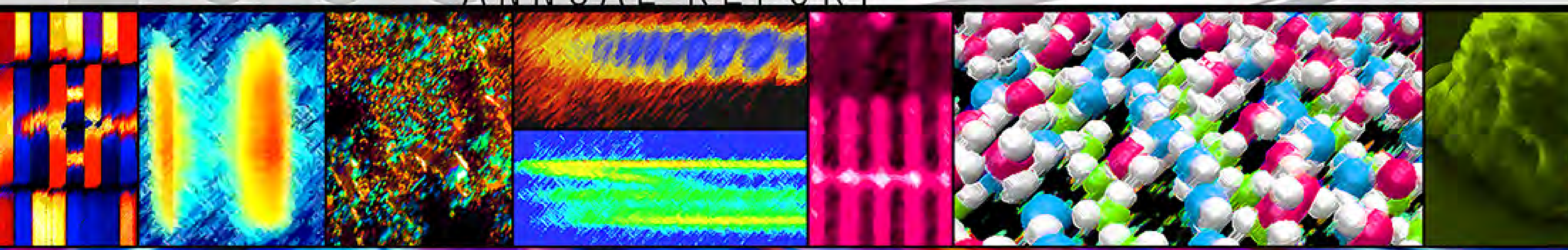
2008 ANNUAL REPORT



OAK RIDGE NATIONAL LABORATORY

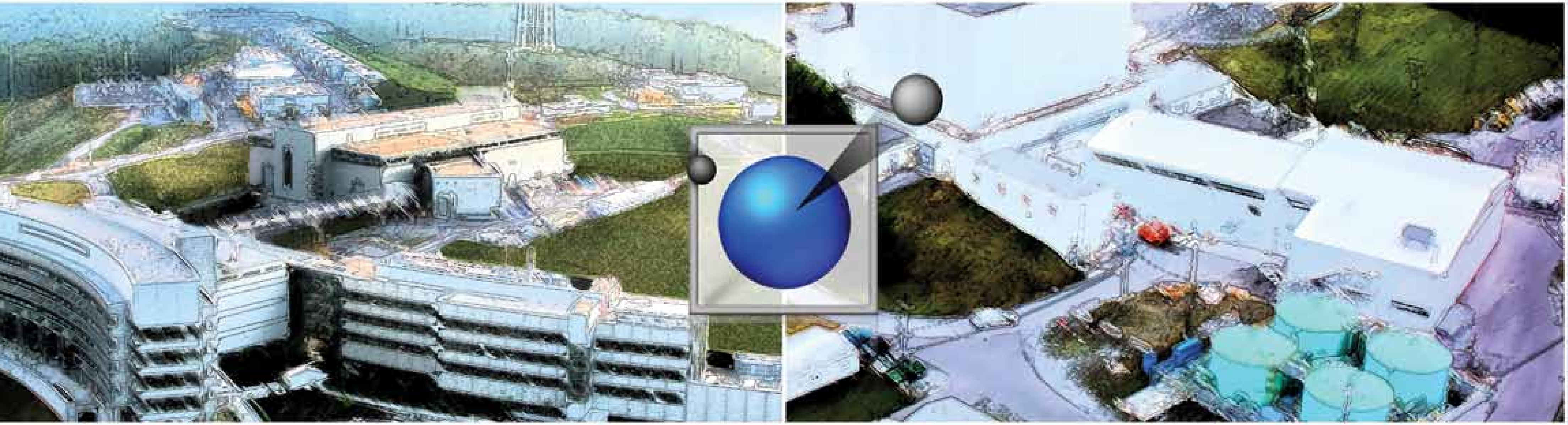
NEUTRON SCIENCES

MANAGED BY UT-BATTELLE FOR THE U.S. DEPARTMENT OF ENERGY

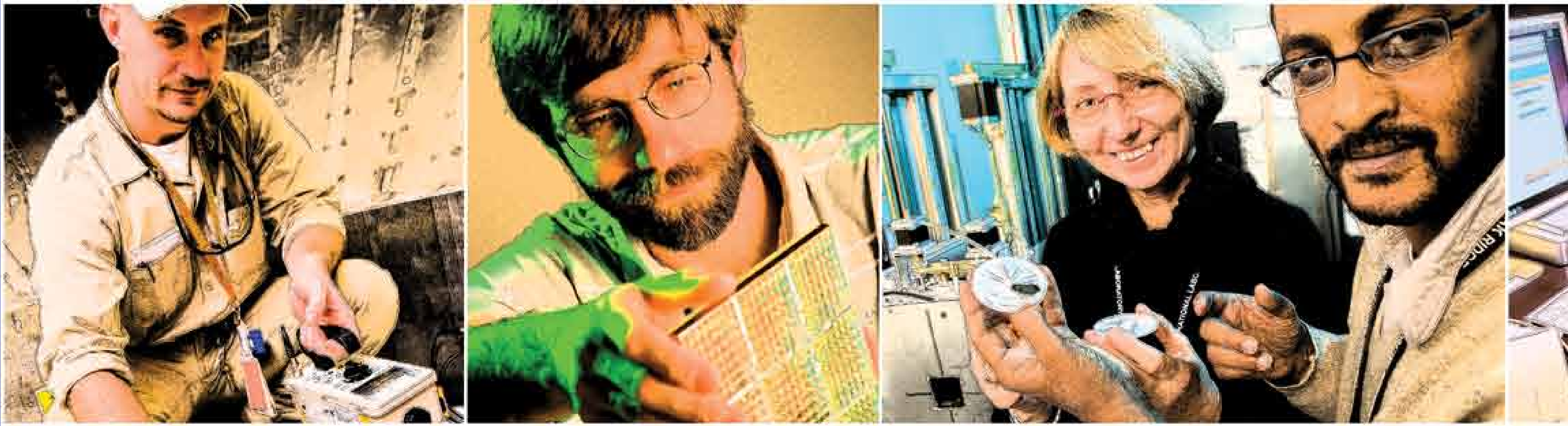
Front and back covers: Artist's enhancements of visualizations from neutron scattering data.

OAK RIDGE NATIONAL LABORATORY
NEUTRON SCIENCES

The Neutron Sciences Directorate is part of Oak Ridge National Laboratory, which is managed by UT-Battelle, LLC, under contract DE-AC05-00OR22725 for the U.S. Department of Energy. SNS and HFIR are funded by the U.S. Department of Energy Office of Basic Energy Sciences.



ORNL Neutron Sciences 2008 Annual Report



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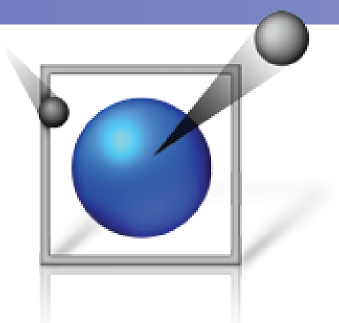
Welcome

Ian Anderson,
Associate Laboratory Director
for Neutron Sciences



When I look back at the changes that have occurred in the past year, I can't help but marvel at the progress we've made in increasing and improving the performance and instrumentation of the Spallation Neutron Source (SNS) and High Flux Isotope Reactor (HFIR), bringing users to our facilities, and producing scientific results. I must thank the staff of the Neutron Sciences Directorate and our sponsor, the U.S. Department of Energy (DOE) Office of Basic Energy Sciences, for its demonstrated commitment to the vision of providing the scientific community with unprecedented capabilities for understanding the structure and properties of materials.

Early in the year, SNS became the official Guinness World Record holder for the most powerful pulsed spallation neutron source. With every increase in power during the year, we continued to break that record and ended the year at more than twice the power that won us the record. In total, beam power was increased by nearly a factor of four to 625 kilowatts. The coming years will remain a challenge as we work to achieve 1.4 megawatts of beam power by FY 2010 or CY 2011. At HFIR, the new cold source operated successfully all year, providing unique capabilities to the research community. HFIR finished the year completing six cycles and beginning a seventh, which allowed us to provide instrument time to students participating in the Neutron and X-Ray Scattering School.

We made significant progress toward providing a full complement of instruments at SNS and HFIR (25 and 11, respectively) by completing 4 instruments at SNS (CNCS, SNAP, SEQUOIA, and FNPB) and 2 at HFIR (Powder and Single-Crystal diffractometers). As we add instruments, the number of users is also increasing. HFIR hosted 258 users, and 165 were hosted at SNS. Improvements were continually made with the Integrated Proposal Management System, making it easier for users to submit proposals and obtain facility support.

As stewards of a national resource for scientific discovery, it is most gratifying to see an increase in the number of publications resulting from work at SNS and HFIR. More than 140 open literature publications were produced, and inside this report you'll find highlights from just a few. I'm also particularly pleased to see our staff being recognized through awards and invitations to share their expertise at meetings such as the National Neutron and X-Ray Scattering School (cohosted with Argonne National Laboratory), the American Crystallographic Association annual meeting, and the 2008 High-Intensity, High-Brightness Hadron Beams Workshop. We plan to take an even greater role in educating various communities (e.g., the public, scientific, and academic) about using neutrons to study materials. This year, for example, we cohosted the workshop on "Leadership in Neutron Scattering Education." We also anticipate that completion of the Joint Institute of Neutron Sciences in 2010 will spark exciting educational and outreach opportunities in collaboration with the University of Tennessee and other institutions.

The past year has provided us with some remarkable achievements thanks to the continued dedication of all our staff and collaborators, and I am particularly proud of the excellent safety record that has been maintained throughout another busy year.

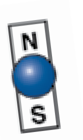
I hope you enjoy reading this report and sharing with us the excitement of neutron science at ORNL.

Ian Anderson

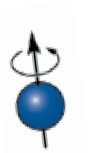
Neutron Primer

Neutron Properties

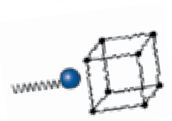
Neutrons are **NEUTRAL** particles.
They
- are highly penetrating,
- can be used as nondestructive probes, and
- can be used to study samples in severe environments.



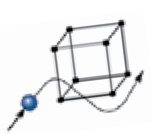
Neutrons have a **MAGNETIC** moment. They can be used to
- study microscopic magnetic structure,
- study magnetic fluctuations, and
- develop magnetic materials.



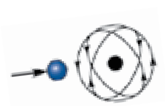
Neutrons have **SPIN**. They can be
- formed into polarized neutron beams,
- used to study nuclear (atomic) orientation, and
- used to distinguish between coherent and incoherent scattering.



The **ENERGIES** of thermal neutrons are similar to the energies of elementary excitations in solids, making them useful in the study of
- molecular vibrations,
- lattice modes, and
- dynamics of atomic motion.



The **WAVELENGTHS** of neutrons are similar to atomic spacings. They can determine
- structural information from 10^{-13} to 10^{-4} centimeters and
- crystal structures and atomic spacings.



Neutrons "see" **NUCLEI**. They
- are sensitive to light atoms,
- can exploit isotopic substitution, and
- can use contrast variation to differentiate complex molecular structures.

Neutrons are useful in research because they reveal properties of materials that other types of probes can't. Why is that?

Neutrality. Because they have no electrical charge, neutrons can penetrate deeply into materials without being attracted to charged particles in the atoms. This neutrality makes neutrons ideal for determining the molecular structure of materials.

Unique sensitivity to light atoms, such as hydrogen. Neutrons can precisely locate hydrogen atoms in a sample. Thus researchers can get a clearer view of molecular structure than with other probes. That's especially important in designing drugs. It also enables neutrons to find hidden water molecules in materials, revealing microscopic cracks and corrosion.

Magnetism. Neutrons act like tiny magnets pointing in a particular direction. Polarized neutrons, which all point in the same direction, let scientists probe the properties of magnetic materials and measure fluctuations in magnetic fields.

Energy. The energies of neutrons closely match the energies of atoms in motion. Thus they can be used to track molecular vibrations; movements of atoms during catalytic reactions; and behaviors of materials under forces such as heat, pressure, or magnetic fields.

Since neutrons are everywhere, why do we need special neutron facilities to make them?

When a stream of neutrons hits a sample of material, some of them go right through it. Others hit atomic nuclei in the material and bounce away. Where they bounce, how fast, and where they land reveal details about the structure and properties of the material. As we sometimes need to shine a bright light on something to see it clearly, researchers need "bright" beams of neutrons to see those fine details. HFIR and SNS are two of the brightest sources of neutrons in the world for research—opening the door to a huge realm of possibilities in materials science.

In addition to the bright neutron sources, the ORNL facilities provide two different types of neutron beams. For some research, it's better to have neutrons available in a series of pulses (as SNS provides); for other research, it's more advantageous to have a continuous source of neutrons (as HFIR provides). Having both types of neutron beams available to users at one location provides an invaluable resource for researchers from all over the world.

For more information about neutrons and neutron scattering science, see neutrons.ornl.gov/science/ns_primer.pdf.

Year in Review

Saad Elorfi and Andrew Church work on Slim SAM.

ORNL Director Thom Mason with the Guinness World Record award for SNS. The record was reached when beam power was ramped up to more than 300 kilowatts, producing 4.8 x 10^{16} neutrons per second. With every increase in power during the year, we continued to break that record and ended the year at more than twice the record-breaking power. In total, beam power was increased to 625 kilowatts—nearly a factor of four.

SNS Now Home to World's First Actively Shielded Magnet for Neutron Scattering

Neutron scattering scientists often need to apply strong magnetic fields to the materials they study, but the stray magnetic fields generated can wreak havoc on their (and their neighbors') experiments. SNS has taken a big step toward solving this problem by commissioning the world's first actively shielded magnet system, known as Slim SAM (SAM = shielded asymmetric magnet), designed specifically for neutron scattering.

Slim SAM not only eliminates the detrimental effects of stray fields but also offers new opportunities for the growing number of scientists interested in polarized neutron diffraction. To produce Slim SAM, a team of ORNL scientists, led by Hal Lee, developed detailed magnetic field profile specifications to ensure superior polarized beam performance. They drafted a comprehensive solicitation package, evaluated vendor proposals, and ultimately guided the winning vendor in producing an excellent design.

The past year was exciting and productive, as research results started to appear in publication, six new instruments were completed, and technology developments continued to rise. Many more users than expected conducted experiments at both SNS and HFIR, and SNS became the official Guinness World Record holder for the most powerful pulsed neutron source.

Science Highlights

High-Temperature Superconductors

Scientists are excited about last year's discovery of a new class of high-temperature superconductors (HTSs). Continuing work begun at other facilities, researchers from ORNL, the University of Tennessee, and the National Institute of Standards and Technology conducted groundbreaking experiments confirming that the iron-based materials were indeed superconductors at 43 kelvin, a higher temperature than any recorded conventional superconductor. This work is helping shed a light on the puzzling phenomenon of how HTSs work, which, when better understood, could have a tremendous impact on energy use.

Protein Studies on Huntington's Disease

Scientists are studying the aggregation of protein fibrils (threadlike fibers) to determine their role in

the development of Huntington's Disease, which is caused by an abnormal sequence of amino acids in the huntingtin protein. Using small-angle neutron scattering, researchers were able to look at samples on a nanometer-length scale, allowing them to capture snapshots of protein structure as it aggregated into fibrils and to determine the rate of aggregation. Data from the experiments are being used by the University of Tennessee Medical Center to better understand how these changes relate directly to Huntington's Disease.

Will Reynolds of the SNS Detectors Group installs a 2-meter-long linear position-sensitive detector into an 8-pack.

High-Pressure Studies

Researchers have been using brucite to discover how hydrogen and deuterium behave differently under extreme pressure. Using a technique called angle-dispersive diffraction, scientists were able to see changes in the core shape of brucite crystals, indicating how close the atoms in the samples become under applied pressure. The work is helping to clarify

GE Energy to Market SNS Detector Electronics

GE Energy, manufacturer of radiation detection equipment, has signed a technology transfer agreement to market the electronics and software developed by ORNL engineers for an award-winning system of sensitive neutron detectors. Developed by Ron Cooper and Rick Riedel of the Neutron Sciences Directorate and Lloyd Clonts of the Measurement Science and Systems Engineering Division, the system was designed to accommodate the large detector areas and high detection rates required by SNS.

The invention, explains Riedel, is called an 8Pack because each module contains eight long parallel tubes. Inside each tube are a resistive wire and helium-3, an important isotope in neutron detection instrumentation. Hundreds of tubes are needed to detect all the neutrons scattered from an experimental sample at a variety of angles.

"The system is modular so that very large detector arrays can be built," says Cooper. "We can have greater than 50 square meters of detector coverage. The system has high rate capability and good position resolution. And it features modern, distributed PC-based electronics."

A solar-powered version, Pharos, won an R&D 100 award in 2007 as one of the year's top technologies as determined by *R&D Magazine*. This portable, cordless system could be of interest for security applications, such as monitoring shipments.

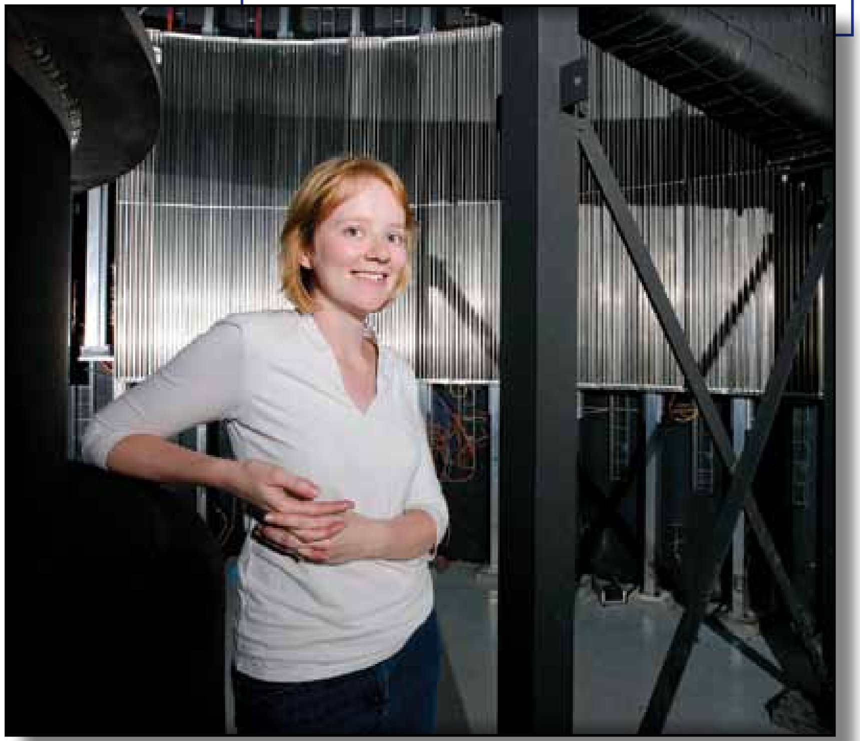
Using the integrated circuit designs and firmware developed by ORNL, GE will build the additional systems needed by SNS. Although SNS is currently the largest customer for the 8Pack system, the market will likely expand to other neutron scattering facilities throughout the world.

"It's exciting that, even as SNS ramps up to its full power of 1.4 megawatts, technologies from its development are already finding their way to the marketplace," says ORNL Director Thom Mason.

fundamental differences between the two isotopes in terms of compressibility. Because of the abundance of hydrogen in the world around us, the potential impacts from these studies are wide ranging and could lead to advances in fields such as medicine, geoscience, and industrial technology.

Biomass Studies

Although biomass from plants offers a potentially abundant source of ethanol, its complex structure makes it difficult to break down and convert to fuel. Understanding the structure of biomass at a molecular level is key to making practical use of this resource. Using small-angle neutron scattering and ORNL's supercomputing capabilities, scientists have been able to see unprecedented levels of detail in biomass structure at both the molecular and atomic levels. This information will help engineers develop new, cost-effective methods for turning biomass into a viable energy source, leading to lower energy costs and reduced pollution.

