OAK RIDGE NATIONAL LABORATORY

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MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

# RECLAIMING AMERICA'S

Spallation Neutron Source

The Next Generation of Materials Research

# OAK RIDGE NATIONAL LABORATORY **REPARENT** • MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Editorial	1 Reclaiming Leadership In Neutron Science
Features	2 Returning Home
	4 Material Value Neutron Tool6 That's Incredible!7
	8 Instruments Of Change
	14 A Historic Partnership
	17 It Took a Village
	17 An Unsung Hero
	18 Unlocking the Cells
	19 Building the Bridge
	20 Making It Last
	21 Under Pressure to Change
Profile	22 Thom Mason
Research Horizons	24 Of Mice and Men
	25 Instant ID
	26 Supernova Discoveries
	27 Hot Technology
	28 And The Winners Are

COVER: Spallation Neutron Source OPPOSITE PAGE: Image of first protons on target produced by SNS Cover design by LeJean Hardin









#### THIS IS No Small Thing

In the summer of 2005, Oak Ridge National Laboratory hosted a delegation of European scientists who came to visit and assess the capabilities of the soon-to-be-completed Spallation Neutron Source. After two days of inspection, the delegation met late one afternoon with the SNS leadership for a final discussion. In a single brief statement, the Europeans summed up the significance of the SNS. "America now has the greatest facility in the world for the study of materials."

This issue of the ORNL *Review* tells the story of how this marvelous facility came to be and how the discoveries that take place at the SNS will strengthen America's competitive position within the world economy. From conception to completion, the story takes place over two decades. The story is one of vision, persistence and courage in the face of skepticism. The experience reminds us how much America can accomplish when we are prepared to marshal the extraordinary scientific capabilities in the Department of Energy's system of national laboratories.

The SNS is a product of an unprecedented collaboration among six Department of Energy laboratories. No single laboratory, including Oak Ridge, possessed the breadth of talent required to design a machine with more than 100,000 separate and interdependent control points that must function with precision. That a project of such incredible complexity could be designed and built by multiple laboratories—operating under different corporate cultures and located thousands of miles apart—defied much of what we thought we knew about science and the political process. The Department of Energy deserves much of the credit for coordinating this partnership and demonstrating that large and complicated projects can indeed be built not only safely, but also efficiently.

In virtually every aspect of its design and construction, the SNS is an imposing accomplishment. The \$1.4 billion, seven-year project was completed on time and on budget, with no compromise in the project's scope and a construction safety record of more than four million hours without a lost work day. We are indebted to the hundreds of men and women, sometimes working in difficult conditions, who made this feat possible.

Over time, the remarkable success in designing and building the SNS will be surpassed by the facility's contributions to scientific discovery. The facility's 24 instruments will enable researchers to see and understand, as never before, the inner structures of a virtually limitless array of materials that shape every aspect of our lives. Our dreams include lighter alloys that will make airplanes more fuel efficient. Miniaturized motors and a new generation of batteries and fuel cells. Time-released drug delivery systems that target a specific body organ. Paints that extend the life of bridges. Advanced electronic materials that store more data and retrieve it more quickly. The list is literally endless and all the discoveries, we believe, are within our reach.

As we embark upon these exciting challenges in neutron science, we are equally enthusiastic about what the SNS will mean for other scientific disciplines. At Oak Ridge, our investments in people and facilities are guided by the belief that future scientific discovery will lie at the nexus of nanotechnology, information technology, and biology. The SNS, together with ORNL's High Flux Isotope Reactor, the Department of Energy's first Nanoscience Center, the world's most powerful unclassified computer, and new facilities dedicated to genomics and bioenergy, will form the foundation for our "nano, info, bio" strategy. With the completion of the SNS, the largest building block is now in place for ORNL's long-term research strategy.

One recent spring day, with the dogwoods and redbuds in full bloom, I slipped out of my office and took the five-minute drive up to Chestnut Ridge. Gazing at this magnificent new facility located against the backdrop of the Smoky Mountains, I reflected on the fact that more than a half-century ago Nobel Laureate Clifford Shull performed ground-breaking neutron scattering experiments in Oak Ridge. For three decades, America led the world in neutron science, then surrendered the lead to Europe. Located in Oak Ridge—the birthplace of neutron scattering—it is fitting that the SNS will restore that leadership to America.

We once again lead the world because the Department of Energy, the Congress, two administrations, and the scientific community possessed the vision and the faith to make it happen. This is no small thing. Together, we can rejoice in a job well done.



Jeffrey Wadsworth Laboratory Director

#### **RETURNING HOME**

The SNS is a story of world leadership lost and regained.

Neutron scattering was born in Oak Ridge at the Graphite Reactor, built under Enrico Fermi in 1943 for the Manhattan Project at the site that became Oak Ridge National Laboratory. The reactor's purpose was to demonstrate the viability of extracting fissionable plutonium, a byproduct of the reactor's operation. The discovery made possible the development of the atomic bomb that ended World War II.

For almost three decades, the United States led the world in neutron science, a leadership based in part on research reactors at Oak Ridge National Laboratory. In the 1970s, the U.S. surrendered the leadership role to Europe, where a new and larger generation of neutron sources was built in France

and Great Britain. The story of the Spallation Neutron Source is also the story of how America, through a series of scientific and political twists and turns, set about to regain the status of world leader in neutron scattering and materials research.

As the war came to a close, health physicist Ernest Wollan had a unique interest in the neutrons produced by nuclear fission in the Graphite Reactor. He built a neutron diffractometer and sought to understand whether neutrons from the reactor could serve as a probe of the atomic structure of solids. In 1945 Clifford Shull joined Wollan in conducting neutron diffraction research. Shull conducted pioneering work in elastic neutron scattering at ORNL until 1955 when he left for a position at the Massachusetts Institute of Technology. In 1994 Shull and Bertram Brockhouse of Canada shared the Nobel Prize in physics for pioneering the use of neutron scattering to study material structure and dynamics.

Significant neutron scattering research continued at the Oak Ridge Research Reactor, which went critical in 1958, and the High Flux Isotope Reactor (HFIR), which began operating in 1966. HFIR's experiments yielded considerable information on the magnetic properties of rare earths and other elements.

#### **Europe Takes the Lead**

In the early 1970s, the High Flux Reactor at the Institut Laue-Langevin in Grenoble, France, began operations. Compared with HFIR in Oak Ridge, the ILL reactor offered higher neutron intensities as a result of improvements in instrumentation, neutron beam optics, and source tailoring, as well as a more open user program. ILL attracted neutron scattering researchers throughout the world seeking to study material Clifford Shull conducting neutron diffraction research at ORNL circa 1945.

structure and dynamics. About a decade later in 1984, the British opened the world's leading pulsed neutron source near Oxford. With these two facilities, Europe had wrested away the leadership in neutron science.

In the search for high-flux neutron sources to produce nuclear materials, researchers realized that, because of limitations in the reactor core power density, the use of a high-energy particle to spall neutrons from a heavy nucleus offered a better path to higher fluxes than nuclear fission for producing a neutron beam. In the 1980s, two accelerator-based spallation sources were built—KENS in Japan and Argonne's Intense Pulsed Neutron Source. Research at both facilities pioneered the development of a spallation target, a pulsed proton beam to produce neutrons in pulses, and time-of-flight scattering instruments.

Beginning in the early 1980s, the U.S. scientific community began aggressively advocating for a world-class reactorbased, neutron source closer to home. Many wanted a higherperformance reactor with a cold source, like the French reactor, to slow neutrons down to make possible research on polymers and proteins. The Department of Commerce responded by installing a cold source, guide hall, and neutron diffractometers and spectrometers at the reactor at what is now the National Institute of Standards and Technology Center for Neutron Research in Gaithersburg, Maryland.

Even with improvements in the existing American neutron sources, a major new facility was needed to satisfy increasing U.S. research requirements and to regain world-class status in neutron science. Since the late 1970s every national panel that reviewed the status of U.S. neutron science recognized the disparity between U.S. and European neutron sources and called for a new American facility.

#### A Twenty-year Effort

In 1984, in response to the President's Office of Science and Technology Policy, the National Research Council appointed the Seitz-Eastman committee to review U.S. needs for materials research facilities. The committee consisted of 22 distinguished researchers, headed by Frederick Seitz, president of Rockefeller University and former ORNL reactor school director, along with IBM vice president Dean Eastman, who later served as director at Argonne National Laboratory. In March 1984 ORNL's Ralph Moon made a presentation on neutron scattering to the Seitz-Eastman committee. The committee's report, *Major Facilities for Materials Research and Related Disciplines*, recommended an intense, synchrotron-based, X-ray source (which was later built

at Argonne and called the Advanced Photon Source), and construction of a new high-flux, steady-state neutron source designed to have a neutron flux 5 to 10 times that of the French reactor. The committee's

Gradually, confidence within the Administration, the Congress, and the scientific community grew until one of the world's largest science projects enjoyed an unprecedented degree of political support.

ceremony occurred.

Significantly, the construction phase of the SNS project got under way less than a month after DOE selected UT-Battelle to replace Lockheed Martin as the managing contractor at ORNL. Skeptics expressed

recommendations also included the development of a plan leading to a high-intensity, pulsed neutron facility.

In 1993 the Department of Energy's Basic Energy Sciences Advisory Committee Panel on Neutron Sources for America's Future reaffirmed the Seitz-Eastman committee's recommendations. The University of California at Santa Barbara's Walter Kohn, who had been a member of the Seitz-Eastman committee, headed the panel. The Kohn Committee concluded that "the nation has a critical need for a complementary pair of sources: a new reactor, the Advanced Neutron Source, which will be the world's leading neutron source, and a pulsed spallation source. The Advanced Neutron Source is the Panel's highest priority for rapid construction. In the Panel's view, any plan that does not include a new, full-performance high-flux reactor is unsatisfactory because of a number of essential functions that can be best or only performed by such a reactor."

In his 1993 report, A Vision of Change for America, President Clinton urged the U.S. Congress to build the ANS. He included the proposed 330-megawatt ANS, to be constructed in Oak Ridge, in his 1995 budget.

