to attach a synthetic cell membrane to the polymer scaffold. "We are taking the first steps in this process. The membrane analogues represent the holy grail in the neutron reflectivity business."

Ankner concedes that the process of attaching the membrane has proven to be tricky. "We're taking a small three-dimensional cell membrane and attempting to spread it out on a flat surface the size of a hockey puck. This goal has been pursued unsuccessfully in a variety of ways. This is our attempt. Our efforts are promising, so we are pushing ahead."

The near-term goal for the team is to assemble a synthetic cell membrane around various biomolecules that have already been attached to the substrate—thus avoiding the chemically problematic issue of inserting biomolecules into the membrane after it has been created.

"In a real cell," Ankner explains, "when proteins or peptides are created, the cellular components that create them inject them directly into the cell membrane one amino acid at a time. The proteins fold and form under the influence of this unique environment."

This process can't easily be duplicated in a laboratory, so researchers typically are forced to find chemical approaches to embedding biomolecules into synthetic membranes—with less than satisfactory results.

*The SNS Liquids Reflectometer is a unique tool used to study synthetic cell membranes and their attached biomolecules.*

"If we can attach them to the substrate and then assemble the membrane around them," Ankner says, "we avoid that whole problem. That's our ambition."

Understanding how cell membranes and other functional areas of cells work may enable researchers to develop bio-inspired systems that apply biological processes to specific tasks in materials and chemical sciences. Lokitz notes that "these functional areas are able to sense and respond to external stimuli; capture, store and convert energy; carry out chemical reactions; and transport a wide range of chemicals."

The ability to engineer and control these cellular features would open up a wide range of possibilities for developing next-generation materials, devices and processes, such as therapeutic agents, drug delivery systems and new methods of diagnosing disease. Ⓡ

*Foreign governments are investing in the SNS.*

# An International Affair

International collaborations have been a hallmark of ORNL since the early days of the laboratory's neutron research program. As the Spallation Neutron Source matures in scope and complexity, these scientific collaborations are more important than ever. As the world's foremost facility for the study of materials, the SNS will be a critical resource for the international neutron community. In return, ORNL will be the beneficiary of a vast wealth of expertise brought to the facility by thousands of visiting scientists.

"ORNL's philosophy opens our user program to international investigators and institutions on the same basis as it does to anyone else," says SNS scientist and administrator Ken Herwig. "That philosophy encourages researchers from every corner of the world to bring their most important scientific problems to the SNS. The result is a creative energy that maximizes our impact in the scientific community."

Herwig notes that because visiting researchers have worked at many different facilities, they bring a range of perspectives and techniques to the research process. "Both their perspectives and their experience enrich the scientific program at SNS," Herwig says.

Currently, barely three years into operation, the SNS has major collaborations with research institutions from Germany, Canada and Switzerland.

## ORNL's German Counterpart

The most extensive partnership to date has been with the German research center, Forschungszentrum Jülich. In many ways a German counterpart to ORNL, Jülich has a research portfolio that emphasizes energy, bioscience and high-performance computing.

A unique collaboration with ORNL has resulted in a major contribution by Jülich to the SNS instrument suite. Drawing on its considerable experience in the design and construction of neutron instrumentation, Jülich teamed with SNS to build the Neutron Spin Echo Spectrometer The instrument will be used to study "soft matter" systems. Researchers use the instrument to delve into a wide range of biological problems, such as how proteins that can encapsulate small molecules might be adapted for delivering drugs to specific targets within the body.

Herwig notes that Jülich not only funded the construction of the instrument but also its operation. "They are embedding their staff in our organization to run the instrument for the benefit of the ORNL user program," he says.

In return for this unique level of commitment to the SNS, Jülich receives 20 percent of the beam time on the Spin Echo, as well as beam time on two additional instruments. Herwig observes that a fifth of the beam time on any SNS instrument is "a sizeable resource." "Jülich also funds an instrument scientist on each of the other two instruments," he adds. "Their commitment to the SNS scientific program is very significant."

Herwig believes the project is a great long-term asset to the SNS. "The Germans brought 20 years of experience to a world-class instrument in a world-class facility that will be available to thousands of users for years to come."

## Canada's "Big" Investment

A second international instrument at the SNS is the VULCAN Engineering Diffractometer, funded by the Canadian Foundation for Innovation. CFI is an independent corporation created by the Canadian government to assist Canada's research institutions.

VULCAN enables users to take measurements of the positions of atoms in materials under conditions of stress that are of particular interest to researchers focused on engineering applications.

"One of VULCAN's unique assets is its sheer size," Herwig says. In contrast to instruments designed to take measurements from minute crystals, VULCAN enables researchers to place objects as large as an engine or a section of an aircraft's wing in the path of the beam.

"We call it an engineering diffractometer," Herwig notes, "because VULCAN is designed specifically to look at materials that are involved in engineering-related problems. Using this instrument, we can push, pull and twist materials while they are in the neutron beam. By subjecting the materials to the same stresses and strains they experience in real-world use, we can better understand how cracks form and spread."

Assisted by the world's most powerful computers, ORNL scientists use data from VULCAN to address a variety of problems associated with material degradation and failure in critical applications.

In return for providing funding to build the instrument, the CFI scientists, like their colleagues from Jülich, receive a share of VULCAN's beam time, as well as beam time on SEQUOIA, an instrument that specializes in studies of magnets and high-temperature superconductors.


## Swiss Magnetism

The Swiss have made two major contributions to the SNS research program. Both of these contributions were provided by the Paul Scherrer Institut, a research laboratory operated by the Swiss government.

The first of the two contributions came in the form of an enormous magnet designed to provide unique environmental conditions for sample analysis.

"We usually seek to control the environment around the sample to meet specialized conditions," Herwig says. "To address a number of scientific questions, we wanted to be able to apply a very strong magnetic field to the sample. The Swiss helped make this possible by funding the construction of a massive 16-Tesla magnet.

Several of the SNS instruments were designed to produce and use beams of polarized—or magnetically identical—neutrons. Polarized neutrons enable scientists to probe magnetic structure and fluctuations in materials.

Herwig explains that, "If all of the neutrons have the same initial polarization direction, we can get more information on magnetic interactions and structure than we could using an unpolarized neutron beam."

The new Swiss magnet is expected to be particularly useful in the study of superconductors and nanomaterials. To ensure that the field produced by the giant magnet does not interfere with neighboring instruments, the magnet is enclosed in a second set of magnetic coils that compensate, or "jam," the magnetic field produced by the primary coils. The Swiss magnet is the first compensated magnet of this field strength to be built for a neutron beam line.