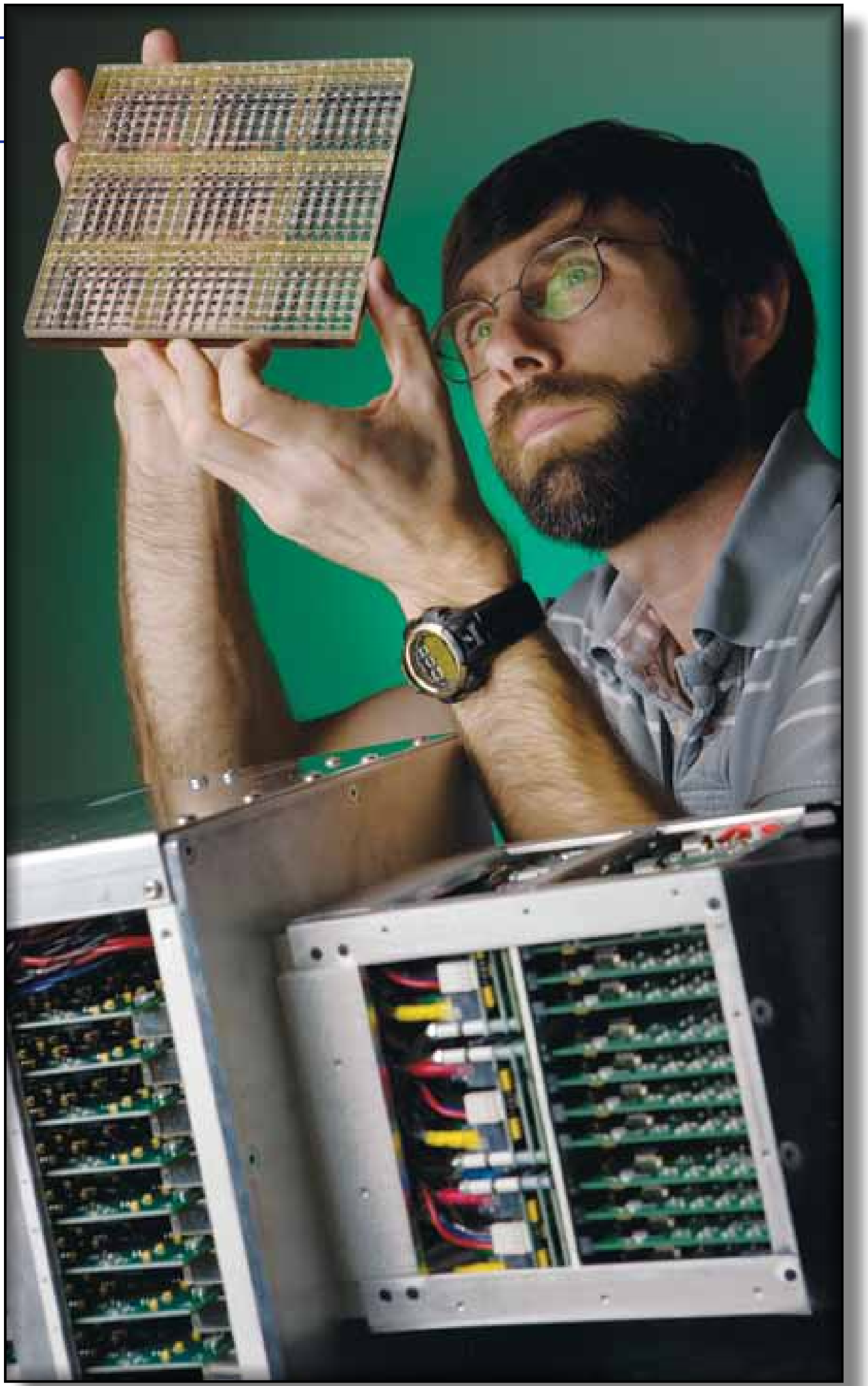


Jennifer Niedziela, scientific associate for CNCS, in front of the instrument's detector array.

Technology Development

Technological and research developments in 2008 were many. Significant enhancements were added for users, including new instruments and expanded experimental capabilities.

Six instruments were completed and are now being commissioned. These are the Powder and Four-Circle diffractometers at HFIR and four new instruments at SNS: CNCS, SNAP, SEQUOIA, and FNPB. Scientists have



Ted Visscher, Detector Group, inspects a parahedral lens on the Anger camera.

been taking advantage of the unique capabilities of CNCS and SNAP, and research results from each instrument has already been published (see "Under Extreme Pressure" and "Frustrated Spin Correlations in Diluted Spin Ice" in the Science Highlights section).

Sample environment capabilities were expanded by commissioning of the world's first actively shielded magnet for neutron scattering—Slim SAM—opening the door for a wide range of experiments (see sidebar on page 7). The scientific scope of several instruments has also been expanded by development of a new Anger camera system with a 1-mm position resolution. The previously unavailable high resolution of this camera permits new opportunities for research on the molecular structure of solid materials, or crystallography. In addition, a contract was signed with GE Energy to market the electronics and software associated with a new award-winning neutron detector system developed at SNS (see sidebar on page 8).

A Wealth of Users

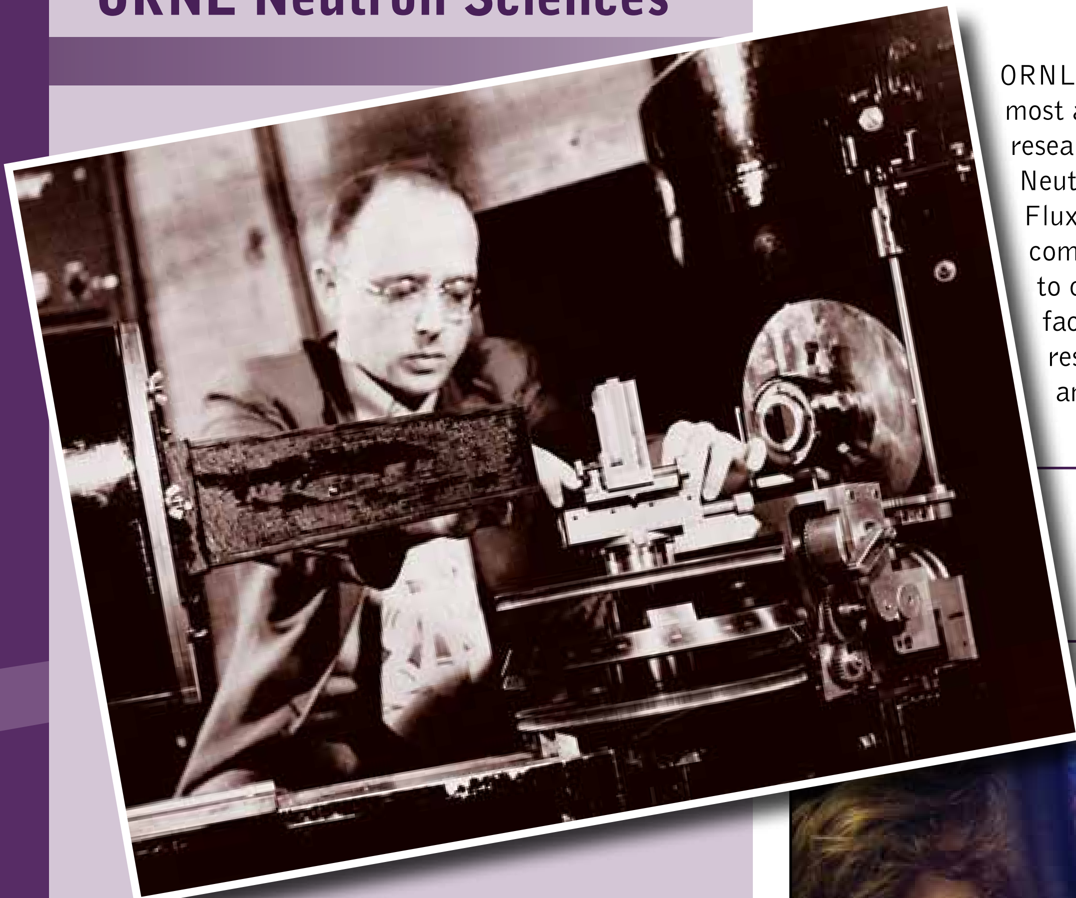
For our second full year of operations at SNS and an upgraded HFIR, we hosted many more users than expected. Our goals of 225 users at HFIR and 75 users at SNS were surpassed with a final tally of 258 at HFIR and 165 at SNS. Users came from a variety of institutions all over the world, mainly from academia, and produced an impressive array of research results. More than 140 publications were authored or coauthored by scientists using SNS and HFIR and by Neutron Sciences staff conducting research at other facilities.

Users Jerod Wagman and Gregory Van Gastell of McMaster University analyze the results of their measurements on high-Tc cuprates at the HB-3 Triple-Axis Spectrometer at HFIR.

Jaime Fernandez-Baca (left), leader of the Triple-Axis Group, with user Hirosha Fukazawa.

ABOUT US

ORNL Neutron Sciences



Clifford Shull conducted some of the world's first neutron scattering experiments using this diffractometer at ORNL.

ORNL has a long history in neutron scattering. In fact, the field was pioneered at ORNL in 1946 by Clifford G. Shull. Shull went on to be a corecipient of the 1994 Nobel Prize in Physics for his groundbreaking work. Today, ORNL is becoming a preferred destination for neutron scattering research, where scientific advancements at these state-of-the-art facilities will continue for years to come.

ORNL operates two of the world's most advanced neutron scattering research facilities: the Spallation Neutron Source and the High Flux Isotope Reactor. Scientists come from all over the world to conduct research at these facilities. The basic scientific research conducted using SNS and HFIR will lead to technological advances that benefit the scientific, business, and industrial communities.

Funded by the DOE Office of Basic Energy Sciences, SNS and HFIR are national user facilities managed by the ORNL Neutron Sciences Directorate. The Neutron Sciences vision is to provide unprecedented capabilities for understanding the structure and properties of materials across the spectrum of biology, chemistry, physics, and engineering and to stay at the leading edge of neutron science by developing new instruments, tools, and services.

The main goal for the directorate is to achieve excellence in science, and all of our activities support this purpose. Through reliable operation and continual development, we strive to capitalize on the capabilities of two of the world's highest-flux pulsed and continuous beams of neutrons. We have a common user program for the two facilities and have integrated operations between them. In addition, we're focusing efforts on reaching out to the scientific community to educate current and future scientists about the benefits of neutron scattering.

Antonio Moreira dos Santos, member of the SNAP team at SNS, aligns diamond anvils before an experiment. The diamond anvil cell is the standard equipment for researching materials under high pressure.

Neutron scattering research impacts many products and technologies that are part of everyday life. Scientists are using neutron scattering to analyze and improve materials used in a multitude of different products, such as medicines and materials for medical implants, chips and thin films for electronics, lubricants and structural materials used in cars and airplanes, and many more. Neutron scattering research could also lead to improved processes that help protect the environment and public health.

Facilities

Spallation Neutron Source

SNS is an accelerator-based neutron source that provides the most intense pulsed neutron beams in the world for scientific and industrial research and development. With its eventual suite of up to 25 best-in-class instruments, SNS will give researchers detailed snapshots of smaller samples of physical and biological materials than previously possible. The diverse applications of neutron scattering research will provide opportunities for experts in practically every scientific and technical field. Moreover, technological discoveries at SNS will provide lasting benefits to the scientific, business, and industrial communities.

High Flux Isotope Reactor

The 85-megawatt HFIR provides one of the highest steady-state neutron fluxes of any research reactor in the world. HFIR fulfills four missions: isotope production, materials irradiation, neutron activation, and research using neutron scattering, which is the focus of this report. The neutron scattering instruments at HFIR enable fundamental and applied research into the molecular and magnetic structures and behavior of materials. HFIR has 11 instruments planned or in operation, including two cold-source instruments in the user program, that greatly enhance the reactor's research capabilities, particularly in the biological sciences.

Operations

Spallation Neutron Source

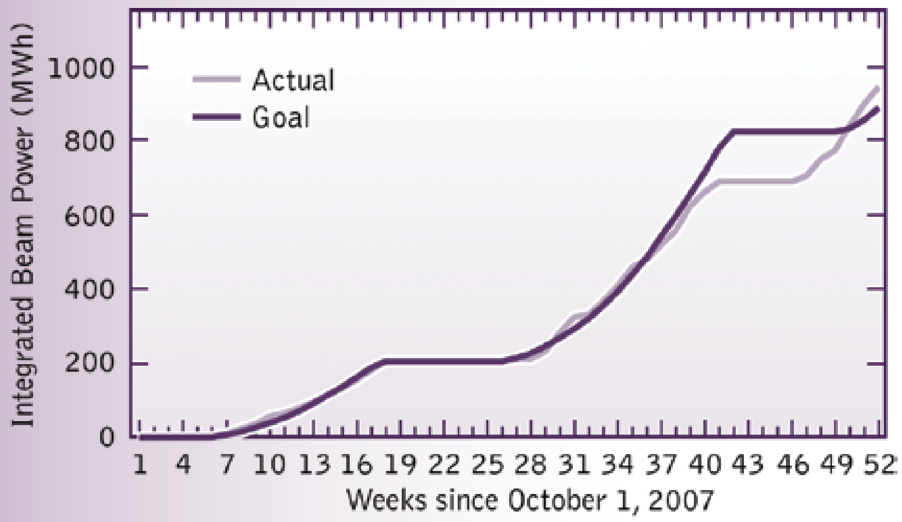
Fiscal year 2008 was the second full year of operation for SNS, and operations progress was significant. Operating power levels, neutron production, and reliability have all steadily increased. By the end of the fiscal year, we had achieved

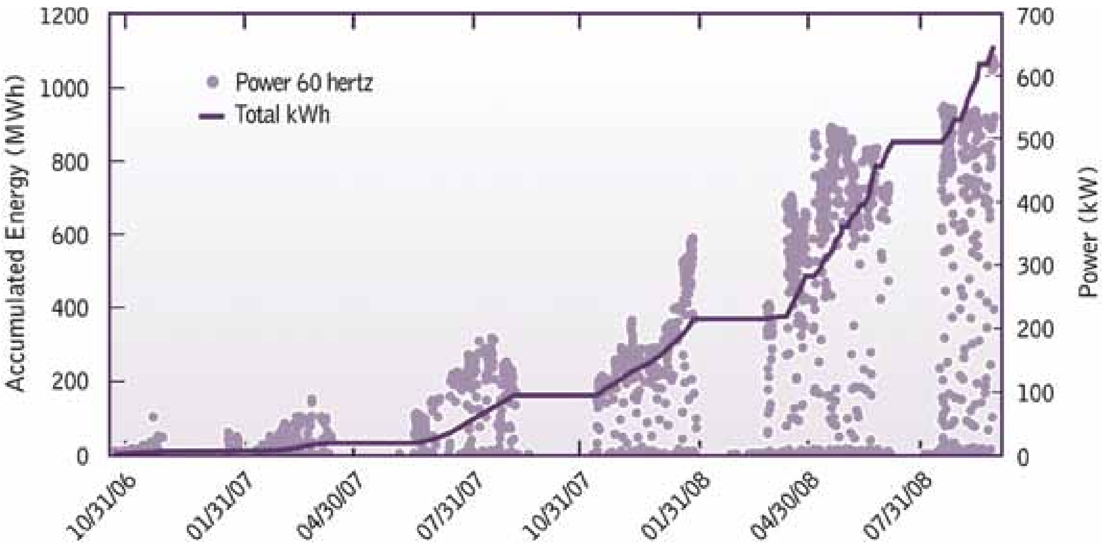
- Continuous operation at 625 kilowatts
- A record number of protons per pulse: 1.1×10^{14}
- 60-hertz beam to target at 625 kilowatts
- 945 megawatt-hours of beam to target
- Accelerator availability of 72%
- 2758 neutron production hours

The graph below left shows the integrated beam power delivered versus the SNS commitment for fiscal year 2008 (October 2007 through September 2008).

The plot below right shows the energy and power on target for fiscal year 2008. For fiscal year 2009, plans are to operate for 4500 hours, reach an operating power of 970 kilowatts, and produce neutrons for 3500 hours. In addition, machine availability is expected to increase to about 88%.

Contact: George Dodson (dodsong@ornl.gov)





High Flux Isotope Reactor

Fiscal year 2008 was highly productive for HFIR operations and marked the first full year of operation with the cold neutron source and a new suite of scientific instruments. By the end of the fiscal year, we had

- Operated for 3550 hours, or slightly more than six cycles.
- Irradiated materials to provide isotopes for medical research and commercial uses and to provide data for fusion reactor design.
- Irradiated and analyzed 221 samples in the HFIR Neutron Activation Analysis Facility in support of nuclear nonproliferation work, forensics studies for criminal investigations, special radioactive source production, reactor materials dedication, and basic science.
- Improved and upgraded HFIR for reliable, sustained operation, including refurbishment of two of its four main coolant pumps, electrical distribution system upgrades, reactor temperature control system upgrades, and building heating and air conditioning system improvements.

Users Hiroshi Kagayama (left) of Kyoto University and Masakazu Nishi (right) of the University of Tokyo analyze data at the Polarized Triple-Axis Spectrometer at HFIR.

The planned operations for fiscal year 2009 will be similar to 2008, with a tentative schedule of 140 operating days provided over six operating cycles. Steady-state operation will eventually provide neutron beams and irradiation services for eight to ten reactor cycles per year. With regular operation, the next anticipated major shutdown—for a beryllium reflector replacement—will not be necessary until after 2020.

Contact: Mike Farrar (farrarmb@ornl.gov)

Complementary ORNL Facilities

Research capabilities at HFIR and SNS are enhanced by the proximity of other ORNL user facilities, most with the same access and training requirements. One of our major goals is to improve integration between the facilities, making it easier for users to access the support they need. Major user facilities at ORNL include the following:

- Center for Structural Molecular Biology (CSMB)
- Bio-Deuteration Laboratory
- Center for Nanophase Materials Sciences (CNMS)
- National Center for Computational Sciences (NCCS)
- Shared Research Equipment User Facility (SHaRE)
- High Temperature Materials Laboratory (HTML)

Center for Structural Molecular Biology (www.cnms.ornl.gov)

CSMB operates the HFIR Bio-SANS instrument. The center develops technologies and methodologies for the structural molecular biology research community and computational tools to reduce, analyze, model, and interpret SANS data.

Bio-Deuteration Laboratory (www.csmb.ornl.gov/Bio-Deuteration)

The Bio-Deuteration Laboratory was designed for in vivo production of hydrogen/deuterium–labeled bio-macromolecules. The laboratory provides facilities and expertise for cloning, protein expression, purification, and characterization of deuterium-labeled biological macromolecules.

Center for Nanophase Materials Sciences (www.cnms.ornl.gov/)

CNMS is a research facility for nanoscale science and technology. The center allows users access to a complete suite of unique capabilities for studying nanoscale materials and assemblies.

CNMS employees work with materials 100,000 times smaller than a human hair.

The NCCS "Jaquar" supercomputer.

National Center for Computational Sciences (www.nccs.gov)

NCCS hosts the Cray "Jaguar" supercomputer, the most powerful system in the world for open scientific use. Jaguar is actually two systems, with a combined peak theoretical performance of 1.64 petaflops, or 1.64 quadrillion floating point operations per second. NCCS is also home to several smaller computers.

Shared Research Equipment User Facility (www.ms.ornl.gov/share)

SHaRE provides access to a suite of advanced instruments and expert staff scientists for the micrometer-to-nanometer-scale characterization of materials in several focused research areas: transmission and scanning electron microscopy, atom probe tomography, x-ray photoelectron spectrometry, and dual-beam focused ion beam and ultramicrotomy specimen preparation and support.

High Temperature Materials Laboratory (www.html.ornl.gov)

HTML helps solve materials problems that limit the efficiency and reliability of automotive systems. The center's instruments can characterize the structural, chemical, physical, and mechanical properties of materials at the nanoscale and microscale over a wide range of temperatures and pressures.

Laura Riester adjusts a specimen for measuring elastic properties using resonant ultrasound at HTML.

Niels de Jonge with SHaRE's scanning transmission electron microscope.

Safety

Doug Abernathy explains the safety warning system for ARCS at SNS.

Safety is critical to the success of neutron sciences work at ORNL. Efficient operation and safety are inextricably linked and are an integral part of every individual's performance plan. One of our primary goals is to operate the best neutron facilities in the world. Achieving this goal means involving staff in all levels of work, from planning through posttask analyses, and incorporating the best ideas from those with the most knowledge of the hazards.

Our facilities are regulated by DOE requirements for reactors (HFIR) and accelerators (SNS). These safety-based requirements are clearly identified to establish safe operating envelopes. Work control processes ensure the integrity of systems created to protect staff, the public, and the environment. In addition to focusing on working safety, staff strive to reduce or eliminate pollution and waste materials, as well as to conserve energy and other resources.

In the spirit of continuous improvement and to avoid complacency, a number of programs are being implemented to move to more in-depth levels of safe operation. One such program is the Management Observation Program, which increases worker involvement and ownership of the safety programs. For example, involving workers in planning activities during the major maintenance periods at SNS reduced the radioactive dose by about 60% from the levels initially estimated for the work. This task-level planning led to using as-low-as-reasonably-achievable goals even more effectively than for previous jobs and resulted in the use of real-time dose feedback that provided immediate dose information to workers. This instant-feedback method is now used for maintenance and other tasks and is implemented throughout the entire work control process.