Despite the backing of the scientific community, the ANS could never get off the ground. Against the recent backdrop of the Superconducting Supercollider project in Texas, which was cancelled after the expenditure of more than one billion dollars, proponents of the ANS could not persuade a skeptical Congress to commit another \$2.9 billion for a project whose benefits, frankly, many did not understand. Opposition to the ANS was compounded by concerns from the State Department about the facility's potential to complicate nonproliferation efforts. Meanwhile, as the debate dragged on without resolution, accelerator technology was making significant strides.

In 1995 DOE regrouped, recommending cancellation of the ANS reactor project and allocating \$500,000 to ORNL for initial scoping studies on a spallation neutron source estimated to be about one-third the cost of the ANS. DOE's Basic Energy Sciences Advisory Committee recommended in 1996 the design of an accelerator-based, spallation neutron source that could begin operation at a beam power of approximately 1 megawatt. concern about "changing horses in the middle of the stream" with a project on which so much was riding for DOE and the scientific community. Questions persisted in 2001 when ORNL Director Bill Madia selected Thom Mason, a 36 year-old Canadian, to take over the SNS project in the same year Congress was being asked to provide an imposing \$281 million in construction funds.

To meet the continually growing needs for an intense source, their recommended design would be sufficiently flexible so as to be upgraded to significantly higher power in the future. On

August 19, 1996, DOE initiated the Spallation Neutron Source

Appleton, work began on the conceptual design of the SNS by

a consortium of six DOE laboratories. The group identified a

wooded 75-acre site on Chestnut Ridge, about one mile from

the main ORNL campus. After a slow start, a team from Argonne

National Laboratory, headed by David Moncton, led the transi-

tion to construction. On December 15, 1999, with Vice President

Al Gore of Tennessee holding the shovel, the groundbreaking

Under the leadership of ORNL's Al Trivelpiece and Bill

project with the formal "Approval of Mission Need."

Time and events proved the skeptics wrong. The partnership among the six DOE laboratories functioned well. Construction went forward on time and on budget. Annual reviews of the project were positive, which in turn attracted international talent. Gradually, confidence within the Administration, the Congress, and the scientific community grew until one of the world's largest science projects enjoyed an unprecedented degree of political support.

On April 28, 2006, ten trillion protons were fired into the mercury target of the SNS, releasing neutrons in a process that would help define American science for decades to come. The result was both tangible and symbolic. At that precise moment, the men and women who gathered around the SNS control room could look back with pride, knowing they are the heirs to the legacy of Clifford Shull and Enrico Fermi, and that they have restored to Oak Ridge—the birth-place of neutron scattering—the world's leadership in neutron sciences. (R)

Shull with Vice President Al Gore at SNS groundbreaking in 1999.

## MATERIAL VALUE

A competitive advantage for the next generation of materials research Over the past few decades, researchers have studied magnetic materials using neutrons produced by research reactors at Oak Ridge and other facilities around the world. The resulting data led to a broad range of commercial innovations, including credit cards, pocket calculators, compact discs, magnetic recording tapes, computer hard disks, magnets for medical imaging devices, and permanent magnets for car seats that adjust automatically. Characterization of material properties by neutron scattering likewise led to improvements in the quality and durability of diverse materials used in airline and military jets, shatter-proof windshields, agricultural pesticides, and hip and knee implants.

Despite these inventions, few people are aware of the extent to which their quality of life is related to discoveries made possible by neutron scattering. With new capabilities in Oak Ridge, the potential for future discoveries is virtually endless.

The accelerator-based Spallation Neutron Source, together with the High Flux Isotope Reactor, will make Oak Ridge National Laboratory the world's foremost center for neutron science. These next-generation user facilities will provide data for computer models that will lead to new physical and biological materials. The resultant quantum leap in the understanding of complex materials will greatly improve the potential for technological breakthroughs in a broad range of consumer products, boosting the competitiveness of American industry.

#### **Natural and Artificial**

Every manufacturing sector is looking for materials that are stronger and more durable under challenging conditions and that are easier to shape into products. Some industries are seeking materials that also can produce a higher-strength magnetic field or conduct electricity, heat, or light more efficiently or hold and read more data in a smaller volume.

The research instruments at SNS will make possible neutron-scattering studies of complex materials of interest to industry. These include complex fluids and soft matter, such as proteins and other biological materials, which are of interest to the pharmaceutical industry. Artificially constructed, multilayered, coated, or otherwise complex physical materials are of interest to the energy, electronic, and aerospace industries. These materials include high-temperature superconductors, optical fibers, nanostructured superlattices, magnetic thin films, polymer-carbon nanotube composites, block copolymers, and materials with correlated electrons, colossal magnetoresistance, or semi-conducting, photovoltaic, ferroelectric, or thermoelectric properties.

Communications and and and and and a second and a second and and a second and a sec

SNS research could lead to improved optical fibers for telecommunications, energy efficient aircraft and new drug delivery systems. Bulk amorphous alloys are a new class of disordered materials of interest to industry. Already this material is being used to make springier golf club heads that help golfers drive the ball farther. The new alloy differs from the typical metal or alloy, which is made of crystalline grains separated by boundaries, like a mosaic. Lacking grain boundaries, bulk amorphous alloys offer high strength, low friction, resistance to wear and corrosion, and the ability to be formed easily into shapes. Because of their combination of elements, these materials can be cast in bulk at a cooling rate slower than normally required to obtain the amorphous state.

During slow solidification, details of the changing positions and motions of the alloy's atoms can be gleaned by neutron scattering. This information on atomic structure and dynamics has been used to construct computer models that guided the development of an aluminum-based, bulk amorphous alloy for making golf club heads with improved elastic properties.

Because its pulses will contain almost 10 times more neutrons than today's best, pulsed spallation sources, the SNS, combined with its instruments, will provide scientists with a comparable increase in the understanding of materials properties. The SNS will enable scientists to trace changes in the positions and motions of atoms and molecules when, for example, a material melts or a metallic alloy switches from magnetic to nonmagnetic or from brittle to ductile. Atomic-level changes can be observed when a geological sample is squeezed at tremendous pressures similar to those near Earth's core.

#### **Smaller Samples**

In another new scientific benefit, the SNS will give researchers the ability to characterize unusually small samples with diameters of less than a tenth of a millimeter. Sometimes only minute specimens are available, such as a newly synthesized, nanostructured material from the Department of Energy user facility located adjacent to the SNS, the Center for Nanophase Materials Sciences.

Small-angle neutron scattering has been used to help explain colossal magnetoresistance—a dramatic change in resistance in a magnetic field, which is present in manganese oxide perovskites. Thin films of these manganites might be useful for making read sensors in smaller computers and magnetic-field sensors. Neutron-scattering studies of oxide superlattice crystals made at ORNL's nanoscience center can help researchers understand and imitate self-organizing behavior that emerges on the nanoscale in chemically complex systems.

> By using neutrons to study lubricants and other complex fluids that spread when a force is applied, researchers have discovered which additives improve fluid properties. Modern oils stick to moving me

tallic engine parts, whereas older oils, when heated during start-up, would spread out and separate from the parts they were supposed to lubricate. The opportunities are exciting. Bridges and other steel structures would need to be painted less frequently. Tiny machines must be lubricated with thin-film coatings, not oil-based fluids. Neutron research on soft matter could lead to time-released, drug delivery systems that target specific body organs.

Neutron-scattering studies of the impact of stress on a variety of materials have led to airplane wings that are more resistant to fracture and oil pipelines that are less likely to corrode and leak. By using neutrons to measure how much distances between planes of atoms have stretched or shrunk, scientists can locate residual stresses in the bulk of materials. These internal stresses, which develop in a component during manufacturing, can predispose the material

to cracking, wear, accelerated chemical attack, and even failure brought on by stresses externally imposed on the component during use. Engineers wish to understand when the component is likely to fail and whether use of a different material and manufacturing process, such as heat treatment, would produce a component that will last longer.

Each new generation of commercial and military aircraft and space probes is expected to travel faster and farther using less fuel. To meet these demands, they must be made of lighter materials held together with stronger, lightweight welds rather than heavy rivets. Neutron-scattering results, combined with computer models, will help engineers select or develop materials and welding processes that meet these needs, thereby providing a competitive advantage to American companies.

Like SNS beams, the race to develop exciting new materials to make innovative technology possible is unusually intense. The SNS will help researchers navigate the world of natural and synthetic materials to find the ones that truly matter.  $\mathbb{R}$ 





#### **Neutron Tool**

A neutron is one of the fundamental particles that make up matter. This uncharged particle, identified in 1932 in England by James Chadwick, exists in the nucleus of a typical atom along with its positively charged counterpart, the proton. Protons and neutrons each have about the same mass, and both can exist as free particles away from the nucleus.

In the universe, neutrons are abundant, making up more than half of all visible matter. But, for research on physical and biological materials, neutrons of the right brightness are in short supply. Just as we prefer a bright light to a dim one to read the fine print in a book, researchers prefer a source of brighter neutrons like the SNS, which will give more detailed snapshots of material structure and, with the help of computer programs, make "movies" of molecules in motion. The neutron has excellent properties for probing matter. The neutron is electrically neutral, able to penetrate materials a few centimeters, sensitive to light atoms in the presence of heavier ones, sensitive to magnetic interactions, and able to cover a range of energies or wavelengths, enabling researchers to probe distances between atomic layers in lattices, magnetic excitations, and slow dynamical processes in polymers and proteins.

Neutrons are especially sensitive to light atoms, such as hydrogen and carbon found in life-giving, organic molecules, and oxygen found in high-temperature superconducting oxides. But neutrons also reveal the presence of heavier elements. Neutrons, which interact with atomic nuclei, complement X rays, which interact with electrons and are, thus, most sensitive to heavier, electron-rich elements.

Each SNS pulse contains neutrons of a range of wavelengths and energies; the highest-energy neutrons have the shortest wavelengths, and the lowest-energy neutrons have the longest wavelengths. Because thermal neutrons move at a slower velocity, their progress can be timed accurately over short distances. Each pulse contains neutrons of all thermal energies, so neutrons of different energies can be separated by letting the neutrons travel a few meters. The high-energy neutrons reach the sample ahead of the mediumenergy neutrons, and the lowest-energy neutrons take the longest to arrive at the sample. Because the neutron energies are spread out in time, the energy of an individual neutron is easily determined by its "time of flight" to the sample. Because thermal neutrons of all energies are available for use in scattering experiments, the time-of-flight technique enables the collection of many data points for each source pulse reaching a sample.