Herwig says the other SNS collaboration with the Swiss is the development of key components of a new instrument called HYSPEC, scheduled to come on line in the next two years.

HYSPEC will be one of the SNS instruments designed to employ a polarized beam of neutrons. The Paul Scherrer Institut is producing a specialized optical component called a supermirror polarization analyzer that will enable researchers to determine whether neutrons change their polarization as they interact with a sample. Unlike other SNS instruments used to study magnetic materials, HYSPEC can also tightly focus the neutron beam, enabling the analysis of smaller samples. This unique capability would be particularly valuable for the study of crystalline materials, such as certain esoteric superconductors that are difficult to grow in large volumes.

Swiss scientists have been allocated beam time across the SNS instrument suite in return for the Paul Scherrer Institut's contributions to the SNS's research program.

## Demonstrating the Benefits

In fewer than three years, the enormous potential of the SNS to expand the boundaries of traditional materials science and extend the reach of neutron science to new fields of study has been demonstrated. The addition of the Neutron Spin Echo Spectrometer NSE, the Paul Scherrer Institut magnet and new optical components, and the recent completion of the VULCAN diffractometer together represent major contributions by the international scientific community to America's research agenda.

There is little question that the U.S. user community, as well as the scientific mission of the Department of Energy, have benefitted—in terms of both the instruments that are available and the quality and breadth of the research being conducted—from an unprecedented level of international involvement in the SNS research program.

As the SNS gradually fills the complement of instruments in the first target station and plans how the 25 additional beam lines in a proposed second target station will be allocated, Herwig expects to see a continued level of international cooperation.

"I expect the model of collaboration we have established to continue," he says. "Without a willingness to undertake this level of collaboration, these instruments and their wonderful capabilities would not be at the SNS. Put simply, our international partnerships extend the reach of our research program in ways we never could have imagined." Ⓡ

# Instruments of Change

## *A remarkable suite of instruments harnesses the power of the SNS.*

Despite its status as one of the world's largest scientific facilities, the true value of the Spallation Neutron Source is not defined by the scale of the buildings and equipment required to generate proton pulses with unprecedented power. For those conducting research at the SNS, a suite of specialized instruments is the secret to providing scientists a unique breadth of opportunity to expand their understanding of the structure and functioning of materials, under a range of real-world conditions. Ken Herwig notes that the long-term development plan for the SNS dictates that the facility seems to always be in the process of adding instruments, some of which are larger than entire buildings that housed earlier generations of equipment.

"We have instruments that have been in the user program several years," Herwig says." We also have instruments that have recently been added to the program, some that are being commissioned, and instruments that are planned or under construction but will not be in the program for another four or five years."

The SNS target station has a total of 19 instruments in various stages of development on the 24 available beamlines. Tentative plans exist for some of the remaining slots, with preliminary concepts for the 25 additional beamlines at the facility's proposed second target station.

### The original three

Three instruments, the Backscattering Silicon Spectrometer (BaSIS) and two reflectometers, were completed as a part of the original SNS construction.

The BaSiS instrument is designed to examine how materials move at the atomic scale over a relatively long range of times—picoseconds to nanoseconds. The instrument also can analyze liquid and solid samples.

One of the most ubiquitous, and most studied, materials on the earth is water. Accordingly, more than half of the publications generated by BaSiS are devoted to the study of water. Much of the recent scientific interest centers around how water behaves when present in much more limited quantities. The very thin layers of water that cover the surface of hydrophilic materials under ambient conditions are one example. Water in these systems may be one or a few molecules thick. The presence of water exerts great influence on the surface properties of the materials. Recent results include the observation of multiple processes occurring in individual water layers.

Across the experimental hall, the Magnetism Reflectometer is used to investigate the surface layers of materials and has the unique capability of studying magnetism in very thin films or multilayers.

The research has applications in the development of materials used for data storage devices, like DVDs and camera memory cards and computer disk drives.

"One buzzword these days is 'spintronics'," Herwig says, "using the spin state of a material's electrons to store or transfer information. With a layered material, the instrument is able to probe the magnetic coupling from one layer to another and determine how well the material might function."

The SNS's third original instrument is the Liquids Reflectometer, designed to look at horizontal surfaces for studies ranging from polymer interfaces to synthetic cell-membranes to liquid surfaces. Researchers have employed the Liquid Reflectometer to help develop a thin polymer film that behaves differently depending upon the acidity, or pH, of its environment.

"If researchers can make a pH-sensitive thin film and wrap the film in a drug, they can control where the drug is released in the body," Herwig says. "The researchers created a layered sample with markers that were visible to neutrons between the layers. Then, as the pH of the sample's environment became more acidic, they could observe the film dissolving layer by layer."

## The next generation

Since the SNS came on line in 2006, instruments have been added at a rate of about two each year. The Wide Angular-Range Chopper spectrometer was designed to explore the movement of energy waves, called phonons, through hard materials.

The spectrometer's most distinctive capability is measuring phonons moving through powders as well as through single crystals. The process has applications in the analysis of superconducting materials, like the recently discovered iron arsenide family of superconductors. Researchers hope to understand how the behavior of phonons changes as a function of temperature and to determine whether phonons play a role in the superconductivity of these materials.

As a complement to this research, the Spallation Neutrons and Pressure diffractometer (SNAP) enables SNS researchers to study a variety of powdered and single-crystal samples under extreme conditions of pressure and temperature. The increased neutron flux of the SNS, combined with SNAP's ability to generate extreme pressure using specialized sample environment equipment, has broadened the pressure range accessible to neutron researchers.

An ambitious goal for SNAP is to reach 100 GPa, a pressure approaching that of the earth's core-mantle boundary. To obtain this extraordinary pressure, sample volumes must be very small, requiring the neutron beam to be concentrated to a similarly small area. To accommodate the small sample, ORNL researchers have designed a mirror that can focus the beam to the exceptionally small width of about 75 microns.

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*The cavernous SNS experimental hall houses an expanding array of analytical instruments. The Powder Diffractometer, located on beamline 11A, is seen in the foreground.*

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"At 100 GPa," Herwig says, "SNAP will reveal phase transitions in materials under high pressure and temperature, particularly the structure of minerals deep within the Earth."

Other state-of-the-art instruments are in the queue. The Powder Diffractometer, or POWGEN, will come online in 2009 and is expected to be the SNS's workhorse in a wide range of structural studies.