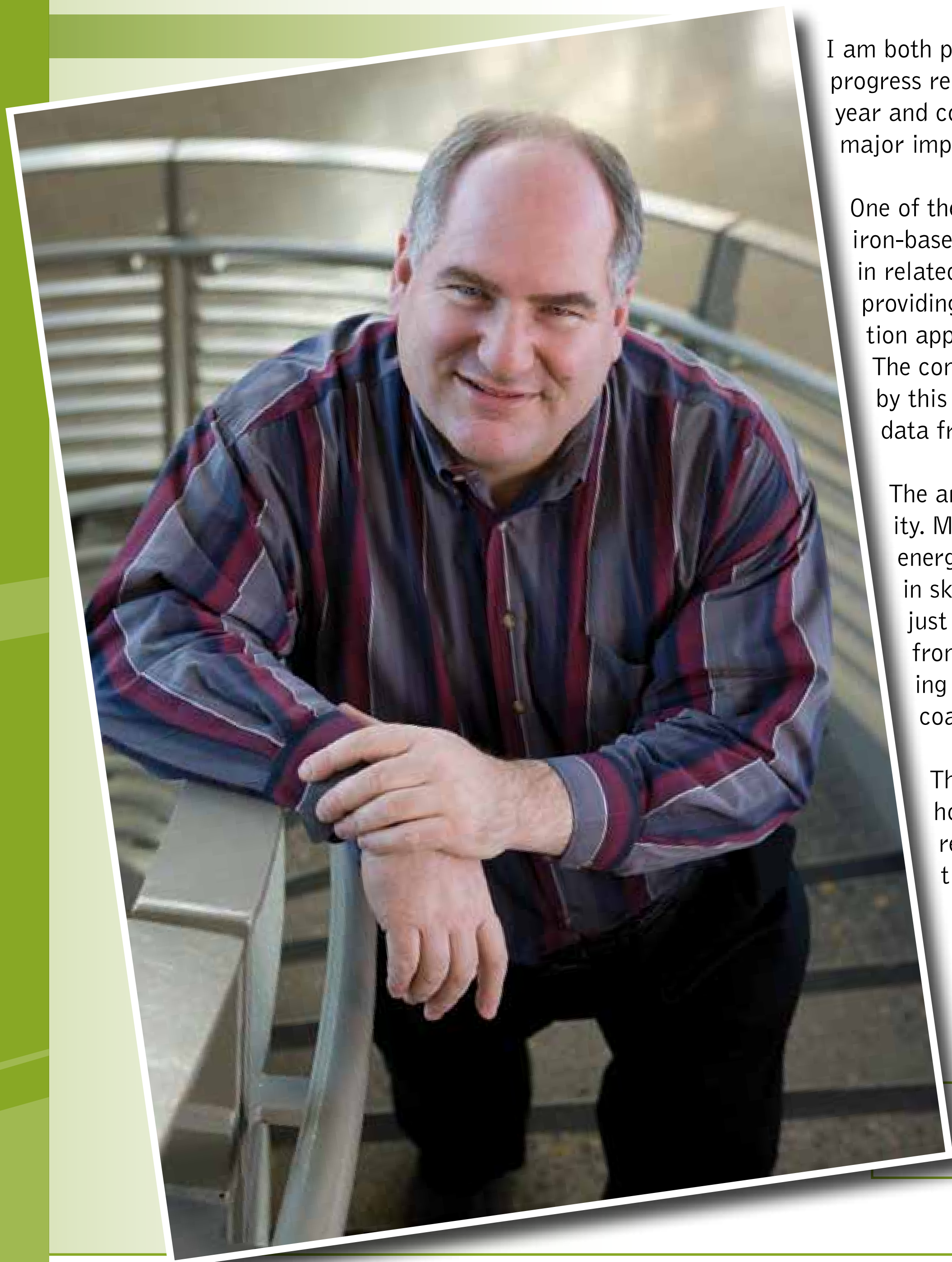
One of our most important successes this year was our outstanding safety record. We worked 1.4 million hours with no injuries that resulted in restrictions or lost workdays.

Contact: Frank Kornegay (kornegayfc@ornl.gov)

Bradley Alcorn demonstrates harness safety in the SNS Target Building.

SCIENCE HIGHLIGHTS

From the Neutron Scattering Chief Scientist



I am both pleased and privileged to introduce the "Science Highlights" section of the second annual progress report of the ORNL Neutron Sciences Directorate. It is exciting to look back over the past year and consider the wide range of neutron science activity and to note how it is beginning to have a major impact on the research community.

One of the year's biggest stories is the rapid advance of knowledge concerning recently discovered iron-based superconductors. Important results obtained at ORNL found antiferromagnetic behavior in related parent compounds, characterized the phonon density of states in the superconductors providing evidence for unconventional behavior, and established that a resonant magnetic excitation appeared below the critical temperature at a wavevector related to the antiferromagnetism. The complementary nature of pulsed and continuous neutron scattering was brilliantly illustrated by this work, which used instruments at both SNS and HFIR, and led to the first publication of data from the ARCS instrument at SNS.

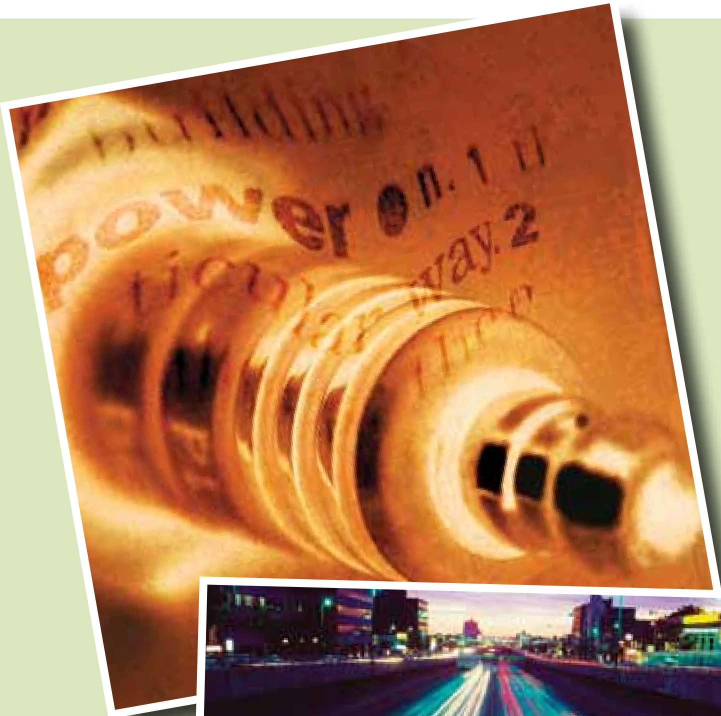
The anticipated explosion of research utilizing the new SANS instruments has become a reality. Much of the basic science work has clear societal relevance: looking for new means of solar energy conversion, finding a cure for Huntington's disease, understanding nanoparticles used in skin care products, and researching new high-temperature alloys used in engine turbines are just some of the examples. Neutron reflectivity has also come into its own with work ranging from biofuels to artificial membranes to magnetic multilayers. High-resolution backscattering spectroscopy was used to probe exotic "spin ice" as well as practical catalysis materials coated with water that resists forming ice.

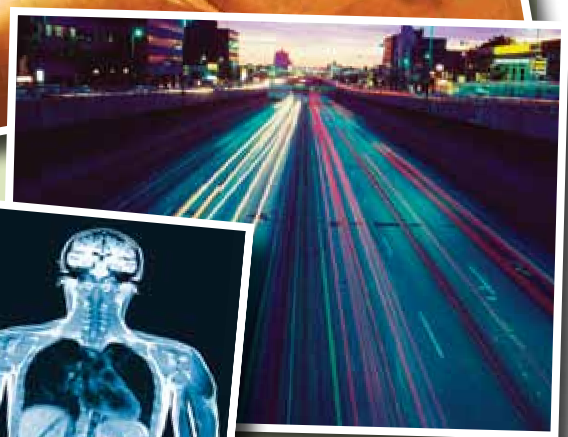
This introduction provides a small taste of the gems found in the work presented here. I hope that you, the reader, will find something both interesting and inspirational. To aspiring researchers, I hope it motivates you to dream about your own experiments. The opportunities for science have never been better—the only missing ingredient is you!

Stephen Nagler
Chief Scientist, Neutron Scattering Science Division

Stephen Nagler, Chief Scientist,
Neutron Scattering Science Division (naglerse@ornl.gov)

Advances in Unconventional Iron-Based Superconductors





Landmark research about a newly discovered superconducting material will lead to more-efficient, less-expensive products in fields such as energy, transportation, and medicine.

In March 2008, Pengcheng Dai, a University of Tennessee (UT)–ORNL joint faculty member and researcher in the Neutron Scattering Science Division (NSSD), attended a conference in his native China. He asked a fellow scientist familiar with a paper in the February 23, 2008, issue of the *Journal of American Chemical Society* why he and his colleagues were so excited. The scientist called the paper "fantastic" and said that the paper reports the discovery in Japan of a new iron-based superconducting material.

After reading the paper, Dai shared their excitement. After obtaining samples of the superconductor's iron-based parent compound made by his colleagues in China, he returned to ORNL to analyze the material's magnetic structure using neutron scattering. The experiments employed instruments at HFIR and the National Institute of Standards and Technology (NIST) research reactor in Maryland.

At about the same time, ORNL staff Michael McGuire and Athena Safa-Sefat became the first team in the United States to report that they had synthesized powders and crystals of lanthanum iron arsenide. In addition, ORNL's Mark Lumsden and Andy Christianson, both in NSSD, were performing neutron scattering experiments on ORNL-made samples.

The original discovery of superconductivity in an iron-based material was made in February 2008 by Japanese scientist Y. Kamihara and colleagues. They initially reported that an iron-based material can conduct electricity without resistance at 4 kelvin (4 degrees Celsius above absolute zero). The elements in the first known iron-based superconducting material are iron, arsenic, oxygen, and the rare earth lanthanum. When LaFeAsO was doped with fluorine, the Japanese discovered that the new material became superconducting at 26 kelvin. Since then several different families of iron-based superconductors have been discovered. The common structural element is the presence of layers of iron atoms arranged in a square lattice.

Any material that is superconducting at more than 30 kelvin is considered a high-temperature superconductor (HTS). The first HTSs discovered and the most explored to date are the copper oxides, or cuprates. The cuprates have been carefully studied for more than 20 years, but condensed matter scientists still lack a complete understanding of how they work. The highest known temperature at which a cuprate turns into a superconductor is 130 kelvin, achieved more than 15 years ago. Scientists throughout the world are excited about the iron-based superconductors because now they have an opportunity to study the electrical and magnetic properties in a new and different system in the high-temperature superconducting class, hopefully gaining crucial insight into the mechanism for superconductivity in these materials.

Clues to how both types of HTS materials work could lead to designs of new superconducting combinations of elements that come close to conducting electricity with zero resistance at room temperature. Such materials would be practical for use in electricity generators, underground electrical transmission in tight spaces, cheaper medical imaging scanners, and extremely fast levitating trains. The reason: these high-temperature, or unconventional, superconductors would not require expensive coolants to chill the

Mark Lumsden (left) and Andy Christianson (right) at HFIR's HB-3 Triple-Axis Spectrometer.

materials to the critical temperature (Tc) at which they become superconducting. Low-temperature, or conventional, superconductors work only if chilled to very low temperatures using expensive liquid helium. HTS materials can be cooled by helium gas or much less costly liquid nitrogen. Unconventional cuprates with yttrium and barium are already being used for superconducting wires and tapes.

The famous BCS theory, formulated in 1957, explains how the conventional superconducting materials discovered in 1911 actually work. BCS stands for the last names of the theorists—John Bardeen, Leon Cooper, and Robert Schrieffer—who received the Nobel Prize in Physics in 1972 for their theory. The theory explains that in a conventional superconductor crystal, the negatively charged electrons attract the positively charged nuclei in the lattice, leaving a wake of positive charges that attract a second electron. The net effect is that the moving, positively charged nuclei (which constitute a phonon or measurement of vibrational energy) provide an attractive interaction to make a pair of electrons, known as Cooper pair. These electron pairs are able to flow more easily between the oscillating atoms in lattice walls, which normally resist the flow of single-file, unpaired electrons in a current. This easier flow creates superconductivity.

The two unconventional superconducting materials—the cuprates discovered in 1986 and the oxypnictides discovered in 2008—possess superconducting and magnetic properties that cannot be explained by BCS theory. Lumsden and Christianson studied the oxypnictides samples synthesized at ORNL using a Triple-Axis Spectrometer at HFIR and ARCS at SNS (see sidebar on page 23). Using ARCS, Lumsden and Christianson compared the lattice vibrations in the conventional superconducting material with those in the iron arsenates. "The phonons we measured in the iron arsenates should induce superconductivity only at a temperature of 2 kelvin using a conventional phonon mechanism, " Christianson says. "Yet measurements show the material's critical temperature is 26 kelvin."

Some scientists predict that magnetic properties of the iron arsenates might make them superconducting at a relatively high temperature. To find out if magnetic fluctuations are the missing piece of the puzzle, Dai's team and Lumsden's team both studied the magnetic structure, or arrangement of electron spins, in the iron arsenides.

In antiferromagnetic materials, the magnetic moments of atoms and molecules are a manifestation of an ordered magnetism. This order exists at low temperatures but disappears when the material passes a certain higher temperature threshold. The existence of antiferromagnetism is easy to detect because neutrons are small magnets.

Undoped iron arsenates, like the parent compound LaFeAsO, are antiferromagnetic when chilled to a low temperature. Using both a powder diffractometer at NIST and HFIR's Triple-Axis Spectrometer, Dai and his collaborators observed very weak magnetic peaks in LaFeAsO, suggesting weak magnetic interactions between layers of iron arsenate molecules (FeAsO). When doped with fluorine and chilled to its critical temperature, LaFeAsO becomes superconducting.

"However, the material's static magnetism disappears when superconductivity pops up," Dai says. "This phenomenon is exactly what we see with the cuprates, except the copper oxide layers become superconducting when the copper atoms each lose an electron."

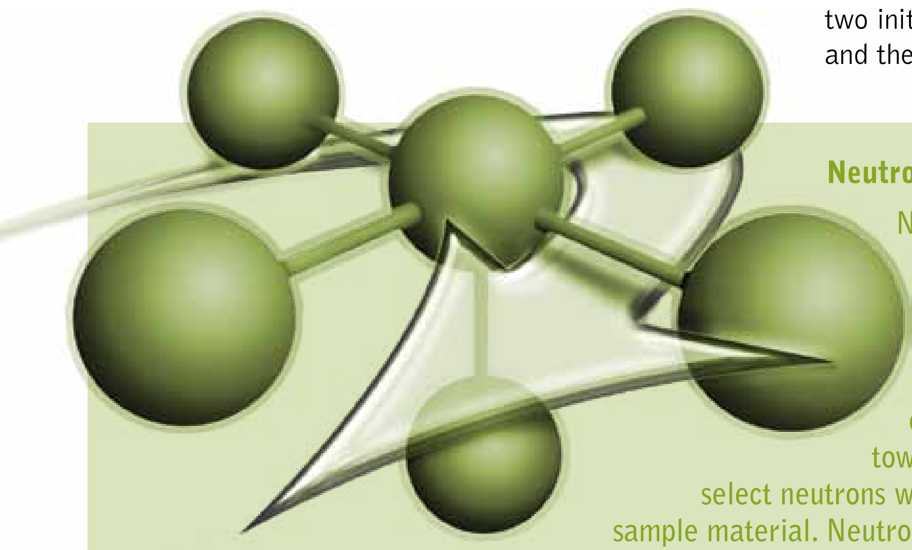
Dai and his colleagues at UT, ORNL, and NIST published a paper on oxypnictides in the May 28, 2008, online issue of *Nature*; it appeared in the June 12 print issue. Clarina de la Cruz of ORNL and UT is the lead author, and Dai and veteran ORNL neutron researcher Herb Mook are also authors. Titled "Magnetic order close to superconductivity in the iron-based layered $LaO_{1-x}F_xFeAs$ systems," the paper was the third-most-cited article on superconductivity in 2008. The authors were shown to be correct in predicting the magnetic structure of LaFeAsO. The experiments at two reactors at ORNL and NIST produced data supporting the theory that subtle magnetism may be responsible for the high-Tc effect. In subsequent work using cerium, published in the October 26 issue of *Nature Materials*, Dai's team showed that the phase diagram of CeFeAsO doped with fluorine is similar to that of the doped cuprates.

In general, if the parent compound LaFeAsO is placed under pressure or doped with fluorine, the static magnetism of the compound is suppressed. The leftover magnetic moments fluctuate in time rather than remaining statically ordered. Under these circumstances, with the absence of magnetic order, the compounds tend to become superconducting.

"We think the surviving magnetic fluctuations are related to superconductivity," Christianson says. "Short-range magnetic fluctuations may be an analog to phonons. One electron enters and interacts with the antiferromagnetic lattice by flipping the spin of an iron atom, causing an unhappy situation. The second electron flips it back, creating a happy situation, energetically speaking. For unconventional superconductors, magnetic fluctuations, rather than lattice vibrations, may lead to electron pairing, the key to superconductivity."

Lumsden, Christianson and colleagues have published two initial papers, one in *Physical Review Letters* and the other in *Physical Review B*. They have also collaborated with scientists at Argonne National Laboratory on a study of spin fluctuations in a barium-potassium-iron-arsenic ($Ba_{0.6}K_{0.4}Fe_2As_2$) material. This paper, published in *Nature*, provides powerful evidence that weak magnetism is strongly coupled to superconductivity in iron-based materials. Since then, the two ORNL researchers and their collaborators have been studying single crystals of iron-based superconducting materials, and several more papers are in preparation. Dai and his colleagues have published numerous papers on the subject in scientific journals and are continuing their research as well.

The scientific expertise of ORNL research staff combined with the availability of in-house synthesis, characterization, and neutron scattering facilities has made ORNL a leader in research of this new type of unconventional superconductor.



Neutron Scattering and Instrument Primer

Neutron scattering is used to examine the structure of materials. In neutron scattering, a beam of neutrons with a known energy and momentum is scattered off a sample of material. The scattered neutrons are detected with special instruments, and the energy and momentum of the neutrons are determined.

At ORNL, two types of instruments have been used to probe unconventional high-temperature superconductors. One type is the Triple-Axis Spectrometer at HFIR. A continuous beam of neutrons travel toward the triple-axis spectrometer to the monochromator, a large crystal that allows the experimenter to select neutrons with the desired energy. The experimenters are able to define the size of the beam needed to probe the sample material. Neutrons scatter off the sample and then off another large crystal called the analyzer. The analyzer is used to measure the final energy of scattered neutrons, which are registered in a final detector.

The other instrument used is ARCS, located at SNS. This instrument is a time-of-flight spectrometer with an array of hundreds of detectors. Time of flight means that the energy of neutrons is measured in terms of the time it takes for them to leave the neutron moderator and reach an instrument detector. SNS produces pulses of neutrons; each neutron in a pulse has its own speed. To select neutrons of a desired velocity, a Fermi chopper is employed. The chopper is a curved tube that rotates at a selected speed to ensure that only neutrons arriving at the desired velocity "see" the tube as straight and shoot through it to the sample.

The capabilities of these two instruments complement each other. HFIR's triple-axis spectrometer has a single detector that measures the positions, energies, and scattering angles of the neutrons in the beam "point by point" on the diffraction pattern. With ARCS, the neutrons are scattered to a huge array of detectors that produces a pattern, enabling a number of features to be measured simultaneously.

Neutron investigation of biomolecules is helping scientists develop synthetic, bio-inspired systems for solar energy conversion.

Bio-Inspired Systems for Solar Energy Conversion

Natural photosynthetic systems in plants have developed a complex machinery for efficient conversion of sunlight to chemical energy, which to the present day has not been matched by humans. ORNL researchers are investigating ways to mimic these exquisite molecular architectures to develop synthetic, bio-inspired systems for the conversion of solar energy to electricity and fuel.

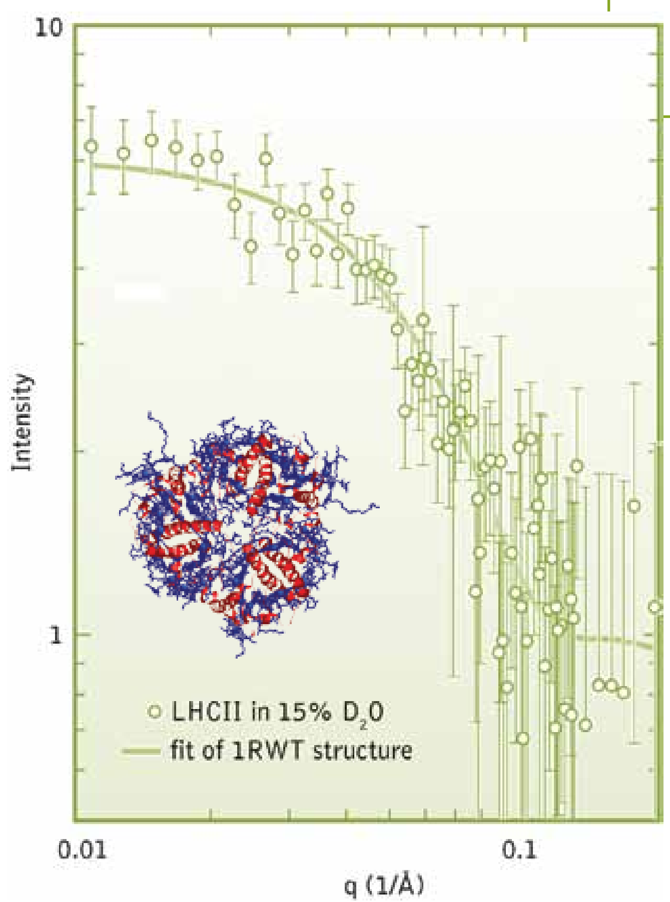
The ultimate goal, says principal investigator Hugh O'Neill of the Chemical Sciences Division (CSD), is to convert solar energy into electricity or fuel, thereby developing a competitive energy source. This goal is one of the key challenges outlined by the DOE's 2005 Basic Energy Sciences Workshop report, *Basic Research Needs for Solar Energy Utilization*. The researchers hope the results of the work will lay the foundation for future photovoltaic devices, which combine the elements of naturally occurring photosynthetic systems of plants with functional polymers that can be engineered to take on desired forms.