With their range of wavelengths, neutrons cover all the length scales of interest to most scientists studying structure, from the size of an atom to that of a metallic crystalline grain or a macromolecule such as a nanocluster, polymer, or protein. Also, neutrons enable researchers to determine the motions, or dynamics, of nanoscale building blocks over a wide range of time scales ranging from ultrafast structural relaxation to vibrations to slow liquid diffusion and protein folding processes—a remarkable time scale that spans 10 orders of magnitude.

Instruments at the SNS include diffractometers and reflectometers, for determining structure by neutron diffraction; and spectrometers, for determining dynamics by measuring vibrations and other motions of atoms and molecules in samples.



## That's Incredible!

Some amazing facts about the Spallation Neutron Source

**Around the world:** The energy of the SNS's ion beam, expressed in terms of voltage, is 1 billion electron volts. The power is equivalent to 666 million 1.5-volt D-cell batteries joined end to end, enough to almost encircle the globe.

**Fast off the line:** The ion beam accelerates through the linear accelerator from a standstill to approximately 90% the speed of light in two microseconds.

**Now that's cold:** The SNS's linac takes advantage of superconducting technology: Approximately two-thirds of the linac's total 1000 feet is chilled with liquid helium to the superconducting temperature of 2 degrees above absolute zero, or 2 Kelvin. By comparison, a December night-game spectator at the Green Bay Packers' Lambeau Field should dress to endure a relatively toasty 275 Kelvin.

**Flurry of punches:** Following 1060 turns around the accumulator ring, 150 trillion accelerated protons strike the mercury target in a pulse that lasts only one millionth of a second. These pulses strike the target 60 times per second.

**Ouch:** The pulses strike the target vessel with enough energy to release neutrons from atomic nuclei for use in research. The force is equivalent to striking the vessel with a 200-pound block of steel traveling at 50 miles per hour.

**Over the horizon:** The SNS requires the tuning of the beam lines to be so precise that Earth's curvature was factored into the construction of the linear accelerator—a tiny but critical difference of 7 millimeters from one end of the 1000-foot linac to the other.

**Fine as frog's hair:** All critical SNS accelerator and target components—independent of size, shape, and weight—were installed to specifications within a mite-sized 0.2 of a millimeter.

**Thick as a brick:** Shielding over the tunnel into the target facility "monolith" consists of 7 feet of steel and 2 feet of concrete. The target facility floor is 5 feet thick. The monolith alone has 12 million pounds of steel shielding and 4 million pounds of concrete.

**Plugged in:** Beam power in the linac is 1.4 megawatts, enough electricity to power 1400 homes. Some 42 MW are required to generate 1.4 MW of beam power. The SNS will use enough electric power to serve 30,000 people, a city the size of Oak Ridge.

#### **INSTRUMENTS OF CHANGE**

# A revolutionary target station and 24 instruments will reshape the study of materials.

The Spallation Neutron Source is the first scientific facility to use pure mercury as a target for a proton beam. ORNL designed and built this "first"—a mercury target in which neutron beams are produced by spallation for use by researchers wishing to analyze materials samples.

"We were ready to take beam on our target in April 2006," reports Tony Gabriel, one of the principal developers of the mercury target. "Like the rest of the SNS project, the mercury target was designed and built on time and within budget." The SNS will soon become the most powerful, pulsed-neutron source in the world for materials and biological research.

One of the principal responsibilities for ORNL staff was the development of the target, where accelerated protons flung from the SNS accumulator ring unleash beams of neutrons by the process of spallation. This specific task was in addition to ORNL's



other responsibilities of managing the entire project, helping develop neutron beam instruments for experiments, and ensuring the SNS works properly by linking the subsystems designed and built by five other Department of Energy national laboratories.

Over the next two years the beam power at SNS will be gradually increased to its full operating level of 1.4 megawatts. This slow ramping up of beam power will give the SNS staff experience in operating at new power levels as well as insight into processes that limit the lifetime of the target. The principal ORNL developers of the target are optimistic that over time the target lifetime will be increased to support reliable user operations and the eventual power upgrade.

#### **A Mercurial Solution**

One day in 1995 Gabriel was invited to a meeting on neutron-source targets in the office of former SNS director Bill Appleton. Present at that meeting was Günter Bauer, a German visitor who was spearheading the development of the European SNS (which was never built). The three men discussed the best-known target options—tantalum and tungsten, which are solids, and mercury, the only metallic element that is liquid at room temperature. Bauer, who had pondered all three elements, convinced Appleton and Gabriel that a mercury target should be developed for the SNS.

"With 120 neutrons and 80 protons, mercury has a high atomic number, making it a source of numerous neutrons," Gabriel says. "Mercury has a high density, which means the neutron brightness can be maintained. Because mercury is liquid at room temperature, mercury does not have to be heated to make it flow. Also, mercury is better than a solid at dissipating the heat deposited in the target by the proton beam. Unlike a solid target, liquid mercury is not damaged by radiation and does not have to be cooled if the proton beam should suddenly shut off by accident."

The mercury target, which is only one cubic meter, will be bombarded 60 times a second with a proton pulse lasting less than a microsecond and consisting of  $10^{14}$  protons. The bombardment of the mercury target with protons dumped from the accumulator ring will lead to the transmutation of only 0.1% of the mercury into radioactive isotopes, which emit gamma radiation. The 20 tons of mercury circulating at one meter per second in the loop of pipes connected to the target module will become radioactive. But this mercury will be recycled, which will prevent escape into the environment.

When the target module reaches the end of its useful life, the mercury will be drained into a storage tank and the module will be retracted via cart into a shielded bay, where the module will be removed from the mercury system's permanent portion. After a new module has been installed through the use of a remotely controlled servomanipulator's robotic arms, the stored mercury will be pumped into the new vessel. Operators in the control room, separated from the target service bay by 40 inches

The SNS target chamber was designed with such precision that workers had to scrape the paint from some components to make them fit.

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of high-density concrete and lead glass windows, will remotely replace the target module and other important hardware, such as the motor that drives the pumps that circulate the mercury completely through the loop in one minute.

The mercury loaded in the target in December 2005 was delivered from the Oak Ridge Y-12 National Security Complex, where the liquid metal had been stockpiled for more than 40 years.

#### **The Pits**

The goal of ORNL's mercury researchers has been to design a mercury target that lasts for weeks instead of days. Because replacing a mercury target requires a week, the best way to reduce downtime is to keep the target in operation as long as possible for SNS users.

"Our research indicates that the target module will last only two weeks if the SNS were to operate at full design power of 1.4 megawatt in 2006, which fortunately for us is not the case," Gabriel says. "We had hoped that the target module would be good for 1250 hours, or about seven weeks, before it must be replaced."

To help address the issues affecting target lifetime, the ORNL researchers designed, built, and operated two test facilities, collected data from reactors and accelerators at ORNL and two other national laboratories, and obtained insights from a dozen international collaborators.

Experiments at a Los Alamos National Laboratory accelerator confirmed predictions that, when short pulses of protons bombard a mercury target, the mercury is heated so rapidly that a pressure wave is generated. Similar tests at Brookhaven National Laboratory confirmed these findings. In 2000 Japanese researchers demonstrated that pressure waves produced by only 100 or fewer pulses on an off-line impulse test apparatus can pit the wall of a stainless-steel container. ORNL researchers quickly prepared for and conducted a series of in-beam tests at Los Alamos, which confirmed that pitting damage occurs after only 100 proton pulses.

"We became aware that the pressure wave could cause cavitation-induced erosion after only a few pulses," Gabriel says. "The pressure wave produces bubbles that collapse near the vessel wall, pitting the inside surface of the target module."

A visiting scientist from Germany suggested that ORNL try "kolsterizing" the inside surface of the mercury target module to make the stainless-steel wall more resistant to pitting. ORNL researchers believe kolsterization, a low-temperature carburization method used to treat stainless steel for commercial products, might extend the life of the SNS target module.

Researchers have found that another way to lengthen target life is to reduce cavitation-induced erosion by mitigating the high-energy pressure wave. "The Japanese SNS will operate at 20 hertz and our SNS will operate at 60 hertz," Gabriel says. "During laboratory testing with their mechanical impulse device, the Japanese found that increasing the frequency level from 20 to 60 hertz substantially reduced the potential for cavitation-induced erosion."

Gabriel believes that operating the Oak Ridge SNS at 60 Hz may generate more bubbles in the mercury, making it "spongy" so as to soften the impact of the pressure wave on the module wall. Researchers are now testing their ability to inject bubbles into mercury at ORNL's Target test facility.

The facility's original purpose was to help researchers design and test remote-handling techniques and gain experi-

ence at operating a large mercury loop. Another ORNL facility, the High Flux Isotope Reactor, was used to test the ability of the target module's stainless steel to resist damage from neutrons released from the mercury by spallation. HFIR's neutrons hardened the steel. "We've had ups and downs in this project over the past 10 years, but we're in an upswing now," Gabriel says. He is optimistic that ORNL researchers can transfer their gift of time to the target.

#### **Translating Power into Discovery**

When the highly energetic pulses of neutrons leave the target, they are traveling too fast to be useful for research. The neutrons are slowed down roughly 1000 times, however, through collisions with molecules of liquid in four moderators designed and built by ORNL staff. One moderator is filled with water. The other three contain supercritical hydrogen.

The SNS Target Building can accommodate 24 research instruments at the end of neutron beam lines of different lengths that link to the mercury target and moderators like spokes of a wheel. The size and nature of the instruments are related to the specific material and properties that researchers wish to examine. To guide neutrons from the target-moderator assemblage to the instruments, designers had constructed beam lines of glass shielded with concrete. The concrete shielding, built to protect workers from neutron radiation, encloses and supports neutron beam optics formed from transparent glass mirrors manufactured by commercial vendors in Europe. These mirrors have complex shapes and a multilayer coating optimized for reflecting neutrons.

For the backscattering spectrometer—one of the three SNS research instruments to go on line this year—the neutrons are reflected along a slightly curved path some 84 meters (90 yards) to reach an experimental sample suspended in the middle of a large tank. The tank wall is partially covered with panels of single-crystal, silicon, hexagonal plates that will reflect, or backscatter, to 112 detectors only those neutrons scattered from the sample that have one particular energy, or wavelength.