POWGEN will enable researchers to predict how materials will undergo structural transitions as they respond to temperature, pressure and magnetic fields. Understanding these changes in the presence of gases is especially important for the study of catalysts and hydrogen storage materials.

Herwig expects POWGEN to be particularly popular for studies of energy-related materials such as cathodes and anodes in batteries and solid oxide membranes for fuel cell applications.

A second instrument scheduled to come on line in 2009 is TOPAZ, a single-crystal diffractometer. Herwig says the instrument can generate substantially more information from analyzing a single crystal of a material than currently can be produced from a powdered sample. The advantage comes from the researcher's ability with a single crystal—unlike a powder—to know how the material is aligned in the neutron beam when taking a measurement. TOPAZ holds promise for a number of potential applications, including analyzing the structure of  small- to medium-sized molecules with pharmaceutical appliocations. One of this instrument's particular skills is finding a material's hydrogen atoms. This unique characteristic is often critical when researchers are required to locate molecular binding sites or to distinguish one molecule from another.

## Producing the science

As intended, the remarkable array of instruments available to scientists at the SNS is channeling the raw power of the facility's neutron flux into the specialized applications needed to illuminate new frontiers in the fields of materials and biological science. The instruments support research that falls into two categories. One is curiosity-driven, without immediate direct application but vital to the creative energy of the scientific process. The other equally important research category is often use-inspired and focused on specific issues such as energy production or storage.

The instruments are producing huge streams of data that in turn have resulted in hundreds of scientific papers. While the majority of these papers are still in the peer review process, they hold the promise of opening new horizons throughout the field of materials research. The expectations for the SNS are high, befitting one of the Department of Energy's largest and most modern scientific facilities.

The self-imposed expectations are equally high for the SNS staff. They are aware of their role at a unique moment in history, asked to attack some of humankind's most critical scientific challenges and equipped with the most advanced instruments available to the scientific community. Thus far, they appear willing and able to meet the challenge. Ⓡ

Technicians replace a sample in the Wide-Angular Range Chopper Spectrometer.

# Unconventional Understanding

## *High-temperature superconductors could revolutionize the use of electricity.*

Superconducting materials, compounds that conduct electricity without resistance, were discovered almost a century ago and are today used in applications ranging from medical equipment to power cables. Scientists are still unsure exactly how the most useful examples of these high-temperature superconductors work. If they can ferret out the details of high-temperature superconductivity, the thinking goes, they should be able to design new kinds of superconducting materials. Since superconductivity could provide major gains in energy efficiency, being able to tailor the new materials for ease of use could be a game-changing technological achievement.

If perfected, high-temperature superconductors could revolutionize the generation, storage, distribution and use of electricity. Currently, a substantial part of all electricity generated is lost to resistance, either in the power grid before getting to users or in the powering of machinery. The potential energy savings from generators, transformers, power cables and motors equipped with superconducting components would make a substantial contribution to addressing America's energy challenge.

The instruments at the Spallation Neutron Source provide a powerful boost to superconductivity research. Their value resides in the capability to reveal the precise position and motions of the atoms inside materials, as well as the magnetic moments associated with these atoms. The Wide-Angular Range Chopper Spectrometer (ARCS) is especially valuable for investigating exotic compounds such as superconductors because SNS's high neutron flux enables the use of small samples, says ORNL researcher Andy Christianson, one of several scientists using ARCS to probe iron-based superconductors. The instrument's huge bank of more than 900 detectors enables coverage of a huge range of neutron scattering angles, from –25° to 133° horizontally and from –28° to 27° vertically. Christianson characterizes the ARCS as providing "a broad view of a wide range of momentum and energy transfer for the excitation spectrum."

Christianson, Mark Lumsden and Takeshi Egami are members of a team that recently used ARCS to obtain the first-ever neutron scattering measurements of magnetic excitations in single crystals of an iron-based superconductor. The ARCS data showed a large spike in magnetic excitations, or spin fluctuations, in a sample of barium-iron-cobalt-arsenic (FBCA) just as the temperature reached 22K and the material became superconducting.

The ARCS results advance the understanding of "unconventional" superconductivity, the type researchers consider to have the most technological potential. In "conventional" superconductors discovered in 1911, vibrations within the atomic lattices of materials compel electrons to form pairs that move through the lattice without resistance. The materials typically acquire superconductivity only at temperatures close to absolute zero, thus limiting their potential uses. In the 1980s, physicists discovered superconductivity in copper oxide alloys, or cuprates, which lose their resistance to electricity at more easily attainable temperatures as high as 138 K. Two decades of research suggest that something other than lattice vibrations causes superconductivity in cuprates, leading to their label as "unconventional superconductors." New revelations emerged in 2008 when Japanese scientists announced the observation of unconventional superconductivity in a class of iron compounds.

The ARCS findings, along with follow-on data from other scattering experiments

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by Christianson, Lumsden and their colleagues, bolster the opinion of many researchers that spin fluctuations play an important role in unconventional superconductivity. The neutron scattering results provide additional evidence that magnetic excitations are key to superconducting behavior in both cuprates and iron-based superconductors.

Christianson says the precise role of magnetism in superconductivity has been an interesting question. "We don't think lattice vibrations by themselves are sufficient to explain electron pairing. Some other mechanism must also be involved. An obvious question is how much magnetism is influencing superconductivity."

"It's a wonderful coincidence that this compound came along just as SNS was available to study it."

The FBCA sample used in the experiment, synthesized in Oak Ridge, comprised three single crystals, each about 7 mm long and 1 mm thick. Because the material is so difficult to synthesize, three crystals were required to form a sample large enough for inelastic neutron scattering investigation, about 1.8 grams. Without the high neutron intensity available at SNS, such a tiny sample could not have been measured. For the experiments, researchers placed the crystals inside a sample canister that could be cooled with liquid helium to within a few degrees of absolute zero.

To produce the sample, a parent compound, barium-iron-arsenic, was doped with cobalt. At low temperatures, the parent compound has long-range or static magnetic order, that is, a regular pattern of spins throughout a sample. When the parent compound is doped with cobalt, the static magnetic order disappears. The change appears to occur when the cobalt "squeezes" the atomic lattice, causing the spins of the electrons to fluctuate. The same sort of effect is produced by applying pressure on the parent compound.

Superconductivity and long-range magnetic order appear to be mutually exclusive—as one appears, the other subsides. Thus doping, by destroying the magnetic order, opens the way for superconductivity to surface when the FBCA sample falls to the critical temperature of 22 K.