The interdisciplinary research team consists of Hugh O'Neill, William Heller, Dmitriy Smolensky, and Mateus Cardoso (CSD and the Center for Structural Biology); Kunlun Hong and Xiang Yu (CSD and CNMS); and Bernard Kippelen (School of Electrical and Computer Engineering–Georgia Institute of Technology). For their research, the team uses the Bio-SANS (CG-3) instrument at HFIR. This instrument is designed for small-angle neutron scattering (SANS) studies and is optimized for investigating the structures of proteins, polymers, colloids, and viruses. The functional polymers used in the research are synthesized and characterized in collaboration with CNMS.

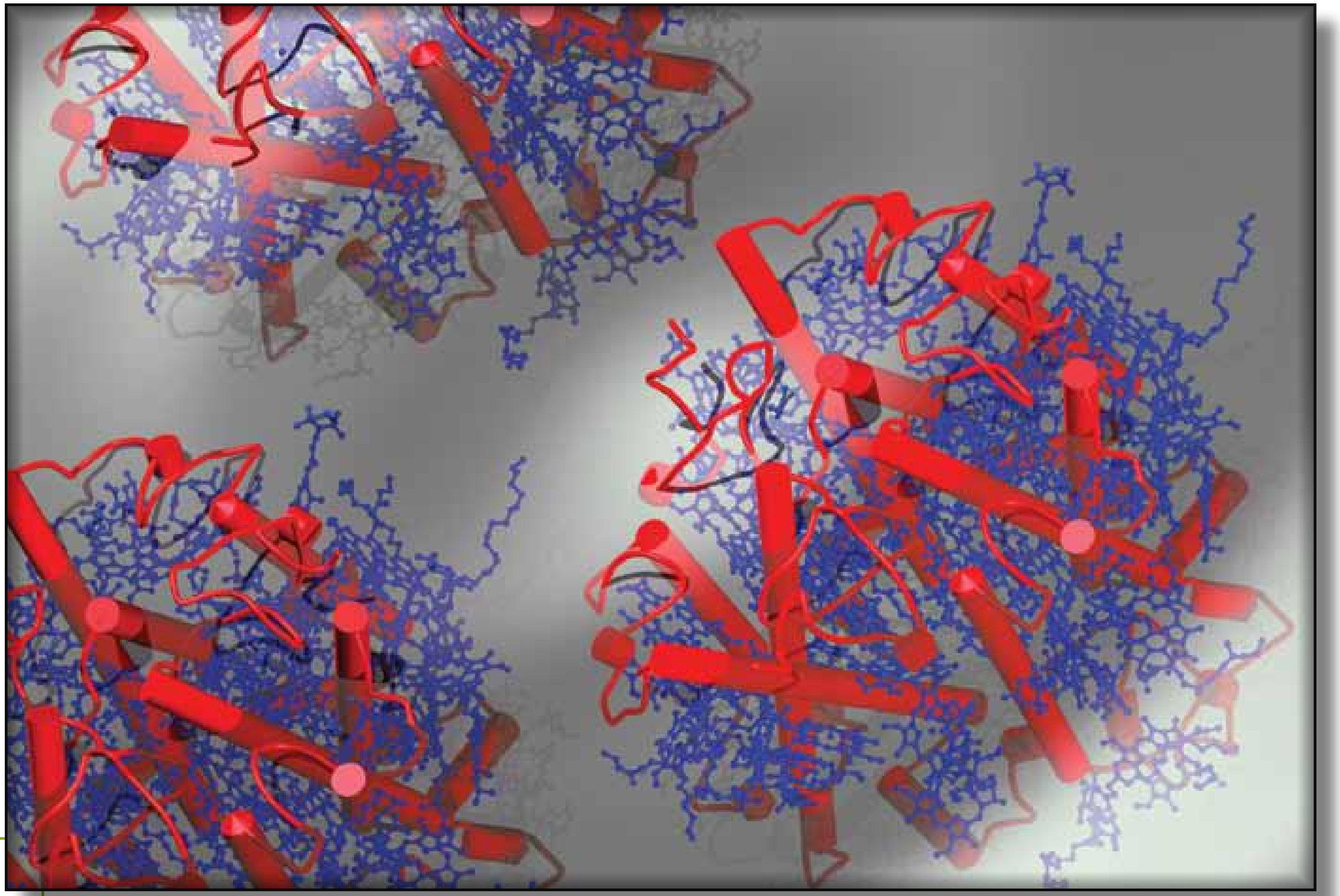
Much of the team's research involves studies of light harvesting complex II (LHC II), a protein complex that is responsible for light capture in plants. SANS experiments were performed with LHC II in detergent solutions containing mixtures of hydrogenated and deuterated water (D_2O). Control of the D_2O concentration allows separate visualization of the protein and detergent, as well as the sample as a whole, through application of contrast variation methods. At the H_2O/D_2O mixture where the detergent is invisible (~15%), researchers could see the scattering profile of the protein, without any significant contribution by the detergent. This study showed that the protein was in its native trimeric state and provides preliminary data for investigating the interaction of the protein with synthetic polymer systems. Beginning in 2009, the group plans to use the Bio-SANS instrument for follow-on structural analysis studies of the polymer-protein systems.

"This fundamental research takes inspiration from nature, utilizing LHC II, and combines it with precision polymer synthesis to produce new photosynthetic systems that will potentially have properties that exceed current biosystems," says Phillip Britt, CSD director. "This project takes advantage of the unique properties of neutrons, which allow only the part of interest to be observed by contrast matching, to study the structure of protein complex in a nonnative environment. These studies will lay the foundation for understanding how the macromolecular structure, or more precisely the three-dimensional orientation of molecules in space, leads to the conversion of light into electricity and how to design new more efficient biohybrid systems."

In future work, the researchers will extend their research by developing synthetic versions of LHC II to replace the natural protein. It is envisioned that synthetic analogues of LHC II could be directly integrated into electroactive block copolymers to produce a self-assembled photovoltaic structure in a configuration that will respond optimally to light.

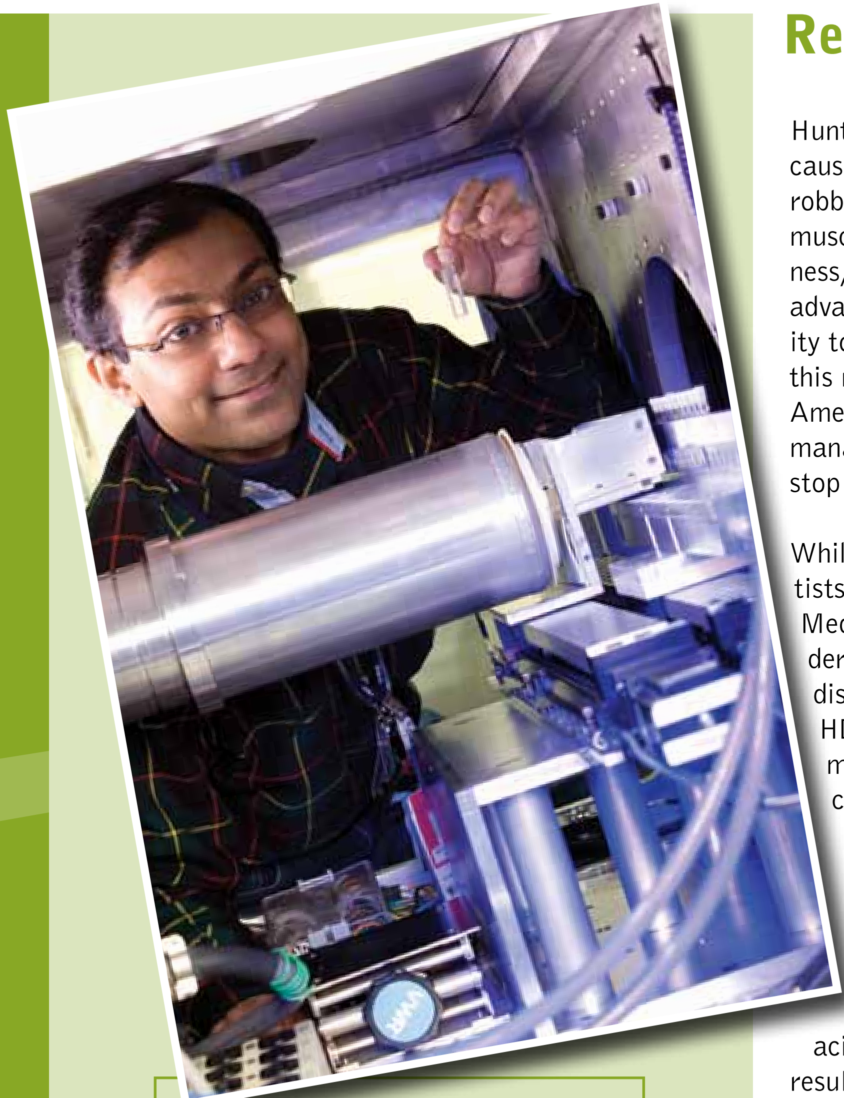


LHC II is the major chlorophyll binding protein in the photosynthetic membrane. This is the first investigation of its structure in solution. The fit of the crystal structure of LHCII (1RWT structure) to the scattering data is shown as a green line.



Artistic rendition of LHC II in a polymer membrane.

Researching a Cure for Huntington's Disease



Sai Venkatesh Pingali, Chemical Sciences Division, with an experiment sample at the Bio-SANS instrument.

Research on the molecular structure of proteins will help us better understand neurological and genetic diseases.

Huntington's disease (HD) is a genetic condition that causes certain brain cells to waste away, eventually robbing its victims of their ability to control their muscles. In its early stages, it can cause clumsiness, forgetfulness, and impaired speech. In its more advanced stages, it can take away a person's ability to walk, talk, and swallow. Available drugs for this neurological disease, first described in 1872 by American physician George Huntington, help patients manage the symptoms of HD, but they don't slow or stop the disease.

While there is no cure for HD, there is hope. Scientists at ORNL and the University of Tennessee (UT) Medical Center are using modern tools to better understand the mechanisms behind this neurological disease. Like Alzheimer's and Parkinson's diseases, HD is caused by a specific protein, huntingtin, that misbehaves. For all cases of HD, a defective gene codes for the troublesome protein.

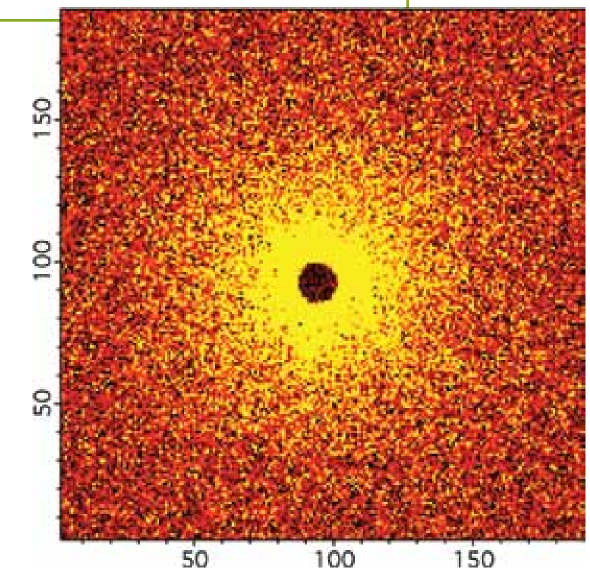
Each protein is made of a combination of amino acids in a sequence dictated by a gene. In a person suffering from HD, the HD protein in many brain cells contains an abnormally long sequence of 40 or more glutamine amino acids in succession. This abnormal repeat sequence results in the formation of fibrils (thin, threadlike fibers) that cause brain cells to deteriorate and die. In a healthy person's brain, the huntingtin protein has only 15 to 20 glutamines in repeat.

At HFIR, Chris Stanley is using SANS to trace in real time the detailed formation of protein fibrils composed of glutamine repeats. Stanley, a Shull Fellow and biophysicist with a Ph.D. in polymer science, came to ORNL with the idea of conducting a study of the growth, or aggregation, of protein fibrils using the Bio-SANS instrument at HFIR. Stanley's mentor, Dean Myles, introduced him to a UT Medical Center researcher, Professor Valerie Berthelier, who is studying the protein specifically involved in Huntington's disease.

At the Graduate School of Medicine, UT Medical Center, Berthelier's group seeks to understand the mechanisms of protein folding and misfolding—correct and incorrect folding of a linear chain of amino acids into a three-dimensional protein. The researchers decipher how these processes are related to normal physiology and disease using chemical, biophysical, and cell biology approaches.

In their current work on HD, they hope to find what makes an aggregate toxic. By identifying small compounds that are capable of altering the shape of the aggregates, they think they will be able to understand the functional role of pre-fibrillar species in the HD

Two-dimensional SANS pattern from polyglutamine fibrils.



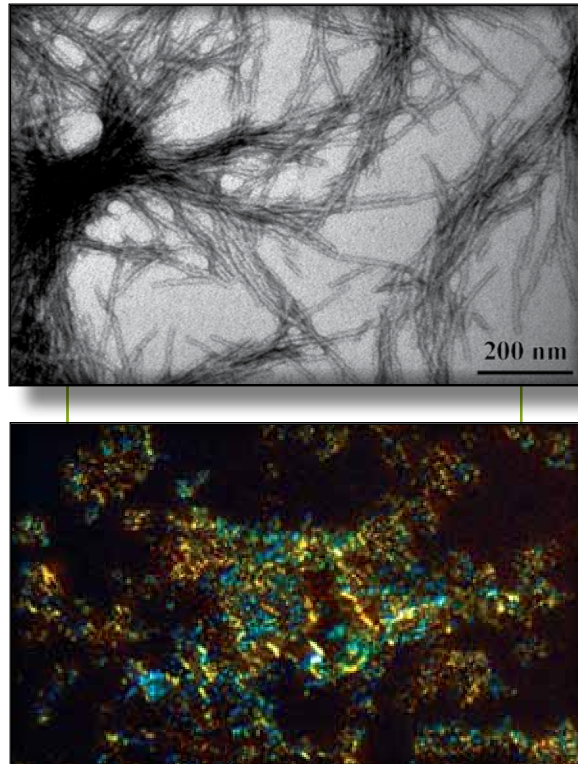
process. Berthelier and Stanley have had a fruitful collaboration so far.

"I am using small-angle neutron scattering to study the structural formation of fibrils to help her understand polyglutamine aggregation in Huntington's disease," Stanley says. "HD is caused by an abnormal polyglutamine expansion in the huntingtin protein, a huge biomolecule that has an interminable site that can be cleaved off as a protein fragment. The resulting small protein, or peptide, fragment misbehaves by aggregating into a threadlike fibril that can turn into neuronal inclusions in the brain, causing brain degradation."

In mouse cell studies conducted by other researchers, no strong correlation has been found between the amount of HD fibrils in the brain cells and real behavioral effects, such as loss of memory and muscular control.

"Something must be happening between the normal, well-behaved protein and the fully formed fibril that is toxic for the brain cells," Stanley says. "We are searching for early intermediates or unusual pre-fibrillar structures that can affect and potentially kill brain cells.

"With the Bio-SANS at HFIR, we can look at samples on a nanometer-length scale. We are doing SANS experiments to identify the structures that form over time with the hope of pinpointing unique structures along the pathway, and possibly even off the pathway, of fibril formation. Valerie and her team can target those unique structures and try to identify therapeutic compounds that inhibit the formation of unique toxic structures. We are trying to get a better handle on what is happening during the formation of the fibril and which part should be targeted for treatment."



Top: Electron microscopy image of polyglutamine fibrils. Bottom: Polarized optical image of stained polyglutamine fibrils.

Using time-resolved SANS, Stanley captured snapshots of the protein structure as it aggregated into fibrils and determined the rate of aggregation. In the experiment, synthetic huntingtin-like peptides having between 22 and 42 glutamines in the repeat were placed in a buffered salt solution in a quartz cuvette. The solution contained deuterated water that, for neutron scattering, provides a high contrast level to observe the scattering from the protein.

"We know when in time that protein structural elements change," Stanley says. "We can determine when changes in size and shape occur during aggregation to form the fibril. We can measure the radius of the cross section of the formed fibrils as well as their mass per length. In future kinetic studies, we will look for changes in the fibril's building blocks when therapeutic compounds are added."

"In future experiments, we're hoping to do a better job of mapping out the pathway of the fibril as it aggregates. We will be able to monitor a larger size range simultaneously in our time-resolved aggregation studies when we use the EQ-SANS instrument at SNS."

Another project that Stanley is engaged in is using SANS to study intrinsically disordered proteins that are responsible for transcription and translation—reading instructions from DNA and producing the requested protein. Because of its plasticity and flexibility, this protein type can bind to different binding partners.

Stanley surmises that the CREB (CAMP response element binding) binding protein, a large binding protein with a short glutamine repeat that performs transcription, might get trapped by an aggregating HD fibril, knocking out the large protein's central transcription function. If SANS can be used to find such a sequestered protein in an HD fibril, the result would suggest one way that a protein fibril could be responsible for the decline and death of a brain cell. Other researchers have speculated about this possible interaction where there are obvious implications for HD.

As more powerful scientific tools become available, HD patients and researchers remain hopeful that a breakthrough might turn an incurable disease into a curable one.

Biomass Studies: Growing Energy

Biomass research can help lower energy costs, reduce dependence on oil, and decrease pollution.

Biomass from plants offers a potentially abundant source of ethanol from the fermentation of component sugars. But its complex laminate structure—consisting of the biopolymers cellulose, xylan, pectin, and lignin often collectively termed lignocellulose—is difficult to disrupt and break down into fermentable sugars. Pretreatment is required to separate the components, detach lignin, and discompose the cellulose fibers for efficient conversion to fermentable sugars.

To learn why lignocellulose is so difficult to break down, a team of researchers is using the Bio-SANS instrument at HFIR and the Cray XT4 supercomputer at the Leadership Computing Facility (LCF) at ORNL to investigate biomass samples from the BioEnergy Science Center (BESC), also at ORNL. Their goal is to visualize the breakdown of plant cell wall structures during biomass processing at length scales ranging from nanometers to microns (one billionth to one millionth of a meter).

This research project, "Dynamic Visualization of Lignocellulose Degradation by Integration of Neutron Scattering Imaging and Computer Simulation," is a high priority because DOE has targeted energy independence through cost-effective production of ethanol and other liquid fuels from renewable biomass as an important part of its mission. DOE says that achieving success in this project will benefit the broader goals of energy security, domestic economy, and pollution reduction. High-resolution visualization and characterization of biomass is also a key task outlined by the DOE's biomass for energy strategy.

Researchers say that their current work will demonstrate the value of using an integrated neutron science and high-performance scientific computing method to solve real-world problems. A second important goal of the research is to develop molecular visualization techniques that can be extended to other fields, such as medical research; this goal would be difficult to achieve without the combined use of neutron scattering and high-performance computing.

Members of the research team from ORNL include Barbara Evans and Joseph McGaughey of the Chemical Sciences Division (CSD); Jeremy Smith, Loukas Petridis, and Brian Davison of the Biosciences Division; Volker Urban, William Heller, Hugh O'Neill, and Sai Pingali of CSD and the Center for Structural Molecular Biology; and Dean Myles of the Neutron Scattering Sciences Division. The team also includes Ida Lee of the University of Tennessee–Knoxville and Art Ragauskas of the Georgia Institute of Technology.

Lignocellulosic biomass, the scientific term for plant leaves, stems, and roots, is an abundant and renewable resource. A wide range of potential sources exist, including stalks and leaves left after harvest; residues from the paper, pulp, and lumber industries; bioenergy crops such as switchgrass hay and poplar trees; as well as municipal wastes such as leaves and tree trimmings. Unfortunately, the processing required to break biomass down into fermentable sugars for alcohol production and creation of other products is more energy intensive and expensive than extracting starch from grains or pressing juice from sugar cane. The structure of plant cell walls, and how those walls are deconstructed or converted at the molecular level, is not fully understood.

Since biomass is a complex, multicomponent, and multiscale material, characterization techniques are required that span a range of length scales from angstroms to micrometers (more than one ten-billionth to one millionth of a meter) and that can differentiate between individual components in the native material. Neutron scattering and diffraction, which probe structures over this range of length scales, can provide a fundamental understanding of the structure at the atomic and molecular level. Neutrons are also excellent at "seeing" order in complex systems, which is also important for understanding why the plant cell wall and lignocellulose structures resist breakdown. The unprecedented detail of these studies of the structure of lignocellulose will help engineers develop new, cost-effective methods for breaking down lignocellulosic biomass and using it in the production of fuels and chemicals.

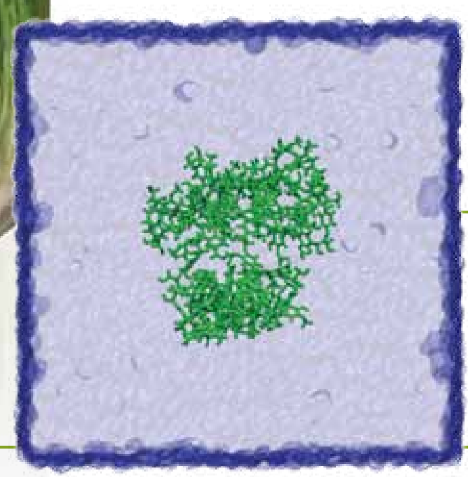
Neutrons are particularly good at locating where critical water molecules are. This is very important, since most of the reactions are hydrolysis, in which a polysaccharide is broken by adding water. In the future, the team will extend their work across a broader suite of instruments at SNS. This information will be complemented by chemical force microscopy, a technique in which nanometer-scale probes are modified with specific chemical groups to spatially map hydrogen bonding and hydrophobic interactions between lignocellulose components.