Each SNS instrument includes a neutron beam line, sample holder, sample environment, and detector system optimized for a particular type of measurement. All the detector systems will use the internationally acclaimed, world-class "event mode" data acquisition system.

Some 80 people are developing SNS neutron scattering instruments, says Kent Crawford, leader of the Instrument Systems Group in the SNS Experimental Facilities Division. He previously worked for Argonne National Laboratory, which has operated the Intense Pulsed Neutron Source as a scientific user facility since 1981. As an SNS partner lab, Argonne was responsible for the development of the instruments, which Crawford describes as "an interesting mix of high precision and massive construction." Argonne instrument scientists initially carried out the engineering work and project management for the instruments and trained or advised ORNL scientists who assisted.

Instrument Development Teams or any other group proposing an instrument must present their proposals to an external Experimental Facilities Advisory Committee, which makes recommendations to SNS management. Thus far SNS management has followed the committee's recommendations. Poor planning had nothing to do with the fact that not all the instruments fit inside the Target Building. Rather than construct a much larger Target Building, SNS management decided to save money by constructing attached "satellite buildings" to enclose 6 of the 17 approved instruments, which stick out of the building because of instrument size and geometry or the need for a very long beam line.

In 2006 three instruments will be "commissioned," or tested with a neutron beam. These instruments, funded by the Department of Energy, are the backscattering spectrometer, the liquids reflectometer, and the magnetism reflectometer. Health and safety considerations are resolved before any instrument is commissioned. Each of the instruments will be used for neutron-scattering research.

While DOE provides funding for most SNS instruments, other instrument funding agencies include a national laboratory in Germany and a foundation in Canada.

The mercury target and the research instruments housing advanced electronics and experimental targets represent the highest plateau of scientific design and construction. As the remainder of the SNS provides the enormous power needed to produce neutrons, the instruments will translate this process into what should be an endless journey of scientific discovery.

## Among the discoveries neutron scattering could make possible:

Drug delivery systems that release a medicine precisely when needed by the body to relieve pain

Lubricants that enable a car engine to generate more power with less emissions

Superconducting wires that carry more power and reduce electricity costs

Manufacturing processes for plastics that do not harm the environment

Lightweight fuel cells that power emission-free vehicles

Cures for diseases through better understanding of how proteins work in the human body

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The accumulator ring, designed and built by Brookhaven National Laboratory, is a product of the multi-lab partnership that made the SNS possible. Photo by Larry Hamill

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## **A HISTORIC PARTNERSHIP**

Six national laboratories joined hands to design and build one of the world's most complex facilities.

At 2:04 p.m. on April 28, 2006, an operator tapped a key stroke that for the first time produced neutrons at the Spallation Neutron Source. With this seemingly simple procedure, Oak Ridge began the journey to become the world's foremost center for neutron science. More important, the event reasserted American leadership in a field that for two decades had been conceded to the European scientific community. The unique partnership that led to this historic milestone is a critical chapter in the SNS story.

The Spallation Neutron Source could not have been built at Oak Ridge National Laboratory without an unprecedented level of collaboration with five Department of Energy national laboratory partners. Quite simply, no American laboratory, including ORNL, possessed the depth of expertise required to design an accelerator-based facility on the scale of the SNS. The solution lay in fashioning a partnership that in effect brought together the capabilities of the entire DOE laboratory system. What the DOE system lacked in talent and equipment would be recruited from around the world.

Six DOE laboratories—Argonne, Brookhaven, Jefferson, Lawrence Berkeley, Los Alamos, and Oak Ridge—composed the partnership to design and construct the SNS. The collaboration, one of the largest of its kind in U.S. scientific history, was an extraordinary collection of talent and experience from a variety of scientific fields. The collaboration was supplemented by additional partners from France, Germany, Great Britain, Japan, and Russia.

The breadth of the partnership was unprecedented. By their very nature, national laboratories are independent institutions that at times compete ferociously for limited research funding. Managed by various combinations of universities, corporations and not-for-profit research institutions, the laboratories represent a myriad of missions, personalities and operational cultures. As policymakers debated the viability of designing the SNS with such a diverse group, many doubted that the parties would even agree on their respective tasks. Against the backdrop of previous experience, the notion that the laboratories could deliver one of the largest and most complex science projects in history on time and on budget defied believability.

The first major challenge for the SNS was political. A commitment of \$1.4 billion to the SNS meant that a number of DOE capital projects at other laboratories would need to be deferred, which in turn would lessen political enthusiasm for the SNS among the respective congressional delegations. The problem was mitigated by the decision to include five additional laboratories as a substantial part of the SNS project in Oak Ridge. Their role was not trivial in either scientific or financial terms. As a result of this strategy, the SNS gained congressional support it might not otherwise have enjoyed during the project's crucial early years.

#### The Sum of the Parts

Spanning the length of seven football fields, the SNS is a scientific tool of enormous size and complexity that accelerates ions and then protons to blazing speeds to produce neutrons for research. At one end is an ion source. At the other end are research instruments on neutron beam lines. In between are 100,000 interdependent control nodes designed by six laboratories that must function perfectly.

The SNS begins with the "Front End," built by *Lawrence Berkeley Laboratory*. Negatively charged hydrogen (H-) ions are

Resembling an airport in size, the SNS was literally carved from the pristine wooded ridge located about one mile from the main ORNL campus. produced in an ion source. Each ion consists of a proton orbited by two electrons. The ions are accelerated to an energy of 2.5 million electron volts (MeV) and then delivered to a linear accelerator.

Los Alamos National Laboratory designed the drift tube linac and the coupled-cavity linac, which are made of copper, operate at room temperature, and accelerate the ion beam to about 200 MeV. They were also responsible for the radiofrequency power systems that provide the accelerating energy for the whole linac.

The bulk of the ion acceleration is achieved in a superconducting linac developed by **Thomas Jefferson National Accelerator Facility.** High-frequency radio waves generated by klystrons are injected into the superconducting cavities embedded in liquid helium, creating an electric field that provides the energy to propel the ions by a factor of 5 to 90% of the speed of light. This velocity corresponds to an energy of one billion electron volts (1 GeV). The SNS today has the world's highest-energy—and soon will have the most powerful--pulsed H- ion linear accelerator.

The ions are passed through thin carbon foils, which strip off each ion's two electrons, converting it to a proton. A 250 km long train of protons is collected in 1060 turns around the ring for a total of 150 trillion accelerated protons in a single, very intense bunch that is kicked out at once. In this way, an intense proton pulse less than a millionth of a second in duration (700 billionths of a second) is produced. The accumulator ring, which was designed and built by **Brookhaven National Laboratory**, produces, stores, and extracts short, intense proton pulses that strike the target 60 times per second.

ORNL designed and built the heavy-metal target, which consists of liquid mercury circulating in a stainless-steel container. The SNS accelerator systems deliver a proton beam with a power of 1.4 million watts to the target.

When a high-energy proton bombards a heavy atomic nucleus, such as mercury, some neutrons are "spalled," or knocked out, in a nuclear reaction called spallation. Other neutrons are "boiled off" as the bombarded nucleus heats up. The process is similar to a pitching machine that repeatedly throws a baseball at a bucket of baseballs, resulting in a few being immediately ejected and many more bouncing around and falling out. For every proton striking the nucleus, 20 to 30 neutrons are expelled.

Corresponding pulses of neutrons freed by the spallation process are slowed down in one of four ORNL-built moderators filled with water or liquid hydrogen. The neutrons are then guided through beam lines to research areas containing special instruments. Once there, neutrons of different energies can be used in a wide variety of experiments. *Argonne National Laboratory* and ORNL had joint responsibility for developing the beam lines and instruments.

Resembling a flashing strobe light providing high-speed illumination of an object, the SNS will produce pulses of neutrons every 17 milliseconds, with at least 10 times more neutrons than are produced at the most powerful pulsed neutron sources currently available. Much like water spraying from a rock being washed by an intense stream from a garden hose, neutrons from a beam will "scatter" from a target material in a way that reveals its structure and microscopic origins of physical, electrical, magnetic, chemical, and biological properties. Some 2000 scientists each year will come to Oak Ridge to perform experiments with these powerful neutron pulses.

#### A Successful Collaboration

"The value of the multilab partnership is most apparent in the accelerator division," says Norbert Holtkamp, an accelerator physicist who previously worked at DOE's Fermi National Accelerator Laboratory and DESY laboratory in Hamburg, Germany. Holtkamp came to ORNL because of the "technical challenges of SNS and the multilab partnership." He points out that four national labs were involved in designing and building the accelerator. "The multilab partnership approach is the right way to build large, complex science facilities, and, surprising to some, it is a better, more efficient way of managing resources. My role in managing the multilab partnership ranged from developing and maintaining expertise to bringing in and phasing out manpower. The facts speak for themselves. The collaboration was a success."

Holtkamp had primary responsibility for the design and construction of the ion source, linear accelerator, and accumulator ring. At the peak of construction of these SNS subsystems, the Accelerator Systems Division had 550 employees. By January 2006, all of these subsystems had been commissioned and were ready for operation. Meanwhile division payroll had ramped down to 180 people.

"But we didn't have to fire 370 people," Holtkamp stresses. "They worked for SNS as employees from six different national labs. When their work for SNS was completed, they returned to their jobs at their home labs. For a large and complex project, the multilab partnership is a much better way to maintain the expertise needed to design and build a facility than the conventional approach of hiring and then laying off large numbers of people."

An SNS colleague used to joke that a properly managed multilaboratory partnership would result in "equal distribution of pain," a phrase that Holtkamp likes.

"Equal distribution of pain also means that everybody has to come out of this project as a winner," Holtkamp asserts. "We felt it important to manage the project so people are recognized for their scientific credentials and feel they are appreciated for the subsystems they built here. They should share the success." of neutrons," he says. "That DOE authorized the power upgrade before construction of SNS was complete is a tribute to the success of the project."

#### **Ready to Lead the World**

A little more than six years after the frigid December morning when Vice President Al Gore turned the first shovel of dirt in the middle of the woods on Chestnut Ridge, the SNS is a reality. Built on time, on budget and on scope under the supervision of UT-Battelle and the Department of Energy, the SNS is a vindication of the belief that the U.S. government is still capable of delivering the kind of large scale projects that have marked the nation's history.