Christianson believes the precise relationship between static magnetic order and superconductivity remains an open question. "One explanation could be competing interactions. When pressure is applied,one is tuned over the other, enhancing the reactions that give rise to superconductivity." He concedes that researchers do not yet know if destroying the long-range magnetic order makes superconductivity happen or enables it to happen.

The magnetic interactions involving superconducting FBCA are two-dimensional, taking place only within each plane, unlike electrons in the parent compound that interact both within and between planes. Two-dimensionality is also observed in the cuprates. The energy of the magnetic excitation measured with ARCS, 8.6 meV, is related to the superconducting transition temperature in a similar way as observed in the cuprates, providing further evidence that the physics underlying superconductivity in the two classes of materials is related.

Theorists will now try to calculate what the experiments have measured, and the ARCS results will allow them to build more reliable models, Christianson notes. "Any theory proposing that spin excitations are the mechanism behind superconductivity must, at a minimum, get the spin excitations right. Theorists have not fully characterized the excitations, but we now know about them in a limited but substantial way.

As researchers pore over the ARCS data, their interpretations may lead in different theoretical directions. Egami notes that for unconventional superconductivity, "there are as many theories as there are physicists. Everyone involved knows the research on iron-based superconductors is tremendously significant because it involves not just superconductivity but also the beginning of 21st century physics, which deals with many-body physics and electron correlations," he adds. "The field resembles quantum mechanics at the beginning of the 20th century."

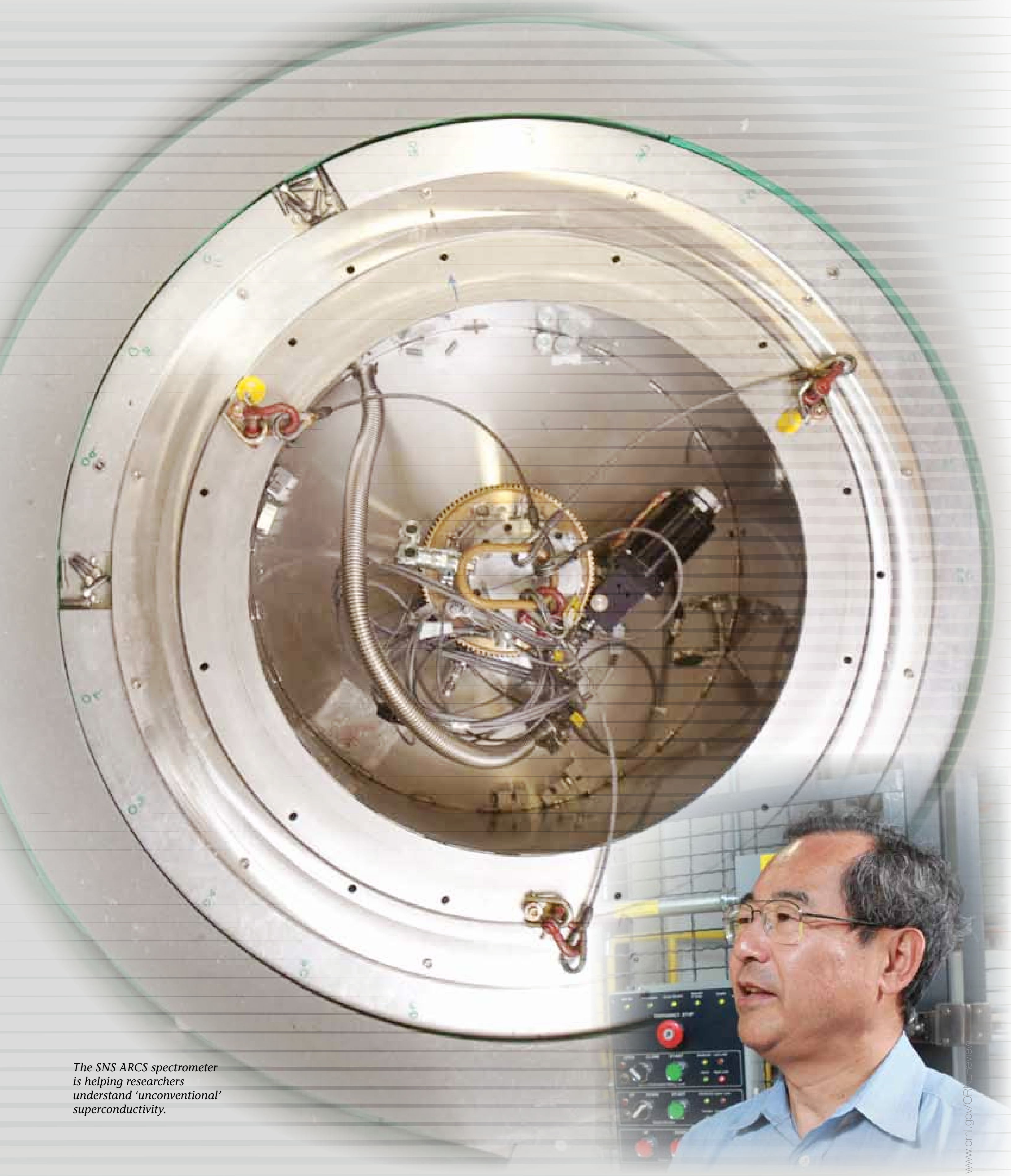
Egami's take from the ARCS results is that just as lattice vibrations are not sufficient to explain unconventional superconductivity, neither are spin fluctuations. "I think both spins and phonon vibrations are involved," he says. "There is an inherent coupling between spin and lattice. Change the lattice and the spin disappears. That effect in this system is profound."

A key advantage of studying the iron-based compounds is that they provide a simpler model for unconventional superconductivity than the cuprates, Christianson says. "We hope that by observing superconductivity in a simpler model we may gain greater understanding."

The hope is that in time researchers will understand the superconductivity mechanism in the iron-based materials, an understanding that will translate back to the cuprates. The goal is the ability to design superconducting materials that operate at higher temperatures.

Egami says the ARCS results lead to the hypothesis that the same mechanism causes superconductivity in both the cuprates and the iron-based materials. "That simplifies the search for the mechanism—we're not chasing dozens of different possibilities. There are signs everywhere, but no one has yet put them all together. The progress using the iron-based compounds is much faster than with the cuprates—probably 10 times faster.

"It's a wonderful coincidence that this compound came along just as SNS was available to study it," Egami notes. "Everyone thought it was impossible for iron to be superconducting. Now that superconductivity has been found in iron compounds, it could be in anything." Ⓡ



The SNS ARCS spectrometer is helping researchers understand 'unconventional' superconductivity.