Computer simulation and modeling will integrate the neutron scattering data with information obtained from other complementary methods, thereby giving scientists a molecular-level understanding of the structure, dynamics, and degradation pathways of these materials. One computer-based method is a numerical simulation of biomolecular systems at the atomic level using a molecular dynamics (MD) approach, which involves the stepwise integration of the equations of motion of many-particle systems. This approach is limited by the restrictions of the available computer processing power and has therefore been applied to systems of at most ~105 particles and a 100-nanosecond timescale.

The increased computer power now available at the LCF allows extensions of the MD computer simulations to micrometer lengths and microsecond timescales, which allows the simulation of lignocellulosic biomass systems. Further extensions using coarse-grained mesoscale techniques will allow the simulation of even larger ensembles of heterogeneous biomass systems, thereby enabling numerical studies of the degradation process of the biopolymers in detail. The best-fit models of the lignocellulose molecules derived from their experimental neutron scattering profiles will then be compared with the results from these computer simulations, providing a combined experimental and theoretical picture of lignocellulosic biomass systems at the molecular scale.

In future work, the interplay between computer simulation and experiment will be enhanced by the development of codes for calculating the relevant neutron scattering structure factors directly from the simulation data; this will require the integration, automation, and optimization of standard biomolecular simulation programs for use in interpreting the results of neutron scattering from lignocellulosic targets. The team will then extend their studies to biological breakdown of biomass by microbes and enzymes, as well as to the growth and formation of cell walls in living plant cells. The understanding of the behavior of water and of molecular order in these systems can clearly be greatly improved by the combination of numerical studies using high-performance computing and neutron scattering experiments on real biomass samples.

This work is supported by programmatic funding from the Genomes to Life Program of DOE's Office of Biological and Environmental Research.



Left: Biomass crops, such as the wheat shown here, are being grown in deuterated water mixtures to provide deuterated lignocellulosic material for neutron experiments. Right: The physical structure of lignin in aqueous solution was modeled using molecular dynamics-based computer simulation paired with scattering data.

Studies of the unique structure of synthetic molecules will help in the development of drugs that can target diseased areas of the body.

Targeted Drug Delivery Systems

An NSSD researcher is using a broad suite of elastic and inelastic neutron scattering techniques to study the structure and dynamics of polyamidoamine (PAMAM) star-burst dendrimers in the hope that these repeatedly branched molecules will become an effective, targeted drug delivery system for the treatment of cancers.

Wei-Ren Chen, who received his doctorate in nuclear science and engineering at Massachusetts Institute of Technology in 2004, is a Clifford G. Shull fellow at ORNL. Chen studies "dendritic molecules," synthetic macromolecules that can be envisioned as polymeric colloidal particles, which are globular in shape. However, dendrimers exhibit additional internal degrees of freedom, such as conformational branch fluctuations characteristic of linear chain polymers, which give rise to rich phase behavior. In addition, dendrimers have properties such as chemical uniformity, an intra-molecular cavity for accommodating exogenous materials, and functionalizable architecture, water solubility, and biocompatibility, which makes them excellent candidates for biomedical applications such as highly specific drug delivery.

"Most of the cancer drugs are very toxic, so they have to be wrapped inside some sort of vehicle when being delivered to the targeted areas inside a human body," Chen explains. "It's very important to know what change takes place in the dendrimer vehicle carrying the drug when it is introduced into the body. So we developed a synergistic approach, combining various neutron scattering techniques—molecular dynamics simulations and theoretical calculations—to systematically study the underlying chemical and physical mechanisms that govern the functioning properties of dendrimers in aqueous solutions at physiologically relevant pH."

Chen works with his supervisor, Ken Herwig, and with Greg Smith, leader of the NSSD's Low-Q Group. "Wei-Ren is the intellectual driver for this. He made a proposal to ORNL's Laboratory Directed Research and Development Program and got funding for this," Herwig says. "Wei-Ren brings a unique combination of a theoretical approach to understand and interpret the data, with a very good understanding of the experimental side, and the ability to carry out precise experiments to provide the data that act as input for the theory."

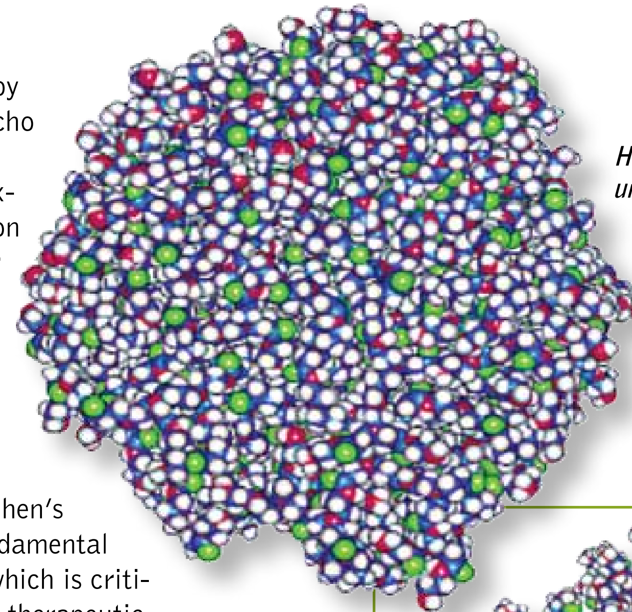
Herwig says that the research, which he calls "very, very hot in the field right now," is a broad collaboration of researchers across the United States, which Chen has been instrumental in establishing. At CNMS, Kunlun Hong is synthesizing the isotopically labeled dendrimer; and the research group at the California Institute of Technology, led by Bill Goddard, is carrying out complementary atomistic simulations to provide the microscopic information that is not accessible experimentally.

"This particular system, this generation of these dendrimer systems, is very exciting. They can be functionalized so that you can add additional groups on the out-surface of the dendrimer so that they can target particular locations, and things like viruses or cancer cells, so they can be like a Trojan horse," Herwig explains. "You functionalize the surface group with something which a virus or cell wants to attract to itself, and then you get it bound onto that substrate cell and then it delivers the targeted drug."

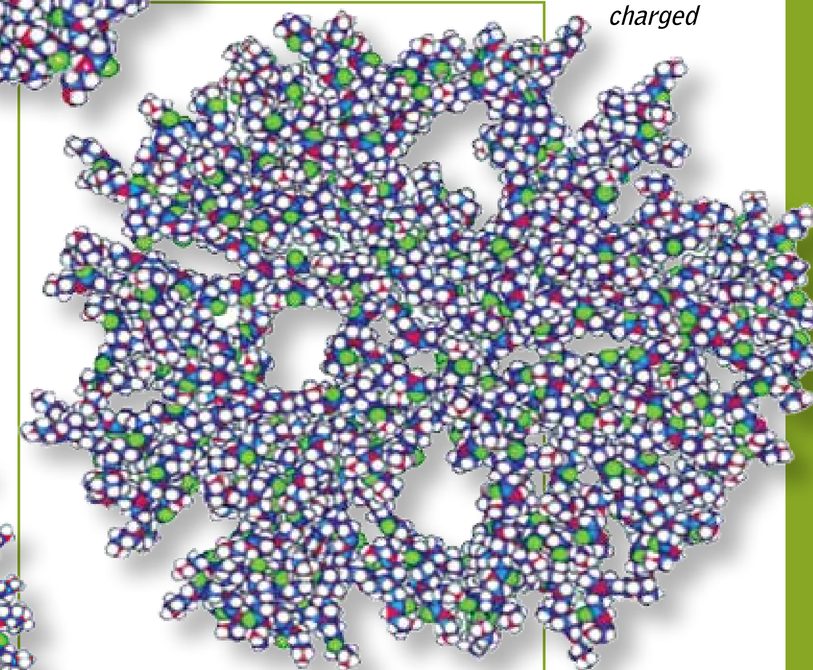
"The other reason there is excitement is that the dendrimer is quite adaptive in its geometry, in terms of how large you make them," Herwig says. "People are also looking at the acidity of the environment (the acidity of a dendrimer/drug preparation outside the body is very different from the acidity it encounters inside), and this is one of the key elements of Wei-Ren's research, to understand how the dendrimers acquire electric charge based on how acidic the environment is and how the dendrimers interact with each other in a solvent."

Chen and his collaborators used the SANS spectrometers available at the HFIR, the National Institute of Standards and Technology, and the Institut Laue-Langevin (ILL) to obtain structural information about dendrimer solutions. They have shown inter-dendrimer interaction is greatly influenced by their unique molecular architecture. Combined with a nuclear magnetic resonance experiment carried out at CNMS, the SANS results provide compelling evidence of the dense-core picture of the dendrimer density profile, a longstanding issue in the field of soft matter science. The findings suggest that the routinely used Stokes-Einstein relation is not valid in estimating the molecular size of ionic soft colloids, such as dendrimers.

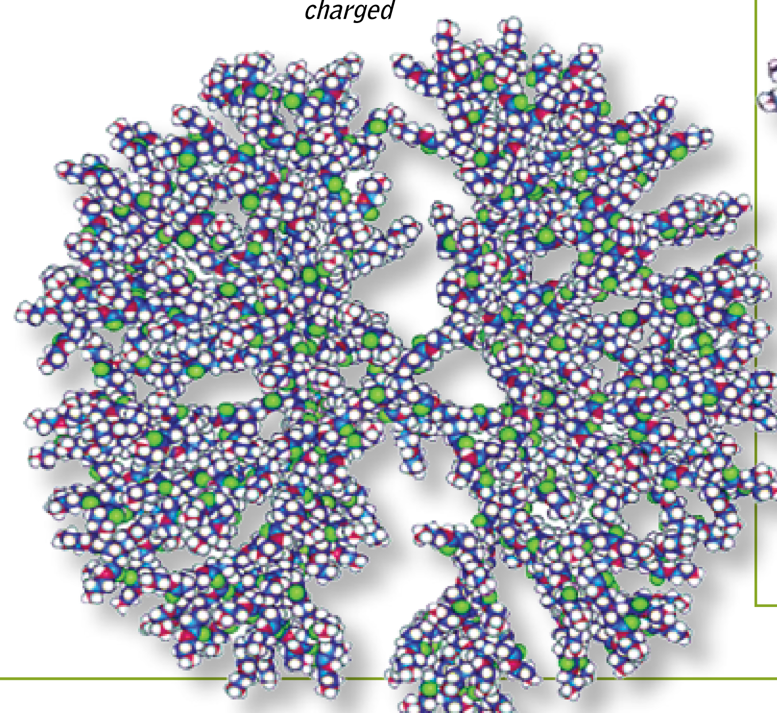
Using a sequence of quasi-elastic neutron scattering instruments, such as the Backscattering Spectrometer at SNS, Chen and his collaborators made the surprising discovery that the individual motions of constituent components of dendrimers show a strong dependence on the pH value of the surrounding environment. This has not been reported experimentally or predicted computationally. The intra-molecular collective dynamics observed by the Neutron Spin Echo spectrometer at ILL shows a similar unexpected dependence on pH value. Molecular dynamics simulation and theoretical calculations are now being carried out to interpret these observations. It is expected that Chen's work will reveal fundamental scientific behavior, which is critical for assessing the therapeutic potential of PAMAM dendrimers.



High pH
uncharged



Neutral pH
primary
charged



Low pH
primary and tertiary
charged

Dense-core to dense-shell transition in dendrimer using pH as a trigger. SANS studies reveal how molecules function within solutions at different pH levels. Simulating levels present in the human body helps determine how drugs will act when administered.

How Nanoparticles Go with the Flow

Nanoparticle studies are leading to a better understanding of the environmental and health effects of the manufactured nanomaterials used in common products such as lotions and skin creams.

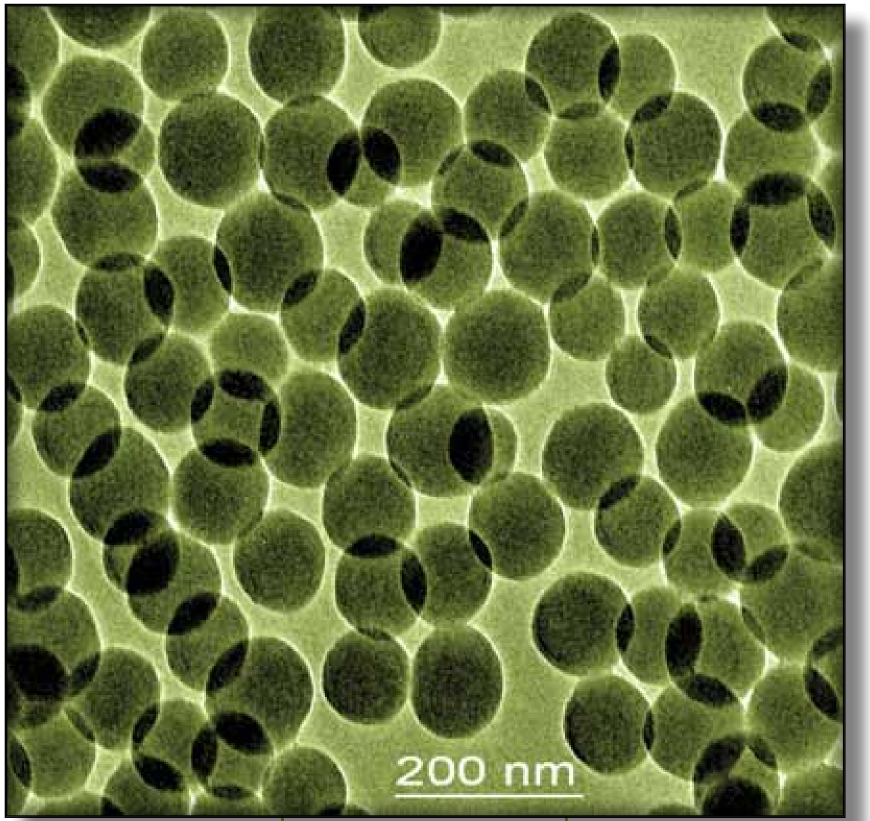
Sunscreen and facial makeup sold at the local drug store consist of particles as small as 30 billionths of a meter, or 30 nanometers. These "engineered nanoparticles"—made of titanium oxide (TiO_2), zinc oxide (ZnO), iron oxide (Fe_2O_3), silicon oxide (SiO_2), and other nanomaterials—are being produced in growing quantities by industrial firms and research laboratories. Concerns are mounting about the effects of these nanoparticles on human health and the environment. The U.S. Environmental Protection Agency is particularly interested in the "fate, transport, and transformation of nanoparticles" to better estimate the environmental and health effects of exposure to manufactured nanomaterials.

Studies indicate that TiO_2 nanoparticles—used in sunscreen to protect skin from ultraviolet light—can penetrate the skin. In some experiments with mice, TiO_2 nanoparticles trigger rapid and long-lasting defensive responses. Other studies show that nanosized TiO_2, SiO_2, and ZnO in water are somewhat toxic to *Escherichia coli*, the kind of bacteria that perform a useful function in the human stomach. Nanoparticles may also act as important carriers of pathogens and environmental contaminants.

Baohua Gu and Wei Wang, both of ORNL's Environmental Sciences Division, are teaming with Ken Littrell, Hassina Bilheux, and Xun-Li Wang, NSSD, to study the behavior of these engineered nanoparticles under environmental conditions. Changes in water chemistry profoundly influence the surface chemistry of these particles, which in turn will affect whether nanoparticles flow as individual particles, or as aggregates that attach to subsurface sediment materials such as quartz sands. The researchers have made the first-ever proof-of-principle measurements of the transport and deposition of nanoparticles in packed sand beds in real time and space. Neutrons made it possible to peek into nanoparticle behavior inside the sand bed.

The data being gathered using neutron radiography at the Technische Universität München, Garching, Germany, and SANS at HFIR will help researchers predict the fate and mobility of nanoparticles in the environment. Specifically, the ORNL team is focusing on the behavior of nanoparticles that Gu and Wang synthesized to ensure that particle size and shape are uniform. For the first experiments, they selected TiO_2 and SiO_2 nanoparticles because of their chemical stability in solution (i.e., they do not dissolve in water) and their surface charge dependence on solution chemistry. Also, these nanoparticles are among the most commonly manufactured nanomaterials.

During SANS experiments at HFIR, the TiO_2 nanoparticles suspended in a solution are pumped into a glass column of packed quartz sand, and a beam of neutrons with a defined width is directed at the nanoparticles in the flow-through system. SANS research can be particularly useful for tracing the fate and behavior of the nanoparticles inside the sand bed. The quartz sand surface normally carries negative charges at neutral pH. When the acidity levels increase, nanoparticles such as TiO_2 will flip their surface charge from negative to positive and start sticking to the negatively charged sand surfaces that previously repelled the nanoparticles. Silica particles cannot be used in this experiment because of their similarity to quartz sand. Some nanoparticles remain as single particles and flow freely through the sand bed, but others attach to each other or to the larger sand particles, eventually clogging the flow through the sand. Aggregates of nanoparticles are formed where coagulation occurs. The neutrons in the low-energy, long-wavelength cold beam "see" only nanoparticles at a given spot. The larger sand particles in the packed column do not interfere with the analysis because of their greater length scale.

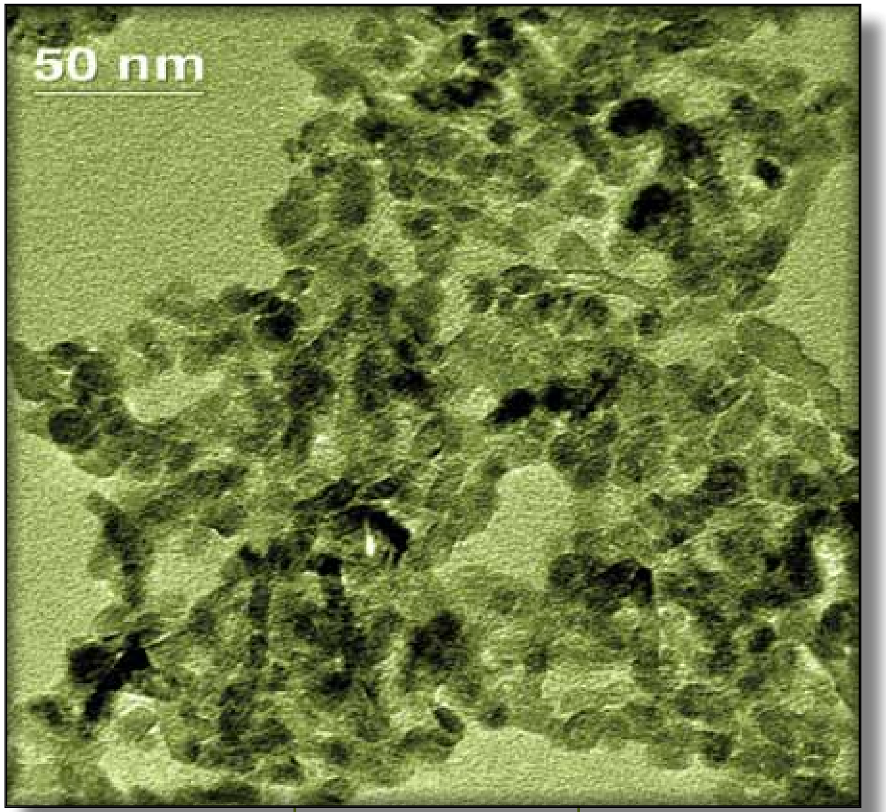


SiO_2 nanoparticles.

In neutron radiography experiments at Garching, the nanoparticles are labeled with a neutron-absorbing element such as gadolinium (as Gd_2O_3). A collimated neutron beam passes through the sand bed to the neutron detector. Because some neutrons will be absorbed by the labeled nanoparticles, they will not reach the neutron detector. The pixilated neutron detector, which has a charge coupled device camera, enables researchers to determine the bulk of nanoparticles as they pass through the packed sand column in real time and space.

"Whether the nanoparticles flow out, attach to each other, or deposit onto larger sand particles depends on the surface and the solution chemistry," Gu says. "Nanoparticles will attach to one another if the repulsion forces are weak between them. For our system, this attachment occurs if the water has higher salt levels. The nanoparticles will coagulate and form aggregates that scatter the neutron beam more effectively."

"What we learn from these experiments," Gu says, "will help scientists better understand and predict how nanoparticles will behave in the environment under different conditions and how they might affect human health."



TiO_2 nanoparticles.

SCIENCE HIGHLIGHTS

Neutron research on developing improved polymers with controllable properties is leading to advances in the biomedical field.

"Intelligent" Polymers for Biomedical Technologies

Proteins, polysaccharides, and nucleic acids are the basic components of living organic systems. Known as functional biopolymers, they exhibit discrete and reversible changes in form as a response to small changes in their environment. The discovery of such cooperative interactions between segments of biopolymers has led researchers to try to create novel synthetic polymers, which are similarly responsive in a controlled way to stimuli. Scientists say the design, synthesis, and characterization of "intelligent," environmentally responsive polymeric materials with controllable properties is important for the emerging biomedical technologies of the next decade.