The SNS was perhaps the most international project ever undertaken. Engineers and scientists joined the SNS Oak Ridge team from 23 states and 15 countries. More than 680 managers, scientific and technical, administrative, and engineering staff worked on the SNS at six locations. An estimated 500 engineers representing all disciplines – chemical, civil, computer, construction, electrical, mechanical, and nuclear—designed, installed, and tested the SNS systems and components. The work force peaked at about 1,300 in November 2002, and included more than 3,800 employees over the seven-year span of the project.

One of the project's most noteworthy accomplishments was an outstanding safety record during construction. An estimated 3000 construction workers worked more than 4 million hours without a lost-time accident.

To some of Oak Ridge's oldest residents, the SNS reminded them of the excitement and energy of the Manhattan Project 60 years earlier. During that marvelous period, hundreds of

The project's scientific quality was apparent even before the SNS was completed. Staff members of the Accelerator Systems Division published hundreds of papers in conference proceedings and scientific journals. The project has also generated patents.

"The SNS from the beginning was designed to be upgraded to double the available beam power and, therefore, the number scientists from America and abroad were thrown together to build something many thought impossible. They succeeded, and in so doing established America's scientific leadership for the remainder of the 20th Century. Their story has been repeated at the SNS, where once again America stands ready to lead the world.  $\mathbb{R}$ 

#### THE NASHVILLE CONNECTION

In some respects, the most important SNS partner was the state of Tennessee. In January 2000, the Tennessee General Assembly rushed through legislation in 16 days that provided the SNS a critical \$28 million sales tax exemption on construction materials that kept the project viable. The state also appropriated \$8 million to construct the Joint Institute for Neutron Sciences, shared with the University of Tennessee and located adjacent to the SNS. Owned by the University of Tennessee on land deeded from the Department of Energy, the facility will provide office and laboratory space for joint UT-ORNL faculty, visiting scientists and engineers from universities, industrial firms, and the international community. Governor Phil Bredesen, himself a physicist, has pledged \$10 million in recurring funds, matched by UT-Battelle, to hire a cadre of world-class researchers to lead the institute.

The Joint Institute for Neutron Sciences will attract the best neutron talent in the

world to interact with the resident staff, students, and user communities in Oak Ridge. Modern computational, communication, and networking services will encourage interactive science and video teleconferencing and provide data acquisition and analysis capabilities for resident scholars and their colleagues around the world.



From Left: Carl Strawbridge, Bill Madia, Norbert Holtkamp, Thom Mason, Jeff Wadsworth, and Ian Anderson

One of the ironies of the SNS story is found in the international flavor of the project team that made possible America's ability to recapture world leadership in neutron science. Many of the SNS project staff have become, or are applying to become, American citizens.

Ian Anderson: Recruited to Oak Ridge from the ILL laboratory in Grenoble, France. Headed design of SNS target and the target's instruments.

**Norbert Holtkamp:** A key figure in delivering what some thought impossible—the integration of six national laboratories in the complex SNS design. Personally led the design and construction of the SNS accelerator.

**Bill Madia:** Became ORNL Director with new UT-Battelle management team in April 2000, just four months after SNS groundbreaking. Instrumental in putting in place management support at the Laboratory and political support in Washington that proved critical to the project's success.



**IT TOOK A** 

Village

**Thom Mason:** Came to Oak Ridge from the University of Toronto to help design the SNS experimental facilities.

Named Director of the SNS project in April 2001 at age 36. Successfully coordinated a variety of construction and personnel challenges, including the hiring of key talent from around the world.

**Carl Strawbridge:** The Naval Academy graduate brought discipline to the construction and kept the project on time and on budget. Provided continuity as other senior managers left and entered the project.

Jeff Wadsworth: British-born and now an American citizen, made SNS a priority immediately after assuming role of Laboratory Director in August 2003. Nurtured partnership with Tennessee Valley Authority to upgrade power for project. Guided the difficult transition from construction to operation. R

## AN UNSUNG Hero

While success is said to have many fathers, the SNS project had at least one critical "mother." Pat Dehmer, as Associate Director for Basic Energy Sciences in the Department of Energy's Office of Science, in her words "didn't have a neutron-free day" from virtually the moment she assumed her job in 1996. Widely respected for both her scientific and political credentials, Dehmer was an articulate and effective proponent for the SNS project within DOE and, perhaps more important, on Capitol Hill. Her passion for DOE's role in America's scientific research community was a driving force in the ability to provide focus amid the distractions that threatened the SNS project's design and construction. **(R)** 

## **UNLOCKING THE CELL**

An unprecedented look into the structure and function of cellular membranes could lead to a new array of designer drugs.

A t least nine Nobel Prizes have been awarded for scientific research based on neutron science, including the 1994 prize bestowed on physicist Clifford Shull, who pioneered neutron scattering at an ORNL reactor. ORNL's Ian S. Anderson boldly predicts that future discoveries resulting from membrane research at the Laboratory's premier neutron sources could lead to another Nobel Prize.

A membrane is a thin, impermeable barrier that encloses a living cell. The cellular membrane is a fluid network of interacting fats, called lipids, criss-crossed by active proteins and other components. These membrane proteins form active channels, sensors, and signaling networks that span the membrane, allowing cells to communicate with the outside world, transport nutrients, and expel waste.

"About 70 percent of all drug targets are membrane-incorporated or membrane-associated proteins," says Dean Myles, director of ORNL's Center for Structural Molecular Biology, which conducts experiments at both the High Flux Isotope Reactor and the Spallation Neutron Source.

"Research at both of these facilities will focus on fundamental problems, including understanding membranes and how proteins interact with membranes," Myles notes. "Researchers will address problems ranging from the breakdown of plant cell walls for bio-energy to the design of therapeutic drugs that protect us from disease.

"In many infections, invading cells release toxins that attack our cell membranes. Neutron scattering can help us determine how and where these toxins attack."

Visualizing such interactions can help scientists identify the mechanism of infection and guide pharmaceutical researchers in designing drugs that block toxin-cell interactions. The process often involves isolating these proteins and determining their atomic structures. The unique value of neutrons is their ability to allow researchers to pinpoint hydrogen atoms in these structures with exquisite detail.

Because heavier hydrogen atoms scatter neutrons differently, scientists can further heighten the visibility of targeted proteins by replacing their hydrogen atoms with deuterium. Users at ORNL's Bio-Deuteration Laboratory label proteins in living cells with deuterium for neutron "contrast variation" experiments. Labeled proteins stand out like beacons against background solvent or membranes. Researchers can then more easily observe how these highlighted proteins interact and assemble into larger protein complexes and molecular machines, thus contributing to the understanding of how these complex systems work in cells.

Biologists use deuterium-labeled lipids to highlight interactions in membranes. Their goal is to determine how and where particular lipids insert in membranes, whether insertions are random or uniform, or, as some evidence suggests, whether particular lipid molecules may coalesce into active units, or "rafts," that travel through the membrane. Cholesterol, for example, is a natural lipid whose interactions with cellular membranes are thought to stiffen them. Deuterium labeling will allow researchers to "see" cholesterol molecules within a lipid sea and to understand their effect on membrane structure and dynamics.

Understanding precisely how membrane and protein dynamics relate to their structure and function remains a major scientific challenge. Ken Herwig, ORNL's Neutron Scattering Sciences group leader, is tackling this problem at the SNS, where he compares the motions of proteins from common microbes and of proteins extracted from thermophilic organisms that thrive in hot deep-sea vents. Understanding how temperature affects dynamics may help explain the remarkable stability of thermophilic proteins at high temperatures that break down most other proteins.

The diverse instrument suite at HFIR and SNS will provide biologists with unique insights into the structure, function, and dynamics of cellular systems. Each year, dozens of researchers will conduct biological research at HFIR using a small-angle neutron scattering (Bio-SANS) instrument. Dozens more will explore biological mysteries at SNS, employing instruments specifically designed to probe dynamics using neutron spectroscopy, or to determine molecular structures using SANS, the liquids reflectometer, and the MaNDi macromolecular diffractometer.

"Neutrons are just a small part of the toolset that biologists use," Myles says. "But, in many applications, neutrons provide critical information that is difficult or impossible to obtain using other techniques."

When they do, the result may be a ticket to Stockholm. ®



#### **BUILDING THE BRIDGE**

Three SNS instruments will explore the new world of nanostructured materials.

The first three instruments to accept beams from the Spallation Neutron Source in 2006 will allow researchers to weigh in on matter at the nanoscale. Both literally and figuratively, a bridge connects the SNS to another major Department of Energy scientific user facility—the new Center for Nanophase Materials Sciences.

Researchers at the nanocenter seek to learn more about biological and polymeric membranes, nanomagnetism, catalysis at the nanoscale, and energy production challenges. Their tools will include the recently commissioned SNS liquids reflectometer, magnetism reflectometer, and backscattering spectrometer.

Proteins buried in cellular membranes allow transport of materials into and out of cells. "Using the new instruments at SNS, we will measure vibrations in membranes and relate these dynamics to the opening and closing of membrane channels and transmission of information and

materials into, out of, and between cells," says Ian S. Anderson, director of the SNS Experimental Facilities Division. "We can determine membrane structure by replacing hydrogen atoms with heavier deuterium atoms, which scatter neutrons differently. In this way, we can highlight the positions of proteins, molecules, and functional groups attached to, or incorporated within, membranes."

To use neutrons to study a membrane's molecular motions, researchers must not restrict motion by fixing the membrane to a solid surface. Studies at ORNL's nanocenter demonstrate that membranes can be suspended over an array of nanofibers, preserving their flexibility and biological function. Furthermore, this "nanostructured scaffold" could be used to insert foreign proteins, for example, into the cell through its membrane. The changes in membrane structure and dynamics that result could be studied using neutron scattering.

The liquids reflectometer can measure how atoms are arranged at the surface and below a few hundred nanometers. The instrument may be useful for determining the part of a cell membrane surface most vulnerable to attack by the AIDS virus or the way bacterial toxins infiltrate and destroy cells by creating pores in their membranes. These structural measurements can be coupled with information on membrane motions obtained from the backscattering spectrometer, providing unique insights into how membranes work.