# Doubling Down

***Plans are under way to double the capacity of the Spallation Neutron Source.***

*The second SNS target station will double the facility's potential research output.*

Although installation of the instruments for the massive target building at ORNL's Spallation Neutron Source has barely reached the half-way point, the promise of discovery is such that managers of the world's most powerful neutron source, while still in its operational infancy, are already planning to double the facility's research capabilities.

Three years after the Spallation Neutron Source produced its first neutrons, the instrument hall in the vast target building remains filled with hard-hatted workers and construction equipment, as the suite of state-of-the-art instruments takes shape. The count of operating instruments, some larger than a suburban home, is currently 13 of an ultimate 25. Beamline power, which has already blown past the previous world record, is approaching one megawatt, with an eventual peak of 1.4 megawatts.

With the installation of the instruments in the SNS target building only about half complete, some wonder if it is premature to accelerate plans for the construction of a second target station and power upgrade. The extraordinary complexity of the project, combined with the high demand for neutron analysis beam time, required that planning for a second SNS target begin almost immediately after the first target began producing neutrons in the spring of 2006.

The Department of Energy officially endorsed the need for a second SNS target in early 2009 by granting the project "Critical Decision Zero" status. At an estimated cost of $1 billion, the second target station will concentrate on nanoscale and biological sciences with an emphasis on novel materials for energy production, storage and use.

Kent Crawford, who led the scientific instrumentation portion of the SNS construction, heads the planning for the second target station. Crawford says the second target station will be very different from the first, designed to serve a burgeoning demand for advanced materials research.

"We have three types of moderators on the existing target station. The two that are dedicated to cold neutrons are pretty much completely subscribed. Cold neutron beams are very popular with researchers and seem to be the direction in which much of future science is headed," Crawford says.

Cold neutrons, literally chilled to nearly absolute zero with liquid hydrogen, have longer wavelengths that make them ideal for probing slower excitations and material structures at longer distances. Both of those factors come into play for more complex materials, from assemblies of nanoparticles to biological systems.

"For the SNS, the ability to examine soft materials and self-assembling nanomaterials is going to be a strong asset for the foreseeable future," Crawford says.

The first target station's capacity to produce very short neutron pulses makes the SNS ideally suited for studies of so-called "fast neutrons" in the thermal range and "time-of-flight" measurement, which is the length of time required for the neutron to go from the source to the neutron detector. Time of flight is a very important parameter in understanding a material's structure.

"A pulsed source is ready-made for time-of-flight measurements. The first target station is optimized for providing high resolution in the timing, but less so for producing high intensities of cold neutrons. The second target station will broaden our capabilities by being optimized for cold neutrons," Crawford says.

The thrust toward cold neutron research means that the second target will differ from its predecessor in several important ways. As envisioned, the second target will be exclusively a cold-neutron facility optimized to produce maximum intensity, which Crawford estimates will enable researchers to improve by as much as tenfold their ability to perform certain classes of research. The first target would remain optimized for different experiments.

Perhaps even more significant, the process of spalling neutrons in the second target would bypass the accumulator ring. The current target receives neutrons at the rate of 60 pulses per second from the accumulator ring, at a pulse length of 700 nanoseconds. If the beam is not channeled through the ring, however, the pulses are lengthened to about a millisecond in length.

As currently planned, one pulse in three will be tapped from the accelerator and sent in long-pulse mode directly to the second target at a rate of 20 pulses per second. The technique would avoid sending protons through the SNS's accumulator ring, which is already operating at world-record levels. The other two short-mode pulses would travel, as they do currently, through the accumulator ring to the first target station.

"Not going through the accumulator ring has two advantages," Crawford says. "Running in the long-pulse mode generates more power per pulse, which enables us to optimize our instruments to that higher power. The second advantage involves risk. The ring is probably the SNS's most complicated system and is being pushed to its limits by the performance we are asking. Not running protons through the ring results in less technical risk."

Bypassing the accumulator ring offers another significant bonus. When the ring is off-line for scheduled maintenance, the second target will still be capable of operation, thus expanding its accessibility to researchers and enhancing the facility's efficiency.

Also being planned in parallel with the second target is another upgrade, a boost in linear accelerator energy from 1 GeV to 1.3 GeV. In anticipation of the need for future upgrades, SNS designers built the linac with the space needed to expand beamline power up to 3 megawatts. The power upgrade, which will further extend opportunities for instrument optimization, will help ensure that the SNS remains the world's foremost neutron scattering facility for decades to come.

One of the key remaining decisions is the composition of the second target. Designers could eventually settle on a second version of the SNS's unique mercury target, the first of its kind. The SNS designers chose mercury for the original target, partly because the element is rich in neutrons and its liquid state allows it to be circulated and cooled. Planners are also considering a target made of tungsten. A little more than a meter in diameter, the tungsten target would rotate at about 30 rpm, slightly slower than an LP record. The rotating solid target would thus distribute heat and radiation damage from the beam.

One potential advantage of the tungsten target would be a projected 10-year service life. The current mercury target must be changed more frequently, although the three-year performance of SNS's original mercury target was considerably longer than many expected.

Although the idea of a tungsten target is not new, Crawford says the use of a rotating tungsten target would, like the use of a mercury target, be the first of its kind. Major design decisions, including the target selection, could come in the fall of 2009.

A precedent exists for twin-target neutron sources. The United Kingdom's ISIS facility has two short-pulse targets, although the power is much lower and the moderators are different. The SNS would be the first long-pulse target, offering researchers a unique analytical tool. If constructed, the proposed European Spallation Source would be a long-pulse system comparable to the SNS's second target.

Researchers already are gathering to plan instrumentation geared to the long-pulse, cold neutrons the second target will produce. Crawford emphasizes that the experience of designing the SNS taught the value of a long lead time for planning. The $1.4 billion construction project that was finished in 2006 began with planning that started in 1995. "We started developing the second target idea immediately after construction was complete. We currently are looking at a potential completion date of 2019," Crawford says. With that kind of long-range vision, the ORNL team seems intent on maintaining their position among the world's leaders in materials research. R

*The first-of-its-kind SNS target is filled with circulating liquid mercury to remove heat generated by the tremendous energy deposited by the proton beam.*

## You have decades of research experience across Europe and the U.S.

# What brought you to the SNS?

I've always had sort of a 7-year, 10-year itch, so the longest I've stayed anywhere has been 10 years. When the SNS project began, I had been working for about 10 years at the Institut Laue-Langevin in France—which at the time was the most powerful neutron source in the world. I was looking for something new to do, and the SNS was the next challenge. It was the most exciting project around, and it was going to expand the boundaries of what could be done in the field. So it looked like the right place to come for an exciting opportunity.