ORNL researchers are working to develop such materials for possible use in biomedical applications. Using the state-of-the-art general purpose-SANS instrument at HFIR, they characterize novel polymeric materials, which are synthesized by materials scientists at ORNL's CNMS. Neutron scattering allows scientists to study the nanoscale structures and interactions of these novel polymers. The research is being conducted by postdoctoral fellow Gang Cheng, Yuri Melnichenko, and George Wignall, all from the Neutron Scattering Sciences Division, and Kunlun Hong and Jimmy Mays from CNMS.

"ORNL has a proven record of using neutron scattering to investigate the solubility and structure of homopolymers and block copolymers in various solvents," says Melnichenko, "and these capabilities have been significantly enhanced by the new instruments available at HFIR and SNS. This research will strengthen ORNL's position as a leader in creating 'smart' functional polymeric materials and characterizing them using advanced neutron scattering methods."

The project involves the synthesis of biocompatible stimuli-responsive homopolymers, block copolymers, and gels, based on methoxy(oligo(ethylene oxide))styrene and methoxy(oligo(ethylene oxide)) norbornene. Says Cheng, "These biomimetic polymers can identify a stimulus (temperature, pH, ionic strength, etc.), evaluate the magnitude of the signal, and then adequately adjust their conformation properties in a direct response." The figure (next page) shows how the scattering intensity from the polymer solutions increases with temperature, revealing at what temperature the polymers collapse. "Understanding the fundamentals of the conformation response and phase behavior of the 'intelligent' polymers is imperative for a variety of applications in biology and medicine," he says, "such as drug delivery, bioseparation, biometric actuators, and surfaces with reversible hydrophobic and hydrophilic properties."

SANS has been used largely for investigation of conformation of the polymers in solutions, due to the appropriate length scales (1–100 nanometers) involved, and the significant contrast between hydrogenated polymers and deuterium substituted solvents," says Melnichenko. "In this project, we use SANS to understand the fundamentals of the conformation response and phase behavior of these polymers, as well as the interplay between the interactions of the backbone and side chains with water molecules. This information is a prerequisite for designing stimuli-responsive materials with desired properties," he explains.

A rapid response to stimuli and biocompatibility are crucial when designing the molecular structures needed for targeted drug delivery inside the human body. To achieve the intended goals, Fengjun Hua and Kunlun Hong, polymer chemists at CNMS, synthesized a series of comblike polymers, consisting of a hydrophobic backbone and hydrophilic oligo ethylene glycol (EG) side chains. The polymers are expected to have low toxicity because of the presence of the EG side chains. By varying the number of EG repeat units in the side chains, the cloud point (temperature at which solids are no longer completely soluble) of their aqueous solutions can be held within the optimal physiological range. And the relative interaction strength of the hydrophobic (backbone—water) and hydrophilic (side chain—water) fragments of the bipolymers can be continuously varied and used to control the solubility and phase behavior of the system.

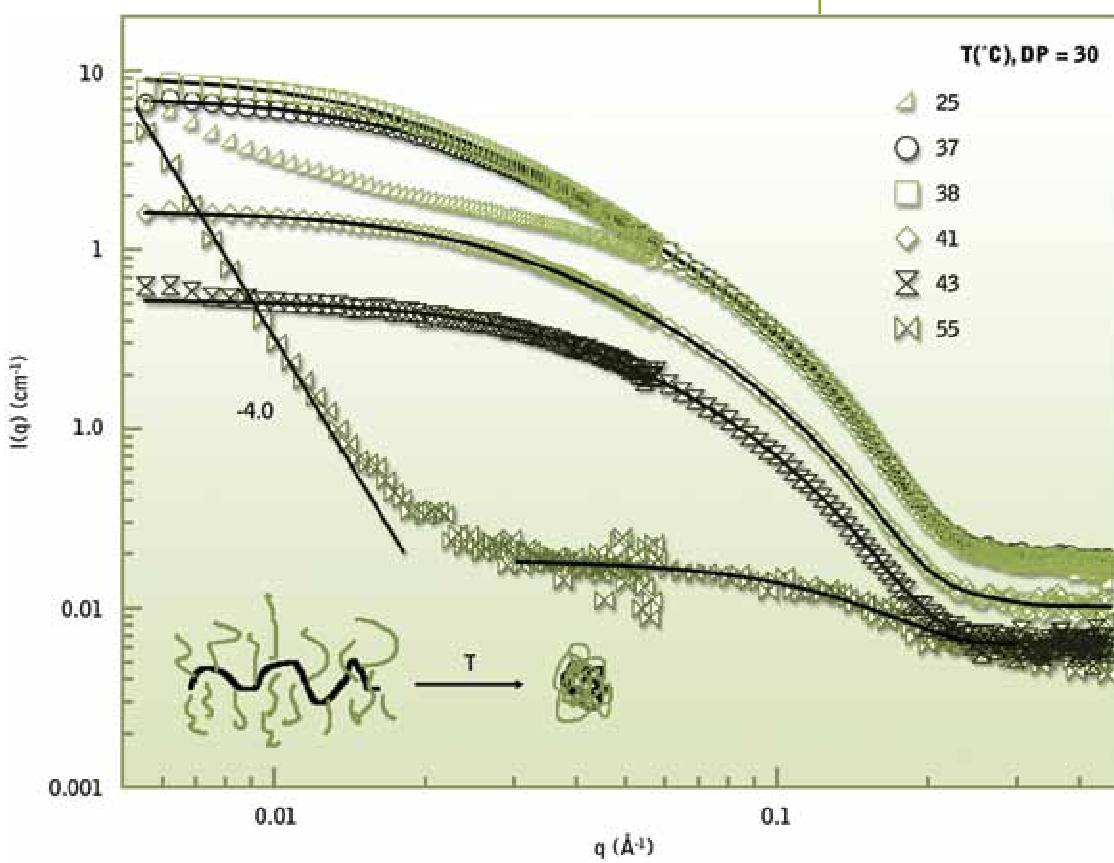
The comblike architecture allows researchers to vary the length and composition of the backbone and side chains independently of each other to achieve the optimized structures and functions. Both the sizes of the polymers and their shapes can be controlled by increasing the molecular weight of the backbone, while keeping the length of the side chain fixed. As a result, a variety of complex and reversible structural transformations and phase transitions can be induced, including coil-globule in homopolymers, micellization of block copolymers, and swelling—collapse transitions in polymer gels.

"These polymers can be dissolved in water only if a sufficient number of the hydrophilic EG side chains are available," Cheng explains. "With increasing temperature, the attractive interaction increases due to increased hydrophobic interactions between backbones and weakening hydrophilic interactions between the EG side chains and water. These findings are important for better design and application of stimuli-responsive materials in the future."

Recent publications resulting from the research include:

G. Cheng, Y. B. Melnichenko, G. D. Wignall, F. Hua, K. Hong, and J. W. Mays, "Small angle neutron scattering study of conformation of oligo(ethylene glycol)-grafted polystyrene in dilute solutions: Effect of the backbone length," *Macromolecules*, vol. 41(24), pp. 9831-9836, December 2008.

G. Cheng, F. Hua, Y. B. Melnichenko, K. Hong, J. W. Mays, B. Hammouda, and G. D. Wignall, "Association and structure of thermosensitive comblike block copolymers in aqueous solutions," *Macromolecules*, vol. 41, pp. 4824-4827, July 2008.



SANS curves of polymer 1 in D_2O at different temperatures. Solid lines are fits to models based on the molecular structure of the polymers. (DP—degree of polymerization).

Neutron scattering research with superalloys is helping scientists develop better materials for engineering and industrial applications.

Superalloy Studies Heat Up

Nickel-based superalloys are attractive structural materials for buildings, precision machinery, and vessels for nuclear power reactors. These remarkable alloys are as strong as steel and possess excellent dimensional stability—that is, they do not expand over a desirable range of operating temperatures.

One type of nickel-based superalloy studied at HFIR is Waspaloy®. This heat-resistant material is used in hot-section components of turbine engines that generate electricity. The constituents of Waspaloy are nickel, chromium, cobalt, molybdenum, titanium, iron, and aluminum. During its manufacture, this alloy is heat-treated to better distribute its precipitates, thus increasing the material's localized "microhardness." The improved precipitate distribution is responsible for the superalloy's excellent mechanical and electrical properties.

Failed tests to drive a pin through Waspaloy samples demonstrate the material's microhardness. The localized spherical inclusions, or solid precipitates, in the polycrystalline material serve as "blocking points" to prevent crack propagation. The heat treatment makes the superalloy more uniform, conferring high electrical conductivity.

The electrical conductivity could be used as a nondestructive measure of performance. If the conductivity suddenly decreases after a long time, the change may indicate that a small crack is about to form in the superalloy, marking a precondition for mechanical failure.

Ken Littrell, lead scientist for the GP-SANS instrument at HFIR, and Rosario Gerhardt and Ricky Whelchel, both of the Georgia Institute of Technology, are using SANS to investigate whether the distribution of precipitates changes in Waspaloy components in turbine engines as a result of repeated thermal exposure and cycling during service. SANS uses beams of cold neutrons, cooled with liquid hydrogen, to produce slower, longer-wavelength neutrons.

The researchers used cold neutrons to strike, at an angle of less than 1 degree, a previously heated Waspaloy sample measuring about 1 square centimeter in area and 1 millimeter in thickness. The results showed that the size of and separation between the inclusions depended on how hot the sample became and how long it was heat treated. Because the low-energy neutrons used had a wavelength about the same size as an inclusion (0.4 to 2 nanometers), these measurements could be made.

"By studying the SANS diffraction pattern, we found that heating time and temperature could be correlated with inclusion size and spacing between these particles," Littrell says. "Smaller inclusions are formed when the Waspaloy sample is heated at low temperatures, and larger inclusions are formed at higher temperatures."

The researchers obtained a previously prepared Waspaloy sample and measured the distances between the inclusions using SANS. Then they heat treated it outside the SANS instrument (ex situ heating) for a nominal two minutes. When the heat-treated sample cooled to its stable configuration at room temperature, the scientists placed the specimen in the SANS instrument. "It took less than five minutes in room temperature to see the effects of heat treatment," Littrell says, indicating that the spacing between the inclusions had increased and become more uniform.

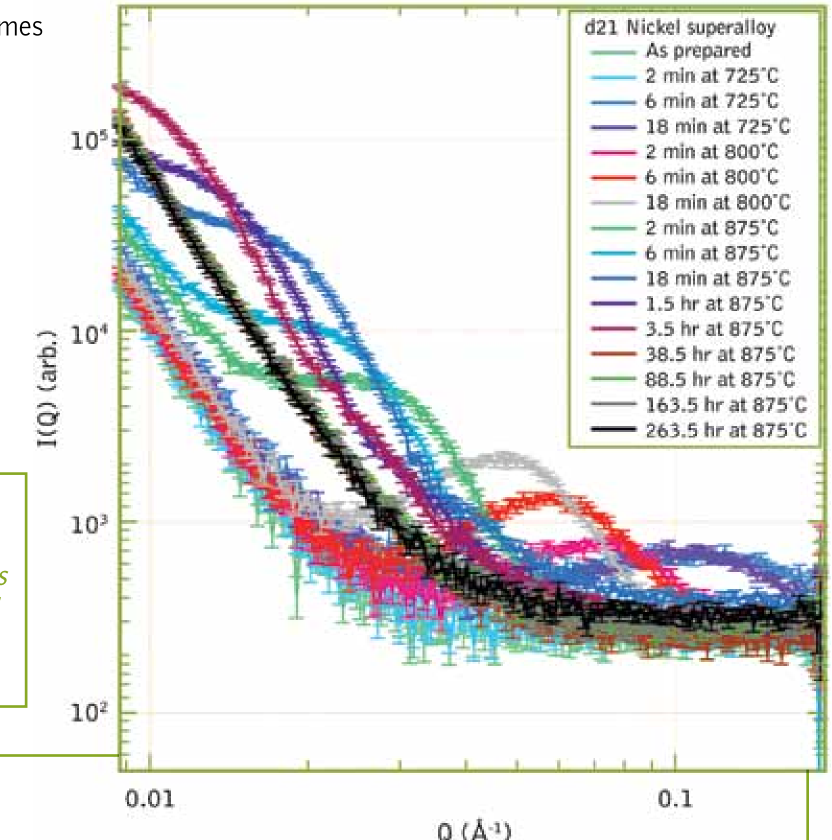
"The diffractions from these correlations show up as a beautiful ring that is faint and broad, spreading to the edges of the detector," Littrell says. "The center of the ring becomes sharper and brighter. Our measurements clearly showed that the distance between the precipitates increases with a higher heat treatment temperature or a longer treatment time."

The peaks in the neutron scattering curves (see image) represent the scattering from correlated spherical inclusions; the positions of the peaks give the average separation between inclusions. The number and density of the inclusions are related to the hardness of the material. Changes in hardness that signal imminent failure of the part can be confirmed by detecting a decrease in electrical conductivity.

The statistical results and measurement times demonstrate that the GP-SANS system at HFIR is suitable for more complex experiments in which superalloy samples are heated while being probed by neutrons.

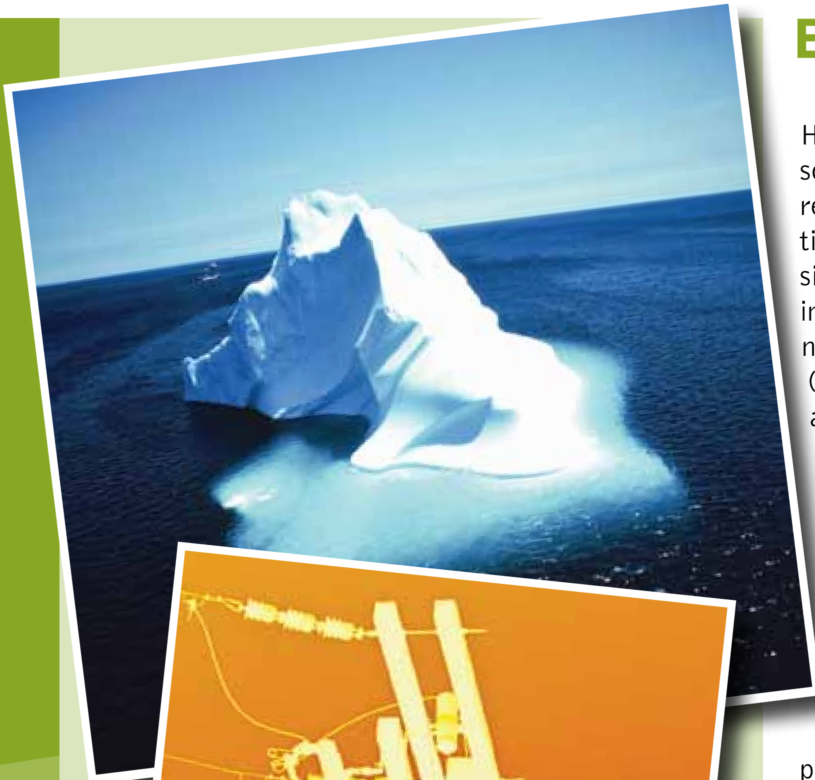
"We want to do real time in situ heating of the Waspaloy sample while probing it with SANS," Littrell says. "Instead of frozen snapshots of the sample before and after heating outside the instrument, we hope to observe the rate of changes in the sample's spacing between precipitates and its composition during the heating process. It will be sort of like making a movie."

Ken Littrell discusses the GP-SANS capabilities with Neutron and X-Ray School students.



The peaks in the neutron scattering curves represent the scattering from correlated spherical inclusions; the positions of the peaks give the average separation between inclusions. The number and density of the inclusions is related to the hardness of the material. Changes in hardness that are signs of imminent failure of the part can be confirmed by detecting a decline in electrical conductivity.

Energy Solutions from Catalysis Research



Catalysis research is playing a key role in developing solutions for energy needs, environmental protection, and the problem of global warming.

How water molecules move at the interface with solids is one of the more urgent questions in current research into catalytic materials. Using a combination of neutron scattering and molecular dynamics simulations, researchers at SNS were able to probe interfacial water dynamics on a time scale from a nanosecond (1 billionth of a second) to a picosecond (1 trillionth of a second). In the process, they gained a fundamentally new understanding of how water engages a surface at varying temperatures. Water is a key element in many catalytic reactions, and the ultimate goal is to develop new catalytic and catalyst-support nanomaterials. Those nanomaterials can then be used as catalysts for chemical production processes in various industries.

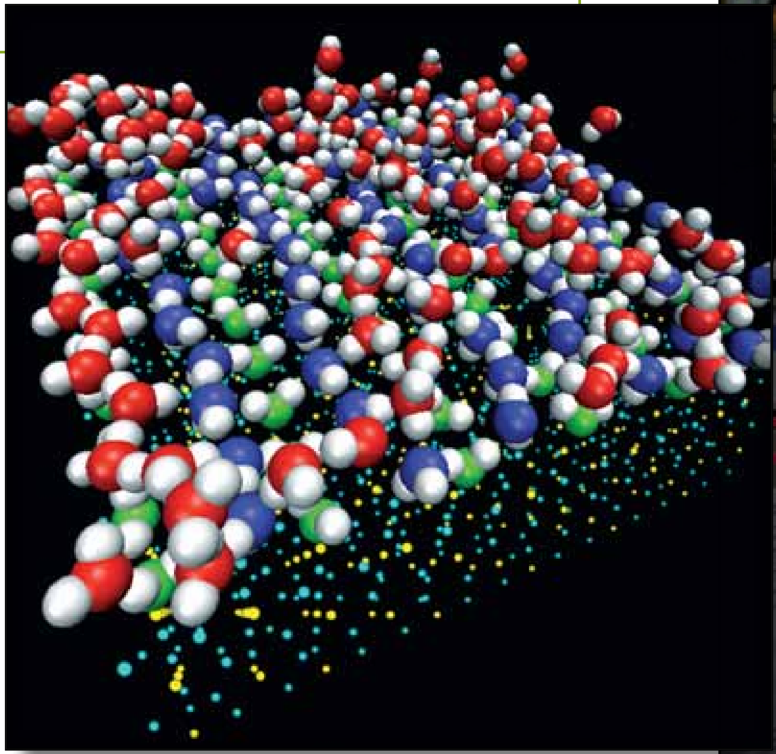
"Catalysis is important for energy and the environment because virtually all chemical production processes are assisted by catalysts of some kind," says Eugene Mamontov, lead instrument scientist for the BASIS. In particular, oxide nano-powders, rutile among them, are commonly used in various applications as catalysts, catalyst supports, or both. In their research, the team studied how water molecules move on the surface of rutile and how the water dynamics were affected by changes in temperature. They used BASIS, which measures subtle changes in the energy of neutrons that are scattered by the sample (in this case, the mobile water molecules on the rutile nano-powder surface).

"Nanoscale Complexity at the Mineral/Water Interface" is a big-umbrella project, funded by the Division of Chemical Sciences, Geosciences and Biosciences, which is part of the DOE Office of Basic Energy Sciences. Led by principal investigator David Wesolowski of CSD, it has a number of participants who combine their expertise in several fields to attain a comprehensive understanding of interfaces. Part of their recent research entailed experiments with water on rutile—a form of the highly refractive mineral compound titanium oxide. The work engaged participants Wesolowski, Mamontov, Lukas Vlcek (Vanderbilt University), Peter Cummings (Vanderbilt and the ORNL CNMS), Jorgen Rosenqvist (CSD), Wei Wang (ORNL Environmental Sciences Division), Dave Cole (CSD), and more than a dozen other researchers. "The scope of this project is very broad, for we are developing a fundamental understanding of the phenomena which occur at water-mineral interfaces," Mamontov says.

"What makes this spectrometer unique is that it utilizes a very high intensity neutron beam; but even more so, its combination of high-energy resolution and wide dynamic range is unprecedented," Mamontov says. "This enabled us to probe the dynamics on a time scale from 1 nanosecond (1 billionth of a second) to 1 picosecond (1 trillionth of a second). In particular, we were able to probe the dynamics of surface water on the rutile sample down to 195 kelvin (-109°F), even though the motions become very slow at such a low temperature." To better understand their results, neutron scientists then used the Computing Center at Vanderbilt University, where the team used molecular dynamics simulations to "label" and track individual water molecules and their motions.

The results of the water on the titanium oxide surface experiment gave the researchers a new understanding of the dynamics in great detail, Mamontov says. "Under ambient conditions, the surface of any hydrophilic material (material that attracts water, such as oxides) is covered by a thin layer of water adsorbed from the atmosphere. If you expose the material to open air for a short time, the surface will

Catalysis research revealed the dynamics of surface water on catalytically active nanomaterials.



Michaela Zamponi (left) and Eugene Mamontov (right), instrument scientists for BASIS.

be covered by adsorbed water. The coverage is thin—only about 2 or 3 molecular layers of water—but these molecules exert great influence on the surface properties of the material, especially in the case of nanomaterials, such as nano-powder oxides, simply because the surface area is so large."

"It's the fact that hydration water is so ubiquitous on the surface of hydrophilic materials that gives broad significance to this research. We found that this thin layer of adsorbed surface water (also called hydration water) does not really freeze; even at temperatures as low as 195 kelvin, it shows some mobility. How this water moves depends on the hydration level (for example, whether we have two layers, or three layers of water). The research has great potential for catalytic and catalyst-support nanomaterials." The team will now conduct further experiments, using different materials hydrated with water and exploring the dynamics of different hydration levels of water on the materials, Mamontov says. "This is an ongoing project and will span at least several years."