Creating an electronic device that packs encyclopedic amounts of information into an amazingly small volume and

retrieves the data incredibly fast is one possible outcome of nanomagnetism research. Such devices require the use of electron spin rather than electron charge to store and transmit information.

> In nanostructured, thin-film, "spintronic" devices, electron spins are relatively aligned to the device's magnetic direction. The read head used to extract the information stored on computer hard disks is a good example of a modern spintronic device. "Polarized" neutrons of known spin reflected and detected by the SNS magnetism reflectometer will provide unique data on magnetic direction and structure in the deeply buried magnetic layers that compose spintronic devices. Such information will guide the development of these devices as well as tomorrow's quantum computers. Most catalytic reactions

responsible for many commercial products occur on surfaces. Because nano-sized particles offer increased surface area, researchers believe they could be ideal catalysts. The SNS instruments will help researchers follow the adsorption of molecules on catalytic nanoparticles and the resulting structural changes. The backscattering spectrometer and planned instruments will probe the dynamic processes of adsorbed molecules, such as diffusion, rotation, and vibration. Future SNS measurements of the atomic structure of catalytic nanoparticles will enable scientists to develop more efficient catalysts for removing pollutants from car exhaust.

Neutron research and nanoscience may light the path toward a "hydrogen-based economy" by improving fuel cells and hydrogen storage systems. The SNS backscattering spectrometer will enable researchers to track the diffusion of hydrogen in carbon nanotubes to predict how well tiny tubes can store and release hydrogen for use in power-producing fuel cells. The instrument will also enable studies of methane hydrates found in the ocean and Arctic permafrost, compounds that are potential sources of hydrogen and temporary storage media.

Over the next decade, the bridge between ORNL's Spallation Neutron Source and nanocenter will symbolize the value of linking two worlds of amazing discovery. Together, they will help shape the future of neutron science and nanotechnology, as well as their impacts on a limitless range of new materials for American industry. R

## **MAKING IT LAST**

Materials that last longer are a primary need of industry.



Non how to improve industrial materials, including materials used in the paper industry itself.

Neutron scattering studies of steel tubes at ORNL provided essential data that helped improve the safety and longevity of the paper industry's recovery boilers, saving millions of dollars. An ORNL effort recently identified alternative tube materials and recommended new operating procedures to prevent the cracking observed in stainless steel–carbon steel tubing used in the boilers. Dozens of kraft paper mills in North America adopted ORNL's recommendations, avoiding the need for additional, costly shutdowns for inspections.

Using neutron diffraction at ORNL's High Flux Isotope Reactor, members of the Diffraction and Thermophysical Properties Group measured tube stresses as a function of temperature and processing parameters. "We found that tensile stresses were induced in the tubes' 304L stainless-steel clad layer, and that these stresses contributed to the stress corrosion cracking," says Xun-Li Wang, a materials scientist with the Spallation Neutron Source's Experimental Facilities Division.

Additional neutron diffraction studies and other tests showed that materials higher in nickel, such as alloys 825 and 625, were far more resistant to cracking than 304L stainless steel, the industry standard. Paper mills began installing tubes made of these super alloys—a success story for neutron scattering research.

The study of mechanical behavior represents a newer application of neutron scattering research. "Consumers want materials that last," Wang says. "The study of mechanical behavior tells researchers what makes materials strong. By measuring the change in spacing between atomic planes, we can 'see' how materials deform at the microscopic level."

Wang leads the development of VULCAN, an engineering diffractometer at SNS, which will be used for more realistic studies of changes in the strength and stability of materials when heated in a furnace or placed under an applied load. The Canada Foundation for Innovation is funding VULCAN's construction. A National Science Foundation grant supports the development of the sample environment, including a load-frame, a furnace, and an electrochemical cell.

An ORNL team helped demonstrate the feasibility of conducting an in-situ welding experiment on a neutron-scattering instrument. They successfully mounted and operated a friction stir welding machine on an engineering diffractometer at the Los Alamos Neutron Science Center. Using a method developed at ORNL, the team was able to determine the weld temperature and stress from the in-situ

data. Their exploratory research is supported by ORNL's Laboratory Directed Research and Development Program.

"We hope to advance this type of experiment at VULCAN to understand better how stresses induced by welding alter the weld's microstructure," Wang says. He explains that in the VULCAN experiments, a focusing neutron guide will increase the intensity of neutrons striking the samples, allowing experimenters to resolve how materials change over time under temperature and applied load. Adding a small-angle neutron scattering (SANS) capability to VULCAN will further allow researchers to characterize structure changes at two different length scales—as small as a few atoms to as large as several grains of metals.

Oxide-dispersion-strengthened ferritic alloys may be studied at VULCAN after it becomes operational in 2008. ODS alloys, which contain both nanoclusters and microparticles, are candidates for high-temperature structural materials in future energy production systems, such as turbines and nuclear reactors.

Using an in-situ SANS facility at Hahn-Meitner Institute in Berlin, Wang and his ORNL colleagues found that nanoclusters formed during fabrication of the ODS ferritic alloy are stable up to 1400°C, explaining the alloy's extraordinary ability to resist creep deformation at high temperatures.

"We are studying how stable these nanoclusters are in the ODS alloy at high temperatures," Wang says. "Soon, we hope to use VULCAN to learn what happens to the nanoclusters under applied load."

Wang's work, along with that of his colleagues at the SNS, will provide a lengthy new chapter to the library of materials science.  $\mathbb{R}$ 

#### **UNDER PRESSURE TO CHANGE**

A new instrument will reveal how materials are transformed under extreme pressure.

By squeezing and transforming matter in specially designed pressure cells and using neutron beams to tease out details of the altered structure, researchers hope to gain an understanding of how Earth's minerals behave when subjected to high pressures similar to those near Earth's core. The technique might also help researchers learn why some microbes survive under high pressure, and how to synthesize hydrogen-rich clathrates like those found on the ocean floor, new materials found in meteorites, and improved, artificial, single-crystal diamonds.

Geoscientists and other physical scientists seeking to uncover the effects of extreme pressures and temperatures on matter will soon add to their tool box a unique research facility being constructed at the Spallation Neutron Source. The new tool, known as the Spallation Neutrons and Pressure (SNAP) diffractometer, represents the next generation of neutron instrument because of a design that uses modern ultrahigh-pressure device technology.

Chris Tulk, a researcher in the SNS Experimental Facilities Division, is guiding the construction of SNAP, which will be available to users in 2008. "In the SNAP instrument, we hope to raise the pressure bar to 100 gigapascals, or a million times atmospheric pressure, which is roughly five times that currently available at neutron sources," Tulk says. "That's close to the pressure of Earth's core mantle boundary, which is approximately 125 gigapascals. With SNAP, we hope to provide useful experimental data for computer models that simulate the pressure and temperature behavior of magnetic materials under 'core-like' conditions."

At the heart of the SNAP instrument is the pressure cell, a small hydraulic press inside of which are cone-shaped anvils made of diamond, sapphire, or moissanite gemstones or tungsten carbide. The sample is held in a gasket and compressed as the anvils are forced together under loads of up to several hundred tons.

According to Tulk, reducing the sample size generally yields higher obtainable pressures. Maximizing the neutron flux at the sample while minimizing neutron scatter from the pressure equipment presents several significant design challenges for the instrument team.

A typical sample size at existing neutron sources is approximately a centimeter, or a half-inch, in diameter. "Our goal is a sample less than 100 microns, or several tenths of millimeters," Tulk says. "Our primary challenge is to focus the neutron beam to make it smaller and more 'needle-like' than previously achieved, while simultaneously locating the sample inside the cell and carrying out neutron diffraction experiments."

At the NRU reactor at Chalk River Laboratories in Canada, Tulk and his colleagues recently "microfocused" a beam using prototype Kirkpatrick-Baez (K-B) neutron super-mirrors, designed specifically for the task by ORNL's Gene Ice. Originally designed to focus X rays, K-B mirrors are very compact. Prototype neutron mirrors are 10 times longer than X-ray mirrors and have a different reflective coating.

Tulk and his associates microfocused a neutron beam down to 100 microns on single crystals of several minerals. "To ensure the beam was focused on our 100-micron sample, we developed a process that included very precise sample movement stages and comparisons of diffraction intensities collected at each step," Tulk says. "We are now trying to refine this process for use with pressure cells."

The researchers had to be sure that the neutron beam was not striking the pressure cell's anvils, producing an overwhelming background. The scientists will then remotely control the anvils, making them squeeze the sample at pressures as high as 20 gigapascals, or 200,000 times atmospheric pressure.

Tulk recently used high-pressure diffraction to study structural changes in glasses under pressure. He structurally characterized the octahedral form of oxide glasses structurally similar to those present in Earth and found that under high pressure, the central atoms in glass are surrounded by six oxygen atoms instead of the usual four.

ORNL, Stony Brook University, and the Geophysical Laboratory of the Carnegie Institution in Washington, D.C., proposed to the Department of Energy an experiment in which SNAP would be used to produce and characterize solid hydrogen in pressure cells. Armed with new tools and new data, scientists believe the research could lead to new methods for storing and releasing hydrogen for fuel cells.

Optical reflection of forsterite sample shown in two mirrors used for microfocusing neutron beams in the high-pressure SNAP instrument at SNS



photo by Lynn Freen

One could say Thom Mason, who assumed management of one of the world's largest and most important science projects at age 36, has science in his blood. His mother was trained as a biochemist and his father received a Ph.D. in geophysics. A lab rat, Mason grew up with the misconception that science was normal. His first brush with administrative management came as manager of the radio station at Dalhousie University in Halifax, where he met his wife Jennifer. Since receiving his Ph.D. from McMaster University, Mason's research took on an international flavor that later proved an invaluable asset to his work in Oak Ridge. He worked at Chalk River Laboratories in Canada, at Bell Laboratories in the United States, at Risø National Laboratory in Denmark, and in the Physics Department at the University of Toronto. He was selected as Director of the SNS project in 2001.