**In general terms, what research capabilities does the SNS provide that its predecessors cannot?**

The SNS is still the most exciting act in town. We're 5 to 10 times more powerful than any other pulsed neutron source—even when we're not operating at full power. Basically the biggest advantage the SNS has is the sheer intensity of neutrons compared with other sources. This allows us to do things that can't be done elsewhere. We can make more difficult measurements and analyze smaller samples than was possible before.

For instance, in the field of biology, neutrons are very good at locating hydrogen in protein crystals. Hydrogen is important because it is usually active in making proteins functional. In the past, the problem was that we couldn't get protein crystals that were big enough to make the measurements in a reasonable amount of time. However, as a result of its high neutron flux, the SNS can make measurements that would have taken six months to a year anywhere else in a couple weeks or a few days. So it's going to enable structures to be measured that couldn't be measured before.

**Could you describe a few of the facility's major accomplishments?**

In operations, our major accomplishment is that we have managed to ramp up to close to the 1MW power level—we expect to be at that level in just a few weeks. We've done this with a machine that is new technology and with a novel target design. Also, the choice of using superconducting technology has proven its worth. It has been a major accomplishment to get the machine to this level in the amount of time we said we would.

Of course now that we have delivered the machine, we are focusing on the science program and the important new results that are being obtained. Some exciting new results have already been obtained on a new class of iron arsenide superconducting materials. The work done at the SNS advances our understanding of so called 'unconventional' superconductivity and is helping theorists get a handle on the basic mechanisms that give rise to superconductivity. A lot of work has also been done on polymers and drug release systems, self-healing polymers, and biopolymers that mimic biological membranes.

We have also done interesting work with layered magnetic films that may have applications in the areas of computers and electronic components, in collaboration with ORNL's Center for Nanophase Materials Sciences.

**What scientific disciplines do you feel will be most profoundly impacted by the SNS?**

One of the areas we will affect the most is biology, because we have such a high intensity of neutrons that we'll be able to measure the structure of protein crystals and biological membranes and understand their functions much better than we were able to before.

Another area in which the SNS will be influential is the study of materials under extreme conditions. One of the advantages of neutrons is that they penetrate materials very easily, so we can look at something we want to study in an extreme environment—under extreme pressures or temperatures. Neutrons can penetrate the test chamber and determine how materials are functioning under those conditions.

Materials are often expected to function under severe conditions that test their limits, so we need to be able to understand how their properties are affected as we push them

# Ian An

harder. This is where SNS comes in with a "tour de force" suite of instruments that is capable of looking at all sorts of materials under real operating conditions. We expect that this capability will revolutionize the materials world. This is an area that we're very good at.

Also we'll have a major impact on nanoscience. Our relationship with the Center for Nanophase Materials Sciences is very important in this area. Neutrons are particularly useful in studying issues at the nanoscale, including those related to biomaterials and the interfaces between materials and nanoparticles that cannot be "seen" by any other technique. In particular the range of instruments available at SNS will enable researchers to study the assembly of nanoparticles into hierarchical structures whose properties can be tailored to perform specific functions. We are already combining the strengths of SNS and CNMS to study biomimetic materials and new polymers with targeted functions.

**I understand you're planning to climb Mount Kilimanjaro. Do you see any similarities between this challenge and that of the construction and operation of the SNS?**

Yes, I look at the ramp-up of power at the SNS—getting it to its full capabilities—as being very much like climbing a mountain. It's a very interesting challenge. I can imagine that the success you feel when you get to the top of Kilimanjaro is similar to what we will feel when we've got SNS at its peak and running at its full capability. Ⓡ

# derson

# Heal Thyself

## *Researchers develop 'self-healing' polymers at the nanoscale.*

Imagine a hip replacement covered with a nanometers-thin biocompatible layer on its outer surface, where it contacts the body, while the rest of it is designed with the strength to cope with any stress the body might deliver.

One could also imagine a multi-layered coating for a doorknob. The outer layer is designed to be microbially resistant, while the remaining layer contains properties that adhere to the doorknob. When an individual with a cold touches the doorknob, the anti-microbial agents immediately kill the bacteria before they can spread. Meanwhile, the adhesive properties keep the coating in place.

A collaboration of polymer scientists at ORNL is using the Liquids Reflectometer at the Spallation Neutron Source to study the dynamics of polymer mixtures. The mixtures comprise repeating large molecules connected by covalent chemical bonds that hold promise for applications as diverse as biocompatible films for human implants; semiconductors; substrates for electronic displays; children's toys; and durable, self-repairing aircraft body materials.