For more information see:

E. Mamontov, D. J. Wesolowski, L. Vlcek, P. T. Cummings, J. Rosenqvist, W. Wang, and D. R. Cole, "Dynamics of hydration water on rutile studied by backscattering neutron spectroscopy and molecular dynamics simulation," *J. of Phys. Chem. C* **112**, 12334 (2008).

Contact: Eugene Mamontov (mamontove@ornl.gov)

Extreme pressure studies with brucite will lead to advances in areas such as medicine, geoscience, and industrial technology.

Extreme-Pressure Brucite Studies

A collaboration using instruments at both SNS and HFIR has investigated how hydrogen and deuterium differ under pressure, to help both the science community and industry clarify fundamental differences in these isotopes. This research can potentially impact neutron scattering, geosciences research, and industrial applications.

Researchers Juske Horita, Antonio Moreira dos Santos, Bryan Chakoumakos, and Chris Tulk used the WAND instrument at HFIR to study the effects of pressure on the compression properties of hydrogenated and deuterated brucite.

Brucite, or magnesium hydroxide ($Mg(OH)_2$), was chosen because it is one of the simplest hydrogenated materials found in nature. It is made of stacked sheets of magnesium hydroxide octahedra, which are composed of magnesium ions with a +2 charge, bonded to six hydroxides with a -1 charge. Each hydroxide in turn is bonded to three magnesium ions. The result is a neutral sheet, as the charges cancel and the lack of a charge means there is no "glue" to keep the sheets together. The sheets are held together only by weak electrostatic interactions.

"Brucite is what we like to call a model system. It is a system that has so little complexity that phenomena that are observed can be traced directly back to the problem that we want to elucidate," says Moreira dos Santos, a postdoctoral fellow at SNS.

The question was whether a brucite sample made with hydrogen and a second made with deuterium, a heavier isotope of hydrogen, would respond identically to pressure. Researchers favor deuterium for neutron scattering samples because hydrogen scatters incoherently and that generates a lot of what scientists call background in the data. The measurements tend to be lengthier and have poor resolution, Moreira dos Santos explains. "Hydrogen is not a very good isotope to work with."

All conditions being equal, scientists prefer deuterium in their samples for neutron scattering experiments. But all conditions are not equal, as Moreira dos Santos and his colleagues have found. The difference between hydrogen and deuterium in the sample can affect neutron scattering research results, as well as studies of hydrogenation of minerals deep in the earth, some of which store water and hydrogen in other forms, and hydrogen storage applications in industry.

Juske Horita, a researcher in the Chemical Sciences Division, made samples of brucite, one with hydrogen and one with deuterium. Then the researchers went to the SNAP powder diffractometer at SNS and applied pressure to each sample, measuring several diffraction patterns in situ, while increasing the pressure. Says Horita, "By the changes that happen as you increase pressure, you can understand what the pressure is doing to the crystal structure at the atomic level, how much the atoms come closer together. You can quantify that and, because you have both hydrogen and deuterium samples, you can see how the one compares with the other under pressure."

Detectors at different angles collected the diffracted neutron beams. Horita explains, "In this technique, called angle dispersive diffraction, at some angles you measure a peak of intensity. There are a lot of neutrons that scatter in that direction, while at other angles there are very few. Crystals are very ordered systems and the positions of these peaks will provide information regarding the positions of the atoms with respect to each other. The periodicity of the crystal is going to be reflected in a sort of pattern."

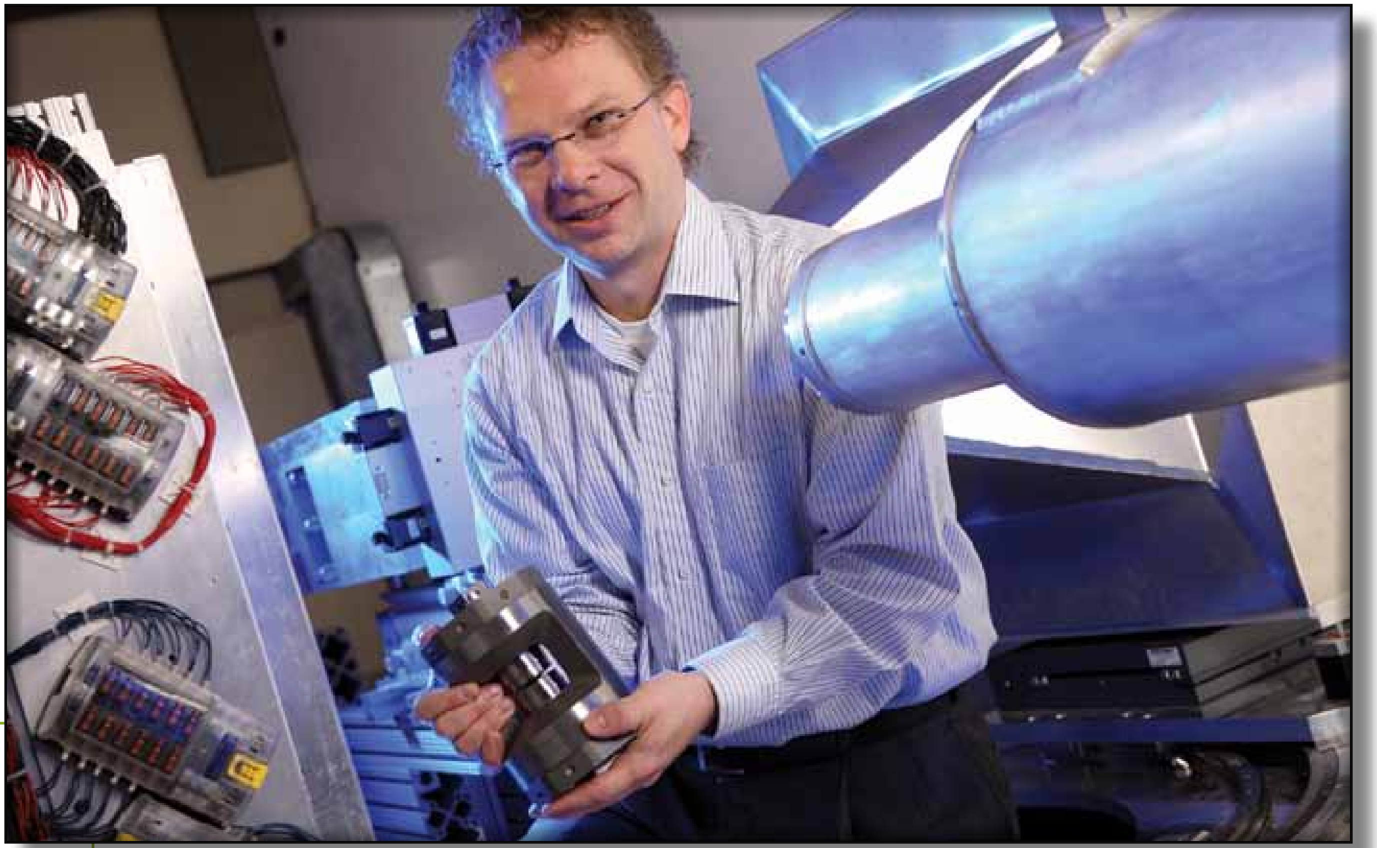
The group was looking for specific changes in unit cell volume (the building block of a crystalline material), which would indicate how close the atoms in the samples became under the pressure applied. What they found was a systematic higher compressibility on deuterium samples of brucite. Moreira dos Santos says this is critically important to him as a researcher. "When I do other sorts of measurements, every time I use deuterium I have to be careful, because things will happen sooner, at lower pressure, than when I use hydrogen. So that will give me clues to establish a standard on what to expect or how to correct the data obtained when doing scientific research on samples containing hydrogen."

The implications may be important across broad fields, from hydrogen storage research to pharmaceutical and even medical research. "When you want to use molecules as a medicine or you want to study mantle minerals underground or you want to study brucite, be careful in replacing hydrogen with deuterium because they are not the same but they actually show a distinctive behavior."

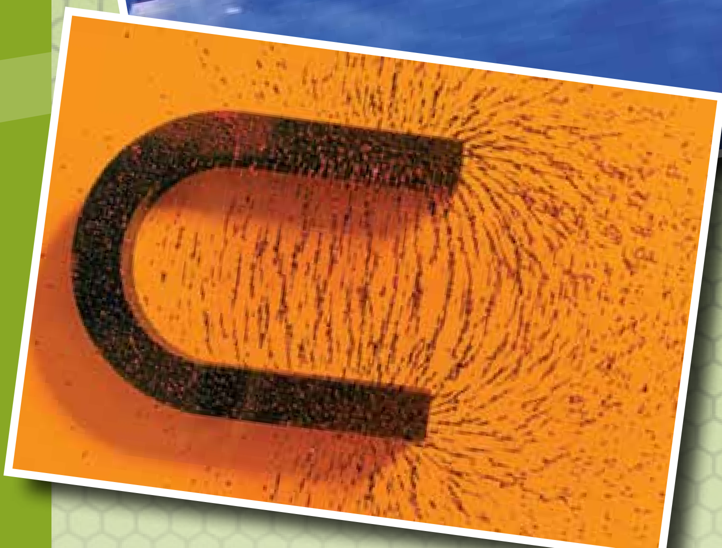
Moreira dos Santos says that a difference in the behavior of hydrogen and deuterium under pressure may be significant at high pressure ranges found in the earth, providing new insight into the abundance of deuterium in nature, and on other planets. "If the deuterium sample is more compressible, deuterium may be more abundant in the earth than previously thought. We mostly measure the things which come to the surface, but of course if hydrogen is less stable under high-pressure conditions, hydrogen will come to the surface first, to escape an adverse environment. If deuterium is actually more compressible, when you compress the rocks it is not such a dramatic change and it may remain in that state. So our estimate for the amount of deuterium and hydrogen in nature can be slightly off."

Finally, the research is important for neutron scattering in hydrogen storage research. "Neutrons are incredibly useful to study hydrogen storage problems, because neutrons can measure hydrogenated samples much better than x-rays. But you still have this background problem with hydrogen. You want to use deuterium, as long as we know what is happening and as long as we have this benchmark.

"If you can just find a good model system it can really open the doors for wonderful research. Horita's work was really important, to find the system in which we were able to isolate the property that we wanted to isolate. Because when you can really clarify something, others can start from that and keep moving forward. This gives us the motivation to move on and do complementary experiments so that we can really probe the bonding of the hydrogen or the deuterium with the oxygen in the structure. This also gives us some ideas to do deeper experiments, to understand the origin of this difference."



Chris Tulk, lead instrument scientist for SNAP, with a Paris-Edinburgh pressure cell.



Studies of spin ice have increased our knowledge of the magnetic relationships among atoms, helping us better understand the other properties of materials.

Magnetism and Molecular Structure

Georg Ehlers and his colleagues are a bit like detectives on an atomic scale. They're looking for clues to explain how changes in molecular structure affect the magnetic relationships among atoms in a material called "spin ice." Because magnetic relationships affect other properties of materials, this research is applicable to a variety of fields.

The term spin ice is applied to materials whose magnetic structure is comparable to the crystal structure of water ice. As one might expect, water ice has been studied in depth, so the similarities between the two materials provide researchers with a model, of sorts, for their investigations. The spin ice Ehlers and his colleagues are studying is basically $Ho_2Ti_2O_7$, where some of the holmium has been replaced with nonmagnetic lanthanum. The reasons for doing this may be a little more obvious if we define a few key terms.

What is a magnet? Everyone has held two magnets together and felt them attract and repel each other. On the atomic scale, the definition of a magnet becomes a little broader—any substance containing atoms that exert a magnetic force on other atoms is considered to be a magnet. The biggest difference between these two situations is that, on the macroscopic scale, a magnet is made up of atoms whose magnetic moments all work in the same direction, acting together. On the atomic scale, however, a magnet can be composed of atoms whose moments point in many different directions—working together or potentially cancelling each other out.

What is a "frustrated" magnet? In a solid material, individual magnetic moments can point in a number of different ways, usually in the arrangement that requires the least energy to maintain. "This is the arrangement of magnetic moments that you would most often find," says Ehlers. "However, a frustrated magnet is a material where the spatial arrangement of the neighboring magnetic atoms prevents the magnetic moments from easily finding this sort of minimum energy configuration."

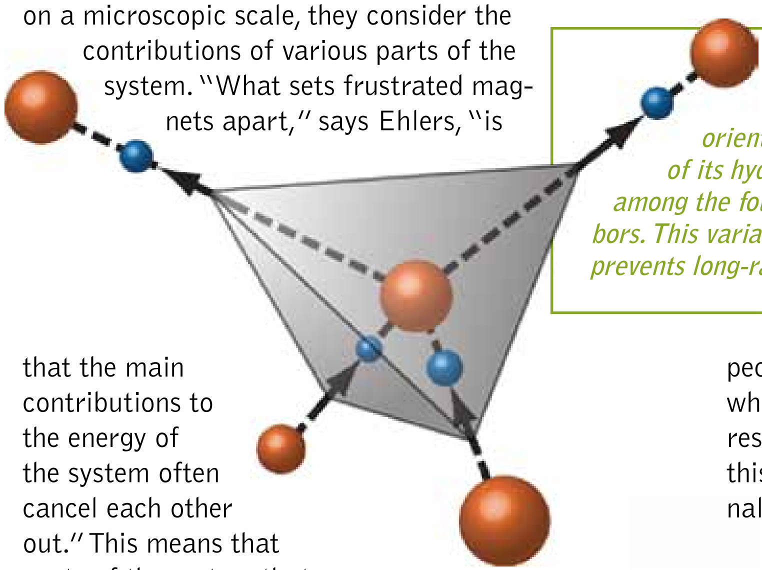
What is spin ice? Spin ice is a type of frustrated magnet. Similar to water, magnetic moments in spin ice can assume any of several different tetrahedral configurations, all with the same ground state energy. But when the ice freezes, the possible varied configurations prevent it from easily finding its "least energy" configuration, or long-range order.

In this project, Ehlers' team (which includes Eugene Mamontov, Michaela Zamponi, Jason Gardner, and K.C. Kam) was trying to determine what happens on the atomic scale when spin ice freezes—and in particular, how impurities in the spin ice, like the added lanthanum, change the freezing process. Ehlers notes that, in water ice, the frustration in the ice is in the hydrogen bonds. However, if you add certain chemical impurities to the water you can eliminate that frustration and make long-range-ordered ice crystals.

"In the spin ice," he says, "we find that the changes resulting from the introduction of an impurity are much less significant than we would expect." Ehlers explains that researchers' expectations in this regard are guided by their experience with other frustrated systems and how the freezing process is altered in these systems when impurities are added. "We found that, in spin ice, the frustration effects are much more resistant to external changes," he says.

However, as it turns out, the frustration effects in the spin ice were not entirely unaffected by these changes. The addition of lanthanum atoms, which are slightly larger than the holmium atoms they replaced, created stress in the structure of the spin ice. "This didn't create long-range order," says Ehlers, "but it created slightly different effects than putting in an impurity which is exactly the same size as the holmium. So, although we were not successful in creating long-range order and relieving the frustration completely, we found that different impurities cause different effects."

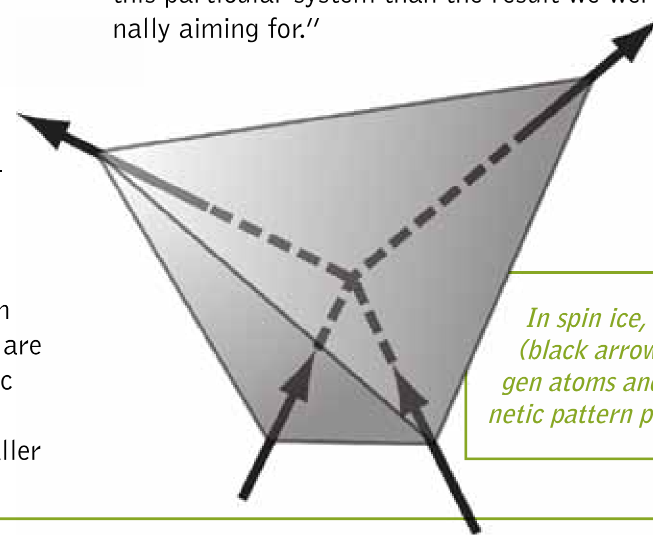
Another, more subtle, finding suggests that influence over the structure of spin ice can come from unexpected places. When physicists describe magnets on a microscopic scale, they consider the contributions of various parts of the system. "What sets frustrated magnets apart," says Ehlers, "is that the main contributions to the energy of the system often cancel each other out." This means that parts of the system that would normally have a negligible impact can sometimes play key roles in determining the magnetic configuration.



In water ice, the central water molecule can take six orientations by moving the locations of its hydrogen atoms (blue circles) among the four hydrogen bonds to its neighbors. This variation in hydrogen arrangement prevents long-range order in the ice crystals.

A system's main magnetic moments are created in the electron shells of atoms, but nuclei also can have magnetic moments. These nuclear moments are about a thousand times smaller than the magnetic moments of the electrons. "In the spin ice system we have looked at, we identified one of these smaller contributors that apparently has a major impact," Ehlers says. "That is the magnetic moments of the holmium nuclei."

The influence of these nuclei appears under fairly specialized circumstances. When spin ice is cooled, it freezes—as does ice—in an irregular, frustrated way until nothing moves. However, at the temperature where the moments of the electrons are frozen, the moments of the nuclei are still dynamic because the nuclei freeze at a much lower temperature. "It appears that the continued presence of dynamics in the nuclear moment system introduces residual dynamics in the system of the electronic moments," says Ehlers. "As a result, the sample has difficulty getting into the truly frozen ice state. We came across something unexpected and new, and it took us some time to realize what it was," he says. "It turns out that this new result should have more impact on the knowledge of this particular system than the result we were originally aiming for."



In spin ice, the direction of its magnetic moments (black arrows) is similar to the position of the hydrogen atoms and the oxygen ions in water ice. This magnetic pattern prevents long-range order in the spin ice.

So what's the next step? "It all depends on what your ultimate goal is," says Ehlers. He mentions several potential avenues of inquiry: continue his group's studies but with other parameters such as external pressure or an electric field, compare the material used in this study with other frustrated materials, and conduct theoretical studies of the importance of other energy terms and their interaction energies.

Regardless of how the research proceeds, Ehlers stresses that much of the data generated by this study could not have been gathered at any other facility. "We were studying something that we thought we already understood fairly well, but the SNS Backscattering Spectrometer allows us to see details ten times more closely than we could before."

For more information see:

G. Ehlers, E. Mamontov, M. Zamponi, A. Faraone, Y. Qiu, A. L. Cornelius, C. H. Booth, K. C. Kam, R. Le Toquin, A. K. Cheetham, and J. S. Gardner, "Frustrated spin correlations in diluted spin ice $Ho_{2-x}La_{x}Ti_2O_7$," *J. Phys.: Condens. Matter* **20**(23), 235206 (April 2008).

G. Ehlers, E. Mamontov, M. Zamponi, K. C. Kam, and J. S. Gardner, "Direct observation of a nuclear spin excitation in $Ho_2Ti_2O_7$," *Phys. Rev. Lett.* **102**, 016405 (2009).

SCIENCE HIGHLIGHTS

Research in Progress

Magnetization Profiles in Nanomaterials

Valeria Lauter and postdoc staff Hailemariam Ambaye at the SNS Magnetism Reflectometer.

Researchers use polarized neutrons, or those with a magnetic spin in one direction, to determine the magnetic qualities of materials. Polarized neutron reflectometry is being used to study the magnetism at the interfaces between different materials in epitaxial heterostructures based on lanthanum manganese oxide (LaMnO). (An epitaxial structure is a thin sheet or film of a material composed of layers deposited or grown in an orderly fashion so that successive layers are aligned atom by atom, forming a single crystal).

The work is being carried out by the Magnetism Reflectometer research team of lead instrument scientist Valeria Lauter, postdoctoral staff member Hailemariam Ambaye, and others in collaboration with Hans Christen and Michael Biegalski of the ORNL CNMS.

Materials can be ferromagnetic (with individual atomic spins aligned in the same direction, as in a permanent magnet), antiferromagnetic (with atomic spins aligned in opposite directions, so that it has no overall magnetic character), or paramagnetic (exhiting magnetic behavior only in the presence of an external magnetic field). In bulk form, $LaMnO_3$ is a well-known antiferromagnet, so it has no overall magnetic character. However, when $LaMnO_3$ is grown in the shape of a thin film, it can acquire new properties at interfaces because of its proximity to other elements. Previous work on these interfaces has shown enhanced ferromagnetism at the interfaces between $LaMnO_3$ and the paramagnetic insulator, strontium titanium oxide ($SrTiO_3$).

A major 2008 upgrade to the Magnetism Reflectometer is enabling dramatically improved studies of nanomaterials. Improvements in background level (reducing interference from other effects), polarization level (degree to which individual neutron spins are aligned), and resolution are enabling researchers to analyze components of the magnetization density of materials at a remarkable resolution of half a nanometer. This advance is providing new insight into how the various atomic-scale magnetic structures interact in different parts of a material. The sensitivity achieved with the enhanced instrument now allows researchers to detect changes in the magnetic state of a layer of material with the thickness of a single unit cell (the smallest bit of a material that preserves its unique structure).