## **Q.** What does the Spallation Neutron Source mean to science and to the American public?

The ultimate importance of the SNS lies in its potential to define our future. Historically, civilizations have been characterized in large part by the materials that shaped their economy, military strength, and everyday life. Stone led to bronze, which led to iron, which gave way to steel, which led in recent decades to silicon. Today's materials—nanomaterials, proteins, and molecules—are much more complex and require far more sophisticated tools to understand them. The neutrons produced at the SNS are one of the tools that will lead to a new age of materials. This change could prove to be as profound as the transition from iron to steel centuries ago.

# **Q.** Completing such a massive project on time and on budget was no small task. What key management decisions made this possible?

The first and most important decision was to build SNS through a multi-lab collaboration. No single lab, including Oak Ridge, had the depth of expertise needed to design an accelerator of such size and complexity. Attempting to coordinate the design of a \$1.4 billion project among six labs was considered by many a risky decision, but overall the effort worked out well. The complications we encountered were far outweighed by the benefits of the collective talent that went into the project. Second, we made a couple of important technology decisions that proved successful. Selecting the superconducting linear accelerator and mercury for the target improved the reliability of operations and the flexibility of future upgrades to the SNS. Finally, we made good hiring decisions over a sustained period. From a handful of people in 1998, we are now up to almost 350 staff composed of some of the brightest scientists and engineers in the world. They came to Oak Ridge to be part of something very exciting.

## **Q.** Why was the decision to incorporate superconducting technology so important?

Dave Moncton was SNS Director when technical director Yanglai Cho led a study in superconducting radiofrequency to determine if European technology advances in superconducting should be considered as a last-minute option. The study recommended that a superconducting linear accelerator should be used because it contains sufficient long-term performance advantages. The advantages include operation reliability, lower electrical costs, and the ease with which the project could be upgraded in the future without adding another accumulator ring. The decision was a hard one made just in time. Six months later would have been too late.

## **Q.** How will the SNS organization change as it moves from construction to full time operations?

One of the advantages of having a multi-lab project is the ability to avoid hiring a large number of design staff in the beginning and then replacing them with a new group of operations staff. Since 1999, we have been on a gradual upward ramp of employees planning to work full-time in Oak Ridge. We are not expecting significant changes as we transition from construction to operations. With the completion of the Cold Source at the High Flux Isotope Reactor, ORNL now has two neutron facilities at which scientists will conduct experiments. The programs will be seamless.

## **Q.** Do you expect the capabilities of the SNS to evolve over time?

Yes. With any project this large, you must plan for the fact that the technology will evolve and improve over the 40-year life of the facility. We have received funding to start a Power Upgrade, and there are plans for a second target building with spaces for additional instruments. During the design and construction of the SNS, ingenious technologies were devised to improve the facility. In Oak Ridge, for example, we developed a revolutionary, event-based, data acquisition system to record in real time neutron arrival times and positions. Our Materials Science and Technology Division designed an antenna that will help extend the ion source's lifetime. Other researchers developed diamond foils for stripping electrons from hydrogen ions leaving the accelerator to produce protons that collect in the accumulator ring. Our laser experts have developed accelerator diagnostics to enhance control of the ion beam. We will always be looking for new ideas on how to improve the SNS.

#### **Q.** Everyone has the same question. How will the SNS change our lives?

Literally everything in our lives is made from materials. If we can better understand how these materials behave, we can invent new drugs, lighter and more fuel-efficient cars and airplanes, more powerful computers, and metals that can last longer than we can imagine. The potential for the American economy is limitless.

## **Q.** Will the SNS reclaim the leadership role for America in neutron science?

Without question. The paradox is that America's scientific leadership will be regained with a remarkably international workforce at the SNS. Many of these scientists are foreign born and now American citizens who bring with them a wonderful breadth of experience and creativity. The same kind of international talent that made possible the Manhattan Project in World War II will make Oak Ridge and the SNS the envy of the scientific world.

#### **Q.** What do you do in your time away from this project?

For the past three years my most important activity has been chairing the Oak Ridge Public Schools Education Foundation. Our first task was to help raise \$55 million for the renovation of Oak Ridge High School. The second task was to raise another \$4 million to establish an endowment for the Oak Ridge school system. We recently reached our first goal, and construction has begun on what will be one of the best high schools in America. As the father of two boys and the person responsible for recruiting some of the world's top talent to Oak Ridge, I could think of few activities more rewarding. **(R)** 



#### **OF MICE AND MEN**

Genetically diverse mice will shed light on how human genes function.

Understanding how genes and the environment interact to control complex genetic traits, such as resistance to certain diseases, is among the most important challenges of biological research. Simulating the genetic diversity of the human population is a critical tool that will help answer this question.

The Collaborative Cross project in ORNL's Life Sciences Division will provide researchers worldwide with a pool of genetically diverse mice that mimics the genetic profile of a typical human population. Because researchers have sequenced the entire mouse genome, which is identical to 85% of the human genome, the mouse genome is an ideal slate for studying complex processes, such as the body's response to chemical, biological, and viral agents.

The ORNL project aims to produce 1000 viable strains of mice from eight original strains over the next seven years. "Part of the goal is to share mice with facilities all over the world," says Dabney Johnson, a genetics researcher at ORNL who headed up the team that wrote the proposal that won \$1.3 million from the Ellison Medical Foundation. The Collaborative Cross has already attracted international attention. Several institutions, including the University of Tennessee, the University of North Carolina, and Jackson Laboratory in Bar Harbor, Maine, are participating in the project.

ORNL's \$14 million Russell Laboratory for Comparative and Functional Genomics, a 36,000-square-foot facility completed in 2004, is a pathogen-free facility for breeding mice. A key part of ORNL's modernization plan, the "mouse house" has space for 80,000 mice, cryogenic storage, and an ideal environment for producing uncontaminated lab specimens.

> "Controlling environmental factors ensures that any differences in a complex process in the mice are genetic," Johnson says. "As an example, exposure to parasites, viruses, and bacteria can change the way

a mouse behaves or responds." Biologists using "clean" mice from the Collaborative Cross can confidently

attribute response differences to genetic factors. Researchers say this mouse population is critical to the development of a community resource for understanding the genetic and environmental complexity of human disease.

Johnson notes that the project generates large amounts of data for use with predictive models and simulations that can be run only by the largest supercomputers. In 2004, ORNL was selected as the site for DOE's National Leadership Computing Facility, which by 2007 will be capable of performing 250 trillion calculations per second and providing a previously unavailable computational capability for genome research.

One complex trait on which these mice can shed light is the human response to pathogens that might be used as weapons. "Los Alamos National Laboratory has discovered a gene that plays a part in the human response to anthrax," Johnson says. "We can change that gene in mice."

Based on their genetic makeup, some people are more susceptible or more resistant than others to infection by a disease agent. If researchers can determine how cells react when exposed to a pathogen, the genes that guide the reaction can be located. How these specific genes differ from person to person might allow biologists to gauge each person's susceptibility to a disease agent.

"We can find biomarkers that point to the first gene in the pathway and confirm it sets off the genetic chain reaction," Johnson says. Pharmaceutical companies can then develop a drug that targets the specific links in the chain and functions as the genetic firewall that protects against the disease agent.

Other potential benefits are emerging. "Suppose we could identify a susceptible population before its members were harmed," Johnson continues. "In a specific population, like military personnel that must be immunized against smallpox, identifying the individuals likely to have a strong response to the vaccine could alert us to the vaccinated soldiers that should be closely observed."

Armed with a modern mouse facility and one of the world's most powerful computers, ORNL researchers are confident they are just opening the door to a new era of biological discovery, where the secrets of humankind will be found among some of Earth's smallest creatures.—Eva Millwood ®

#### **INSTANT ID**

Detecting biological threats in five milliseconds might be the difference between life and death for modern soldiers.

The scenario is frightening. A terrorist group modifies clusters of anthrax bacteria so they resemble pollen grains. The life-threatening powder is

deposited on the ground in anticipation of U.S. troops. The challenge to both scientists and military planners is to detect this camouflaged biological warfare agent in time so that soldiers could safely avoid the contaminated area.

Two ORNL researchers are confident their unique tandem mass spectrometry configuration, a type of hybrid mass analyzer, and its operating method could be further developed to sense such a threat. They also believe that the hybrid mass analyzer, developed with funding from ORNL's Laboratory Directed Research and Development Program, is a strong candidate for the next-generation technology needed by the U.S. military to detect known and unknown biological warfare agents.

"This instrument, which might be up to 1000 times faster than current tandem mass spectrometers, could be the basis for a next-generation detector of chemical and biological threats," says Doug Goeringer. "Proper use of the instrument by proteomics researchers would significantly speed up data acquisition for protein identification. Each protein is identified based on its molecular weight and its unique sequence of amino acids coded for by DNA. Bioinformatics software, by sorting through all the data, could then identify protein biomarkers of specific microbes."

The analyzer was conceived by Goeringer, a scientist in ORNL's Chemical Sciences Division, and Scott McLuckey, a former ORNL researcher. CSD's Marc Wise helped Goeringer build the instrument prototype. Wise led the development of the ion trap mass spectrometer at the heart of the Block II chemical biological mass spectrometer (CBMS) used by the U.S. Army on its ground reconnaissance vehicles to detect chemical warfare agents in war zones. This year the Army is testing the mass spectrometer's ability to detect biological warfare agents.

The hybrid mass analyzer, which separates ions based on their mass-to-charge ratio, consists of a radiofrequency ion trap, a gas-filled radiofrequency quadrupole collision chamber, and a time-of-flight mass spectrometer arranged in a tandem configuration. The instrument can be operated to generate a three-dimensional mass spectrum of parent ions and associated product ions, formed when the parent ions' internal energies are raised until they fragment into lighter-weight ions.

Unlike the CBMS, the new instrument can almost simultaneously analyze a heterogeneous population of ions whereas the CBMS focuses on analyzing one homogeneous population at a time. The CBMS ion trap repeatedly selects one type of parent ion to store, fragment into product ions, and mass analyze, while expelling all other types of parent ions from the sample. The trap is then refilled with another sample, and the process is repeated multiple times.

"In our device no parent ions are thrown away from the trap because it is used only to store and sort them," Goeringer says. "The ions dissociate in the collision chamber, and the resultant fragment ions are subsequently mass analyzed in the time-of-flight spectrometer, which is about 1000 times faster than the ion trap. Thus, the ion trap doesn't have to be refilled each time the next type of parent ion is analyzed."