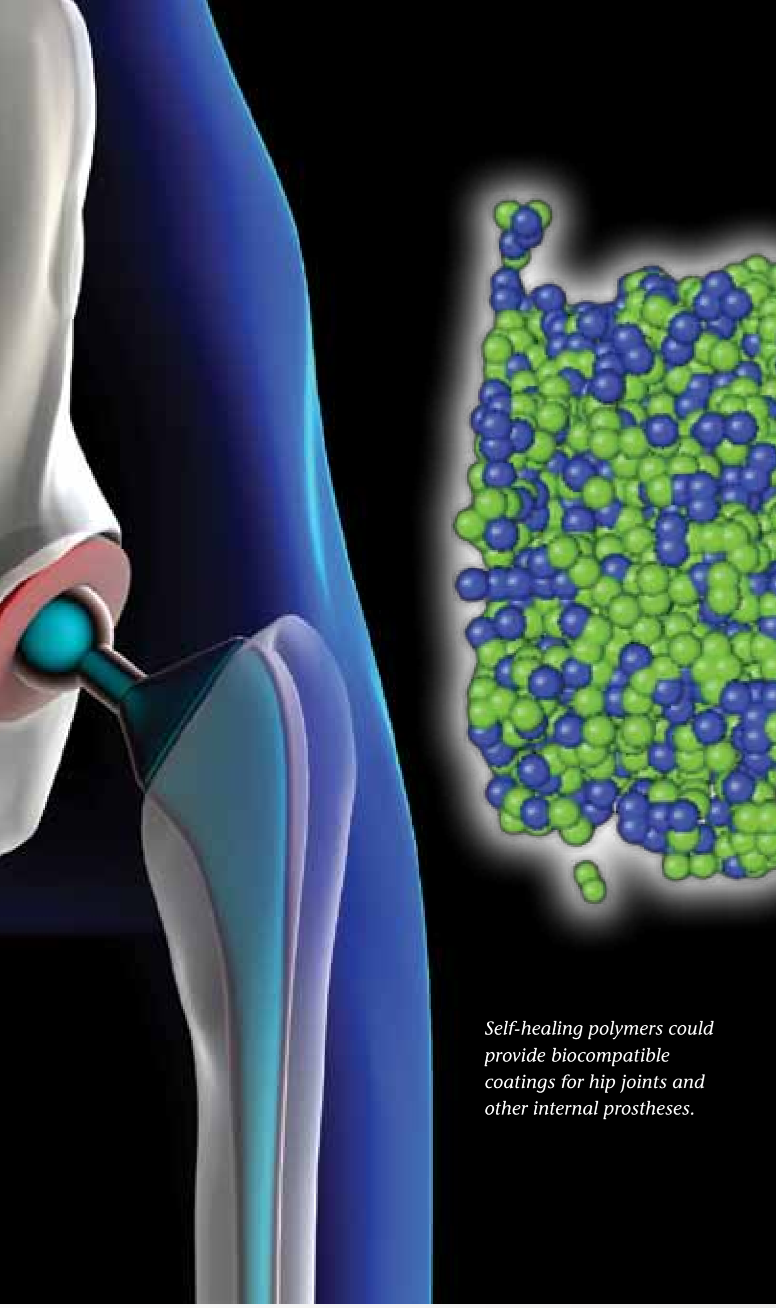
Polymers in nature include cellulose, the main constituent of wood and paper. Familiar synthetic polymers include nylon, Teflon and silicone. Mark Dadmun, professor of chemistry at the University of Tennessee and a Joint Faculty appointee in the Chemical Sciences Division at ORNL is exploring what he calls "self-healing materials"—polymer mixtures in which one critical component moves quickly to the surface while the matrix (the understructure) gives structural rigidity. Specifically, Dadmun is looking at the dynamics of a copolymer (the targeted, surface material) in a matrix (the homopolymer, the bulk of the material). "We design our process so that the copolymer comes to and saturates the surface. We retain a portion in the matrix so that if we lose it at the surface, we simply force the copolymer to the surface again."

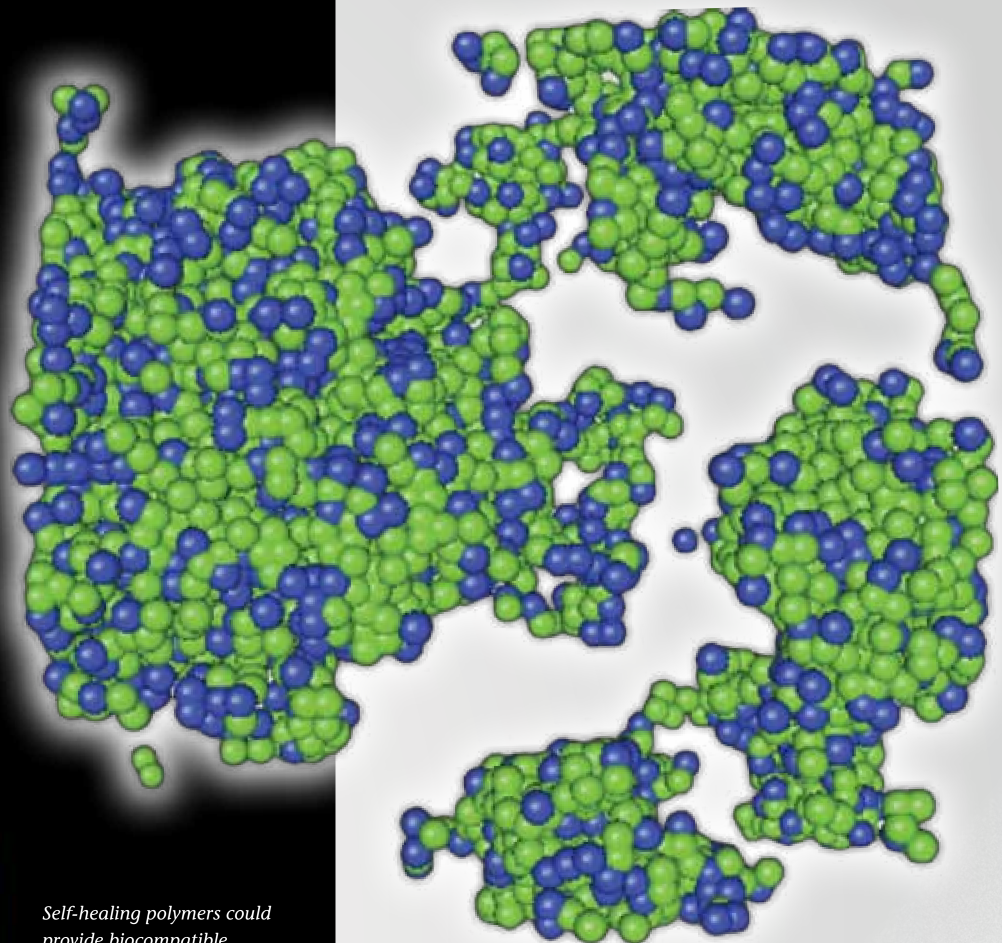
Dadmun works with instrument scientist John Ankner at SNS and materials scientist Joe Pickel at the Center for Nanophase Materials Sciences, as well as UT & ORNL Distinguished Scientist Jimmy Mays. Pickel and Mays synthesized the polymer samples. In the self-healing materials, they target the key properties of biocompatibility, microbial resistance, adhesion and flammability.

"Our goal is to design a system in which the majority of the component has the stability we need and the strength to be a suitable matrix," Dadmun says. "We have a separate polymer designed to bloom to the surface, with the potential to provide the surface-sensitive property we need. Because we started with a mixture and forced it to the surface, if the polymer is washed off a reservoir of material would continue to rise to the surface."

Dadmun stresses that finding a copolymer that migrates to the surface is not difficult. More difficult is finding one that gets there fast enough, a process that involves the material's thermodynamics. What the researchers seek to learn is how the specific structure of the copolymer affects the speed with which it migrates to the surface.

The researchers began the experiment with a silicon wafer. They coated the wafer with a thin film, a mixture of deuterated polymethyl methacrylate as the matrix polymer, and a branched copolymer of methyl methacrylate and ethylene oxide. As they





*Self-healing polymers could provide biocompatible coatings for hip joints and other internal prostheses.*

heated this sample, allowing the mixture to approach thermal equilibrium, the graft copolymer containing ethylene oxide diffused to the surface. The process enabled the measurement of the water contact angle to verify that the copolymer segregated to the surface.