"The CBMS ion trap requires 5 seconds to analyze ions of 25 different chemical warfare agents, toxic industrial chemicals, and environmental pollutants," Wise says. "Those same 25 different ions can be identified in only 5 milliseconds by the hybrid mass analyzer."

The CBMS can detect bacteria but not viruses because this instrument focuses on fatty acids found only in bacteria. The practical benefits of the hybrid mass analyzer stem from its ability to identify quickly harmful viruses, as well as bacteria, because the technology can detect proteins found in both types of biological threats.

In situations where the difference between life and death can be measured in seconds, the hybrid mass analyzer may prove as valuable to modern soldiers as the helmet was to their predecessors. (R)

## **SUPERNOVA DISCOVERIES**

A partnership with high-performance computing helps astrophysicists understand how stars explode.

A rmed with the computational power of ORNL's National Leadership Computing Facility, now capable of 40 trillion calculations per second, computational astrophysicists with the ORNL-led TeraScale Supernova Initiative have made new scientific discoveries regarding the explosions of massive stars.

John Blondin of North Carolina State University and Tony Mezzacappa, TSI's leader and a corporate fellow in ORNL's Physics Division, used Blondin's computer code to produce a three-dimensional (3D) simulation of a core-collapse supernova on 5000 pro-

cessors of NLCF's Cray X1E supercomputer. Their discoveries relate to the shock wave generated when a star collapses and the core's inner part rebounds into matter falling inward. They discovered that, in 3D as well as 2D simulations, the shock wave becomes unstable, and this "standing accretion shock instability" induces rotation in what was previously a spherically symmetric configuration.

"The SASI induces counter-rotating flows of stellar matter on the inside of the star," Mezzacappa explains. "As matter spins and accretes on the central object of the simulated star, the process deposits angular momentum on the central object, spinning it up. We started with no spin and our simulation generated an object that spins at tens of milliseconds—just like a pulsar, which is a rotating neutron star."

Scientists have known for some time that supernovae are dying stars reborn as neutron stars. Pulsars are like lighthouse beacons, but their pulses are radio waves rather than visible light. The TSI simulation provides a plausible mechanism for explaining how a supernova can morph into a newly born, fastspinning pulsar after forming and flinging into space elements responsible for life on Earth.

"We predict that SASI, along with neutrino transport and the magnetic field from within the star, will affect how the shock wave generates the explosion," says Mezzacappa.

Blondin and Mezzacappa also found that 3D simulations of supernovae are far more realistic than 2D and 1D simulations. In a 1D simulation the only dimension is the radius. In a 2D simulation, the radius and latitude are the dimensions. A 3D simulation adds longitude. "In our multidimensional simulations we also take into account neutrino direction, neutrino energy, and time," Mezzacappa adds.

The 3D models run thus far at ORNL simulate only fluid dynamics. Mezzacappa and his colleagues plan to add neutrino transport, magnetic fields, and more realistic particle and nuclear physics to the models.

ORNL's Raphael Hix, who was recently selected for the 2006 Young Inves-

tigator Award by Sigma Xi, The Scientific Research Society, has shown that understanding reactions involving neutrinos and nuclei in supernovae can help astrophysicists get a better grasp on both how shock waves disrupt the star and which chemical elements are formed in the process. During core collapse, electrons captured by nuclei slam protons, resulting in the emission of electrically neutral, almost massless neutrinos. These events significantly affect the location of the birth of the shock wave.

During the explosion, neutrinos are also involved in nucleosynthesis—the formation of new elements in varying abundances in supernovae, including many elements found in our bodies and our planet. Proper consideration of the neutrinos interacting with nuclei in the outer layers results in predicted nuclear compositions much more like those observed.

TSI is a five-year research program funded by the Department of Energy. The proposed, five-year Petascale Supernova Initiative will include at least 37 investigators from 15 universities and 4 DOE national laboratories, led by ORNL.

The initiative's proposal is to simulate supernovae even more realistically by developing codes that will run on NLCF's planned petascale supercomputer—a machine that would make a thousand trillion calculations per second—in about three years. What has not been promised is a real supernova in our Galaxy, which would supply observational data to neutrino and gravitational wave detectors on Earth that could be used to validate the astrophysicists' codes. To better understand stellar death and rebirth, researchers are wishing *for* a star. **R** 

## **HOT TECHNOLOGY**

# Using nanotechnology at 600,000°C per second, researchers are laying the groundwork for new consumer products.

Researchers at ORNL have developed a rapid heating technology that could revolutionize the manufacturing of products made of materials whose functionality is maintained at the nanoscale. Called pulsed thermal processing (PTP), the technology enables researchers to control precisely the diffusion of atoms and the merging of nanoparticles to generate desirable electrical, optical, and magnetic properties in thin films and nanoparticle systems.

The researchers believe PTP could be used to produce affordable and more efficient solar electric cells; flexible digital displays that can be rolled up; light-emitting diodes that make digital clocks and traffic lights glow; and thin-film batteries needed to energize medical implants and radiofrequency identification labels on consumer products.

ORNL's research tool used for PTP is the most powerful light source in the world—a high-density plasma arc lamp that provides "white light" nearly matching the sun's spectrum, including infrared, visible, and ultraviolet light. The light source produced by Mattson Technologies is a direct-current arc that ionizes gas inside a water wall-insulated quartz window.

ORNL's Materials Processing Group in the Materials Science and Technology Division has demonstrated that the latest upgrade of the Mattson lamp can make various nanomaterials functional by delivering a flash of light as short as 1 millisecond at a power density up to 20,000 watts per square centimeter over an area almost as broad as a flat-panel computer screen. The lamp can heat surfaces up to 600,000°C per second. "We are trying to reduce the flash time to 0.1 millisecond," says Craig Blue, the division's associate director for technology. Decreasing the pulse time generates less 'heat soaking'—the amount of heat absorbed by the layers underneath the surface.

Guided by computer modeling of materials' thermophysical properties, the group conducts experiments with funding from ORNL's Laboratory Directed Research and Development Program and industrial firms. Modeling enables prediction of the "thermal profile"—the temperature on the surface and underlying layers based on the lamp's distance and the selected wavelengths of light and power density delivered to the sample. "We can filter out wavelengths we don't want," Blue says. Unlike laser processing, PTP can rapidly heat the entire surface area with one flash, potentially creating a uniform microstructure or nanocrystalline structure that has uniform electrical, optical, or magnetic properties. The technology is capable of thermally influencing the surface without thermally affecting the substrate.

"We have shown that the lamp can achieve critical annealing temperatures of 500 to 700°C for thin-film silicon in solar electric cells and thin-film silicon transistors for flat-panel displays," says team member Ron Ott. "The multibillion-dollar photovoltaic and thin-film transistor industry would like to anneal silicon on inexpensive polymer substrates, but inexpensive polymers cannot be heated to more than 150°C. PTP is the only process that can simultaneously heat the surface of the thin film or nanoparticle system to over 500°C and limit the substrate to 150°C over broad areas."

Laser processing currently used by the thin-film transistor industry is expensive, time consuming, and environmentally unfriendly because of the gases the technology uses. Laser light scanning surfaces creates non-uniform microstructures, resulting in non-uniform electrical and optical properties and stresses that can lead to cracking.

Solar cells made of inexpensive, amorphous silicon convert about 5% of sunlight into electricity. PTP, which offers high throughput at a low cost, introduces nanocrystals into the matrix, creating more charge carriers, increasing electron mobility, and doubling the photovoltaic efficiency to about 10%.

Ott proved in an LDRD project that the lamp could increase data storage 1000 times by chemically ordering magnetic ironplatinum nanoparticles.

Researchers from ORNL and Caterpillar, the world's largest manufacturer of construction equipment, worked together to use PTP to coat bearings. Caterpillar now owns a Mattson lamp and is prototyping the technology.

Researchers already are thinking beyond the laboratory. "We and Mattson envision a third-generation lamp at ORNL that would be a dedicated user facility for industry," Blue says. "Before buying a lamp, each user could collaborate with us to develop the process science for making prototypes. The user's experiences could then be transferred to the factory environment to make marketable devices." ®



Ward Plummer, an ORNL-University of Tennessee Distinguished Scientist, has been elected to membership in the *National Academy of Sciences*. Plummer is director of the new Joint Institute for Advanced Materials that will be built on the UT campus. He also supervises research at the Department of Energy's Center for Nanophase Materials Sciences at ORNL.

Theoretical astrophysicist W. Raphael Hix received the 2006 Young Investigator Award of Sigma Xi, The Scientific Research Society for his research in nuclear physics, novae, supernovae, X-ray and gamma-ray bursts, and stellar

structure and evolution, including nucleosynthesis—the cosmic origins of the elements that make up the universe.

> Yuri Melnichenko has been elected a *fellow of the American Physical Society* for his studies of polymer materials using small-angle neutron scattering techniques.

> > Peter Cummings has been elected a fellow of the American Physical Society for his contributions to the

Ward Plummer, elected to the National Academy of Sciences molecular understanding of industrially relevant fluids and processes and for his national leadership in applied molecular modeling and computational nanoscience.

**Cam Hubbard** was elected a **distinguished** fellow of the International Centre for Diffraction Data, in recognition of his extensive contributions to the ICDD and the field of X-ray powder diffraction.

Andrew Payzant was elected a *fellow of the International Centre for Diffraction Data* in recognition of years of leadership and service to the ICDD beyond that normally associated with membership.

Brian Davison has been elected to the College of Fellows in the American Institute for Medical and Biological Engineering.

Tim Burchell received the Hsun Lee Lecture Award given by the Institute of Metal Research, Chinese Academy of Sciences, for significant contributions to materials science and engineering.

Panos Datskos received the Charles Stark Draper Award for Most Outstanding Tutorial at last year's 51st International Instrumentation Symposium (IIS) of the Instrument Society of America. His tutorial, entitled "Using MEMS and NEMS as Sensors," was ranked first.

Elliot Volkin, co-discoverer of messenger RNA and a retired ORNL biologist, received **Penn State University's Distinguished Alumni Award**, the University's highest award for an individual. Former ORNL Director Alvin Weinberg ranks the discovery of mRNA by Volkin and the late Lazarus Astrachan as the most significant ever at ORNL and one of the most important events in the history of molecular biology. ®

#### Next Issue...



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