"We could determine the presence of additional ethylene oxide from the copolymer in the mixture at the surface," Dadmun says. "Our ultimate goal is to use the liquids reflectometer to extract information on how quickly it gets to the surface."

Neutrons are ideally suited to study the copolymer's dynamics because, Dadmun says, "with neutrons we are able to label the material selectively." In Dadmun's samples the matrix is deuterated polymethyl methacrylate and the copolymer is an undeuterated polymethyl methacrylate, grafted to undeuterated ethylene oxide. The various neutron scattering properties of the deuterated and undeuterated materials enable researchers to observe the location and movement of the copolymer in the composite material as a function of the "annealing time," or the heating and slow cooling.

As it is heated, the copolymer tends to migrate to the surface. The experimenters observe the time dependence of the intensity of neutrons scattered from the copolymer near the surface, which can be analyzed to provide detailed dynamics of the copolymer diffusion process. "We thus can analyze the data to determine the diffusion coefficients, as well as other precise dynamic information about the surface segregation process, including the volume and speed."

Dadmun knows from previous experiments that the polymer chain is actually collapsing. "The polymer is changing its conformation away from conventional behavior in the homopolymer because of the repulsive interaction between the polymers. The changes cascade from repulsive interaction, to conformation, to dynamics, which ultimately changes the properties. The cascading effect enables us to correlate the structure and thermodynamics of the copolymer to its dynamics," he says.

"If you think of a polymer chain with long arms, those long arms make it very difficult to move. But because of this odd repulsive interaction they might actually be retracted, and, therefore, may be moving faster. We do not yet have clear evidence of this phenomenon, but this is one of the things our team is trying to determine."

Dadmun is cautious about predicting the future for these polymers. "All of the applications may not be commercially viable, because ultimately it may take too long for the polymers to get to the surface. If the process does prove viable, however, the result will be a wide range of applications. That, after all, is why we do the research." Ⓡ

# ...and the WINNERS are...

## Accomplishments of Distinction at Oak Ridge National Laboratory

Researchers and engineers at ORNL have won eight coveted **R&D 100 Awards**, presented each year by *R&D Magazine* in recognition of the year's most significant technological innovations. The competition for the awards includes national laboratories, universities and private industry.

With its total number of awards at 148, ORNL has won more R&D awards than any other DOE laboratory.

ORNL researchers received recognition in 2008 for the following inventions:

***Alumina-forming austenitic stainless steels*** - invented and submitted by a team led by **Michael Brady** of ORNL's Material Science and Technology Division.

***Artificial Retina*** - submitted jointly by **Oak Ridge National Laboratory**, Argonne National Laboratory, Lawrence Livermore National Laboratory, Los Alamos National Laboratory, Sandia National Laboratories, University of Southern California, California Institute of Technology, North Carolina State University, the University of California at Santa Cruz and Second Sight® Medical Products.

***Fire-resistant phase change material*** - developed and submitted jointly by **Jan Kosny** of the Energy and Transportation Science Division at ORNL, Tim Riazzi of Microtek Laboratories and Doug Leurthold of Advanced Fiber Technology.

***Mass-Independent Kinetic-Energy-Reducing Inlet System for Mass Spectrometers*** - developed and submitted by **Peter Reilly** of ORNL's Chemical Sciences Division.

***Methodology for Estimating the Life of Power Line Conductor-Connector Systems Operating at High Temperatures*** - invented by **Jy-An John Wang** of ORNL's Materials Science and Technology Division, **Edgar Lara-Curzio** of the Materials Science and Technology Division, **Thomas King Jr.** of the Energy Efficiency and Electricity Technologies Program and submitted by John Chan of the Electric Power Research Institute, Joe Graziano of the Tennessee Valley Authority and Tip Goodwin III of PBSJ Corporation.

***PulseForge 3100*** - submitted jointly by Stan Farnsworth of NovaCentrix and a team led by **Chad Duty** of ORNL's Materials Science and Technology Division.

***Superconducting "Wires" by Epitaxial Growth on SSIFFS (Structural, Single-Crystal, Faceted, Fibers)*** - invented and submitted by **Amit Goyal** of ORNL's Materials Science and Technology Division.

***Thermomagnetic processing technology*** - developed and submitted jointly by **Gerard Ludtka** of ORNL's Materials Science and Technology Division, Aquil Ahmed of Eaton, Aashish Chourey of American Magnetics and Ronald Akers of Ajax TOCCO Magnethermic.

**Gary A. Baker** has received the **Young Independent Scientist Award** and the **Presidential Early Career Award** from the U.S. Department of Energy.

**Jeff Bielicki, Brian Egle, Chad Parish** and **Wyatt Tenhaeff** have been awarded **Alvin M. Weinberg fellowships** by Oak Ridge National Laboratory.

**Gregory R. Hansen** has been recognized as a **Distinguished Inventor** by Battelle Memorial Institute.

**UT-Battelle** has received the **Mentor of the Year Award** from the U.S. Department of Energy, Office of Economic Impact and Diversity, Office of Small and Disadvantaged Business Utilization.

**Louis K. Mansur** has received the **Mishima Award** from the American Nuclear Society for his international leadership in understanding fundamental mechanisms of radiation effects in materials.

**Sharon Robinson** has received the **Robert E. Wilson Award** from the American Institute of Chemical Engineers. She has also been elected a **Fellow** of that organization.

**James Bentley** has been elected a **Fellow of the Microscopy Society of America.**

**Craig Blue** has been elected a **Fellow of the American Society for Metals International.**

**Amit Goyal** has been elected a **Fellow of the World Technology Network** and has also qualified as a **Finalist** for the organization's **World Technology Network Award** in the Materials category.

**Hua-Tay Lin** has been elected **Secretary of the Publication Committee** of the *Journal of Materials Engineering*. Lin has also been awarded the **Lee Hsun Lecture Award** by the Shenyang National Laboratory for Materials Science and the Institute of Metal Research of the Chinese Academy of Sciences. ®

## next issue

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Editor—Jim Pearce
Designer—LeJean Hardin
Illustrator—Andy Sproles
Photographers—Charles Brooks, Curtis Boles, Larry Hamill, Jason Richards
Web developer—Dennis Hovey

Phone: (+1) 865.574.7183
Fax: (+1) 865.574.0595
E-mail: ornlreview@ornl.gov
Internet: www.ornl.gov/ORNLReview

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