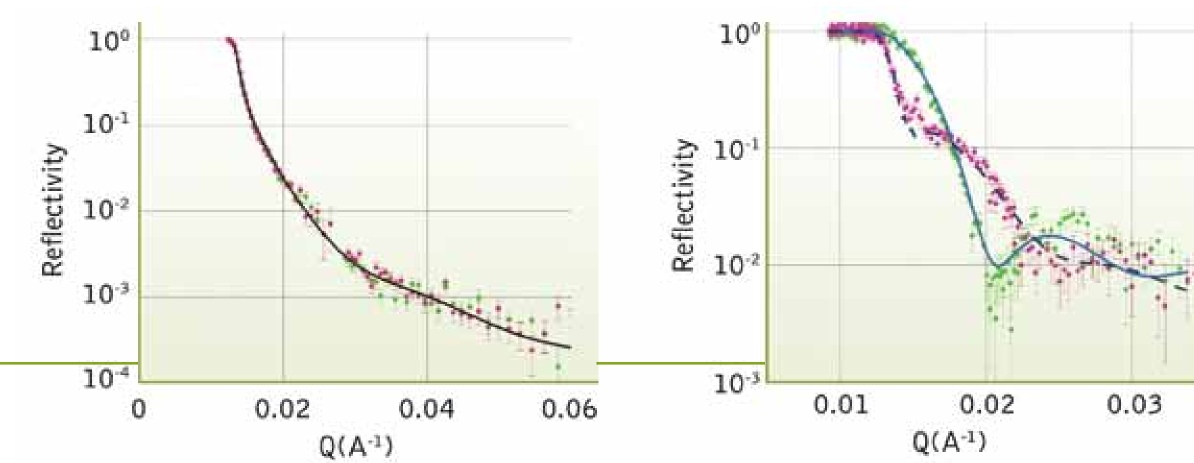


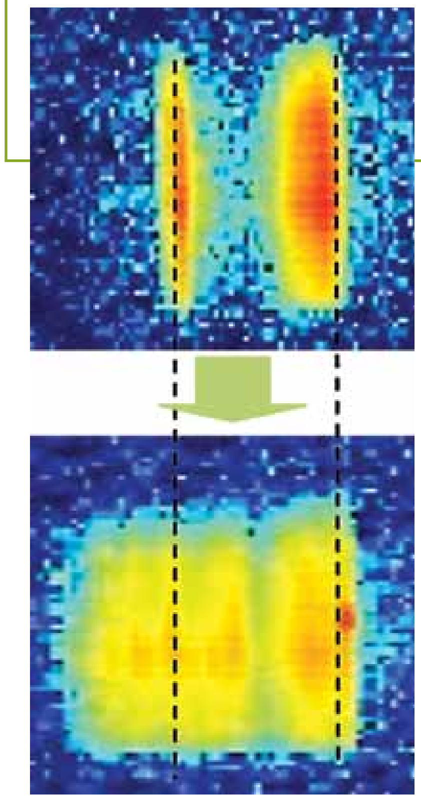
Figure 1a. Neutron reflectivity profiles R+ (green points) and R- (magenta points) as functions of momentum transfer for an $SrTiO_3$/$LaMnO_3$ bilayer film on $SrTiO_3$, measured with polarized neutrons and an applied magnetic field of H = 1 Tesla, applied in the plane of the film (left, T = 300 kelvin; right T = 5 kelvin). The solid lines correspond to the data using a model with a depth-dependent scattering length density.

Preliminary results have revealed that the observed magnetism depends on the stacking order of atomic layers at the interface between the two materials. (Different types of interfaces can be formed using pulsed-laser deposition.) Neutron reflectometry can be used to determine the magnetic depth profile of different epitaxial structures with a resolution of less than a nanometer. "The magnetization profile obtained from the reflectometry experiment (see Figure 1a) will provide information that cannot be obtained using any other measurements," Lauter says.

Additional promising nanomaterials research was conducted by Sunil Sinha (University of California–San Diego) and Elizabeth Blackburn (Birmingham University, UK). The team used neutrons to map out the magnetization at the interface of the ferromagnetic and antiferromagnetic layers in the prototypical system (Py/CoO) and observed how the magnetization changes as the material enters the exchange biased state (Figure 2). When an exchange-coupled bi-layer film of a ferromagnet and an antiferromagnet is cooled in an external magnetic field through the ordering temperature of the antiferromagnet, an exchange bias—a shifting of the hysteresis loop—is observed. "Although this effect has already been exploited to develop several new industrial applications using thin film materials, a detailed microscopic understanding of the physical mechanism underlying this effect has proved elusive," Lauter says. The goal of these studies is to search for traces of pinned magnetization, which is thought to be responsible for the observed magnetic behavior.

The epitaxial film imposes an elastic strain (temporary displacement of atomic positions) on the SrTiO substrate. In the course of the experiments, an unexpected effect of this strain was observed below the structural phase transition temperature (the temperature at which the preferred arrangement of atoms within a material changes, ~105 kelvin in this case). "It was observed that the domain state in the substrate can be altered by application of a magnetic field to a magnetic film, and neutron reflectometry has been shown to be sensitive to the resulting minute changes in the surface," Lauter says (see Figure 1b). The research team is continuing to investigate this fascinating and previously unreported effect.

Figure 1b. Experimental intensity maps of incident and reflected neutrons integrated over neutron wavelengths from 2 to 5 angstrom. The dashed lines correspond to the positions of the reflected (left) and the incident (right) intensities at temperatures of 300 kelvin (top) and 5 kelvin (bottom). Drastic changes in the profiles of reflected neutrons give evidence of structural modifications at temperatures below the substrate's phase transition.



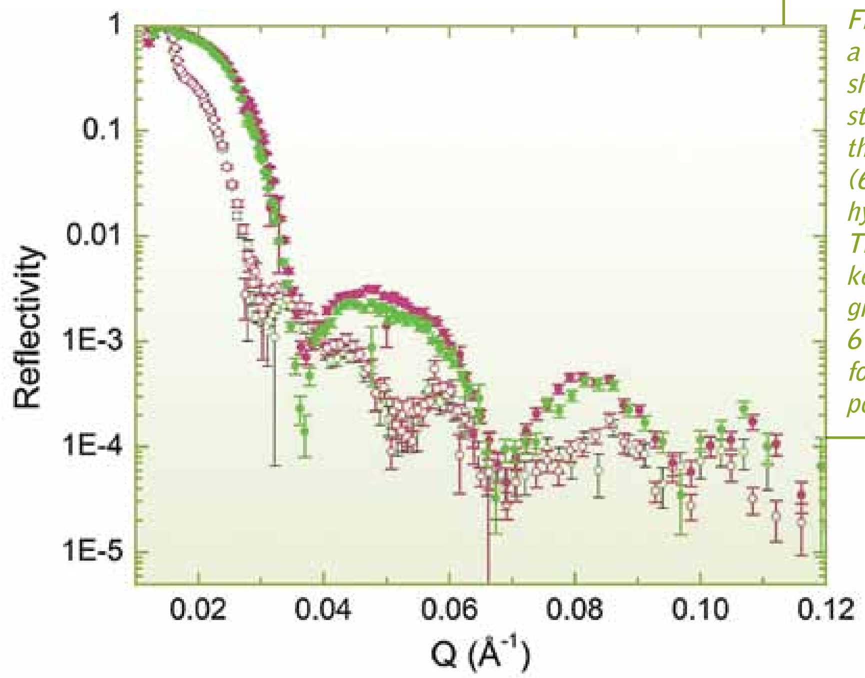


Figure 2. Reflectivity data for a Py/CoO thin film material showing results for the normal state (room temperature) and the exchange-biased state (6 kelvin). The inset shows the hysteresis loop for this sample. The data were taken at 300 kelvin (green solid for R+ and green open points for R-) and 6 kelvin (magenta solid point for R+ and magenta open points for R-).

Research in Progress

Synthetic Membranes: Copying Mother Nature

Studies with "manufactured" biomaterials promise advances in medicine, such as more effective drugs and methods for diagnosing disease.

Imitating the biological complexities found in Mother Nature is no easy task. Nevertheless, scientists working at SNS and the nearby CNMS are trying to emulate the molecular activity that occurs at biological interfaces—the boundary areas within living cells. The researchers are building bio-inspired, biocompatible synthetic membranes to help them understand the interactions between synthetic materials and biomolecules.

"We're taking our inspiration from Mother Nature," says researcher, Brad Lokitz. "In the body and in nature, lots of biological processes happen at interfaces and membranes, so we're trying to mimic nature in a very basic way to gain some insight into these processes."

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

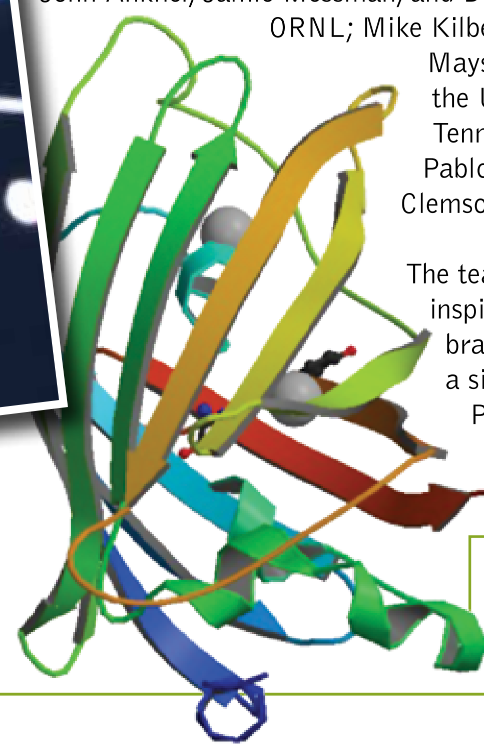
The team's bio-inspired membrane starts with a silicon base. Polymers are then attached more or less evenly across the surface of the silicon. These polymer strands provide a framework, or scaffold, for the biomolecules that are added later.

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

It has taken several attempts to come up with a process that results in a polymer framework that has a uniform thickness and is evenly distributed across the surface, but the results have been worth the trouble. "In order to use neutrons to study the sample, it needs to be very uniform on the molecular level," says Lokitz. "The rougher the surface is, the less information you can extract from it, so we want the surfaces to be as molecularly smooth as possible. Just now we're getting to the point that we can reproducibly prepare samples that are sufficient to take over to SNS and obtain good results."

The team is using the SNS's Liquids Reflectometer to study both the polymer scaffold itself and the attached biomolecules. One of the reflectometer's specialties is using neutrons to investigate the boundaries between hard and soft matter—like the bio-inspired surface Lokitz and his colleagues are working with.

Lokitz notes that having SNS right next door to CNMS provides a synergistic opportunity to perform nanoscience research at two state-of-the-art facili-



This green fluorescent protein (GFP) variant is shown as a representative protein for future binding studies.

ties. "We can create our samples at CNMS, walk next door, and test them at a world-class facility. As we're running our test, we pretty much get immediate feedback. If we see that we need to do something different, we can go back to CNMS, tweak our procedure, and then go back next door to continue the testing."

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

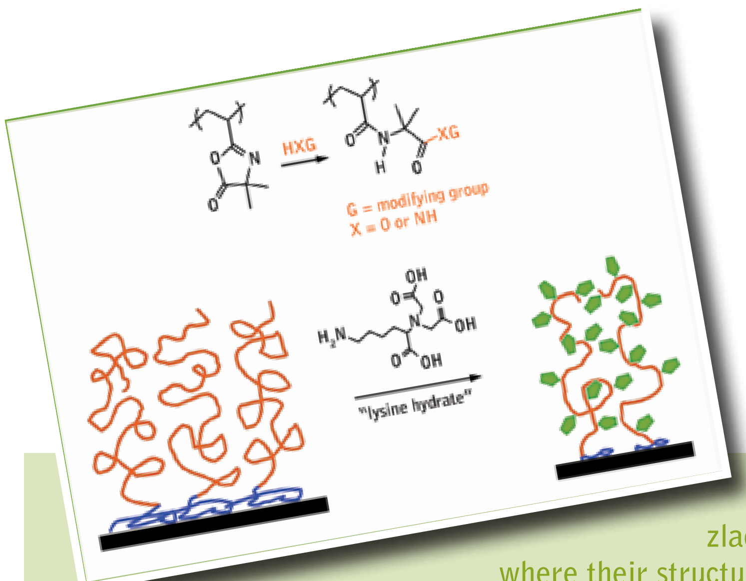
The Liquids Reflectometer is able to characterize the thickness, density, and orientation of the polymers. It is also very sensitive to small changes in density or thickness, so it provides researchers with an opportunity to study minute variations in the scaffold or the attached biomolecules.

"We can look at the surface with just the polymer attached and get an idea of the layer thickness and composition." Lokitz says. "Then when we functionalize the layer—attach the biomolecules—and look at it again, the instrument is sensitive enough to notice those small changes."

"For example," Lokitz says, "Right now we're using lysine hydrate as a model compound and are evaluating its ability to bind proteins after it's attached to the scaffold. "

Overall, the project aims to develop expertise in using neutron scattering to prepare and investigate soft material scaffolds that can be used to create bio-inspired membranes. Because interfaces play a key role in biological processes, developing robust platforms that can be used to examine structure-property-function relationships of biomolecules attached at interfaces is crucial to bridging biology and biological processes to the development of next-generation materials, devices, and processes.

Brad Lokitz examines a sample at the SNS Liquids Reflectometer.

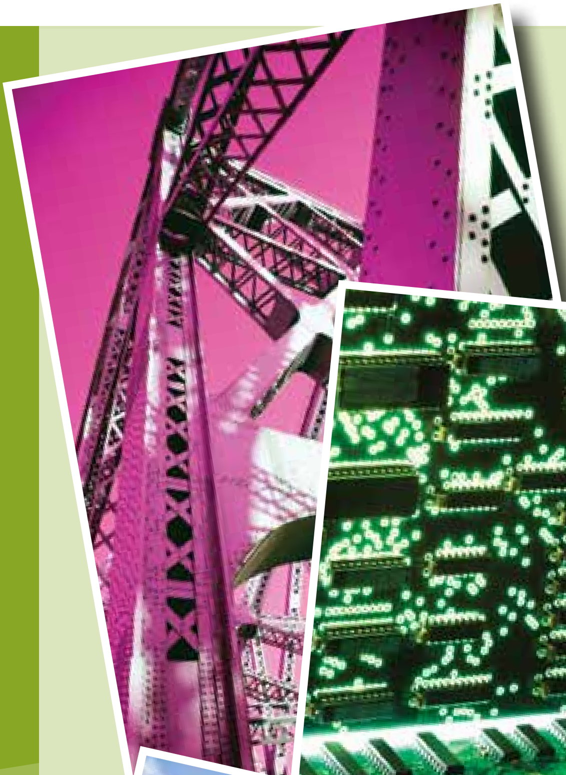


The research team has made scaffolds based on a novel class of block copolymer called vinyldimethylazlactone (VDMA). The VDMA block copolymers allow proteins and enzymes to be confined to interfaces, where their structure and stability can be examined at the molecular level. This knowledge can provide a foundation for developing more complex bio-inspired systems.

Above: reaction of VDMA with lysine hydrate. Once the polymer scaffold (orange) is attached to the substrate (blue), biomolecules (green) are attached to the individual polymer strands. Researchers then examine the scaffold to see how the biomolecules affect the structure of the scaffold, how being attached to the scaffold affects biomolecules, and whether the biomolecules can still perform their biological functions.

Research in Progress

Magnetic Behavior in Manganese Nanoparticles



Research on the magnetic properties of ubiquitous elements such as manganese will have almost endless applications—from engineering to electronics to environmental protection.

Manganese is present in rail switches, tools, axes, safes, batteries, and an additive in unleaded gasoline. Manganese works with several enzymes in the body and is a required trace element for all known living organisms. Manganese ore is often found in combination with iron ore.

Both manganese and iron have magnetic properties. Andy Christianson, a Shull Fellow at ORNL who is interested in the physics of manganese oxide (MnO) nanoparticles, explains the different magnetic properties of both elements.

"If I pick up a piece of iron, it may not act magnetic because the domains are pointing in different directions," Christianson says, explaining that a domain contains electrons that spin in one direction, either up or down. "If a strong magnetic field is applied to the iron piece, the domains line up in the same direction and an external magnetic field results."

Manganese is antiferromagnetic. In materials that exhibit antiferromagnetism, the magnetic moments of atoms or molecules, usually related to the spins of electrons, align in a regular pattern with neighboring spins (on different sublattices) pointing in opposite directions. Like ferromagnetism, antiferromagnetism is a manifestation of ordered magnetism.

Christianson is looking for evidence that the magnetic behavior of bulk MnO is different from that of MnO nanoparticles. ORNL's Sheila Baker is working on synthesizing MnO nanoparticles in a uniform size—about 8 nanometers across. If bulk MnO has long-range antiferromagnetism, Christianson believes that some MnO nanoparticles could exhibit a different magnetic or nonmagnetic property from what is detected.

"MnO is a classic antiferromagnetic system," Christianson says, adding that he uses neutrons to detect magnetic excitations, or spin waves. "We picked manganese oxide because we wanted to start with a material as simple as possible."

Neutron scattering is the best method for measuring spin waves, Christianson says. "Neutrons will scatter from spin waves. Neutrons entering a sample will either create a spin wave or destroy a spin wave in the material before being deflected toward a detector."

A relationship exists between the energy of a spin wave and its wavelength: as a spin wave's energy decreases, its wavelength gets larger.

"If the energy is small enough, the spin wave would have a wavelength that is bigger than the nanoparticle, which is impossible," Christianson says with a smile. "What we expect is a gap in the spin wave spectrum that is due to this size effect."

The MnO nanoparticles are encapsulated in a hollow aluminum tube filled with helium. Christianson then cools down the sample to find the temperature at which the antiferromagnetic order appears. Below that temperature he can detect spin waves using neutron scattering.

During cooling of the nanoparticles, the helium gas transfers heat evenly, keeping the nanoparticles at the same temperature. Christianson and his colleague Mark Lumsden have cooled the MnO nanoparticles down to their antiferromagnetic ordering temperature of 118 kelvin (room temperature is 300 kelvin).

Using a helium-3 refrigerator, the scientists have cooled the sample all the way down to

500 millikelvin, or 0.5 kelvin, just barely above absolute zero. At this extremely low energy for the spin waves, they have tried to measure a gap in the wavelength spectrum.

"We want to track the magnetic properties of the nanoparticles, such as the ordering temperature at which they become antiferromagnetic and begin producing spin waves, as a function of particle size," Christianson says.

Christianson, Lumsden, Baker, and their colleagues Steve Nagler and William Heller have not yet published any papers, but they have a lot of interesting preliminary data. They obtained their data from the HB-1A Triple-Axis Spectrometer and the GP-SANS instrument at HFIR, a chopper spectrometer at the NIST, and the Backscattering Spectrometer at SNS, "from which we obtained interesting data that we don't understand," Christianson says.

An important part of this study is the synthesis of nanoparticles of different sizes for comparison. Sheila Baker has been synthesizing 8-nanometer MnO nanoparticles and capping them with hairlike organic ligands that have two purposes: (1) they allow the chemist control over size and (2) they protect each nanoparticle from contaminants that could alter its size and composition.

Another group of scientists not associated with ORNL studied MnO nanoparticles embedded in porous glass. Finding that the nanoparticles have a higher ordering temperature than does bulk manganese, the scientists speculated that pressure from the glass could have raised the temperature at which the particles magnetically order. The ORNL group found that the MnO nanoparticles capped with organic ligands have a slightly lower ordering temperature than bulk manganese—the lowest of the three cases.

Mark Lumsden (left) and Andy Christianson (right) examine a sample of a new FeAs-based superconductor.

"It's as if our nanoparticles are under negative pressure," Christianson says. "It may be that the lower the pressure is on manganese oxide molecules, the lower is the magnetic ordering temperature."

Transmission electron microscopy (TEM) images of the nanoparticles Baker makes show the size distribution—the percentages of nanoparticles that are slightly larger or smaller than the desired size. X-ray diffraction experiments also confirm that the nanoparticle consists of MnO instead of other manganese oxide states (such as Mn_2O_3). In conjunction with TEM data, they can determine whether the nanoparticles are single crystalline.

Next steps for the team include continuing to improve the size distribution of the nanoparticles and replacing the hydrogen in the organic ligand caps with deuterium. Because deuterium has a smaller incoherent cross section, ligands made with it will produce less background noise.

Research in Progress

Biofuels Development for Energy Alternatives

Biofuels studies will help reduce future needs for gasoline and other petroleum products.

Improving the efficiency of breaking down cellulose with an enzyme, known as enzymatic hydrolysis, is a key technological hurdle to reducing the cost of producing ethanol from lignocellulosic material for alternative fuels. A group of researchers at SNS and their collaborators are using neutron reflectivity (NR) to understand how they can speed up the catalytic process and help meet new national goals to produce biofuels alternatives for industry and transportation.

Team members are principal investigator Michael S. Kent, Jaclyn Murton, and Blake Simmons of the Joint BioEnergy Institute (JBEI) and Sandia National Laboratories; Jim Browning, John Ankner, and Candice Halbert of ORNL's NSSD; and Bulent Akgun from the National Institute of Standards and Technology.

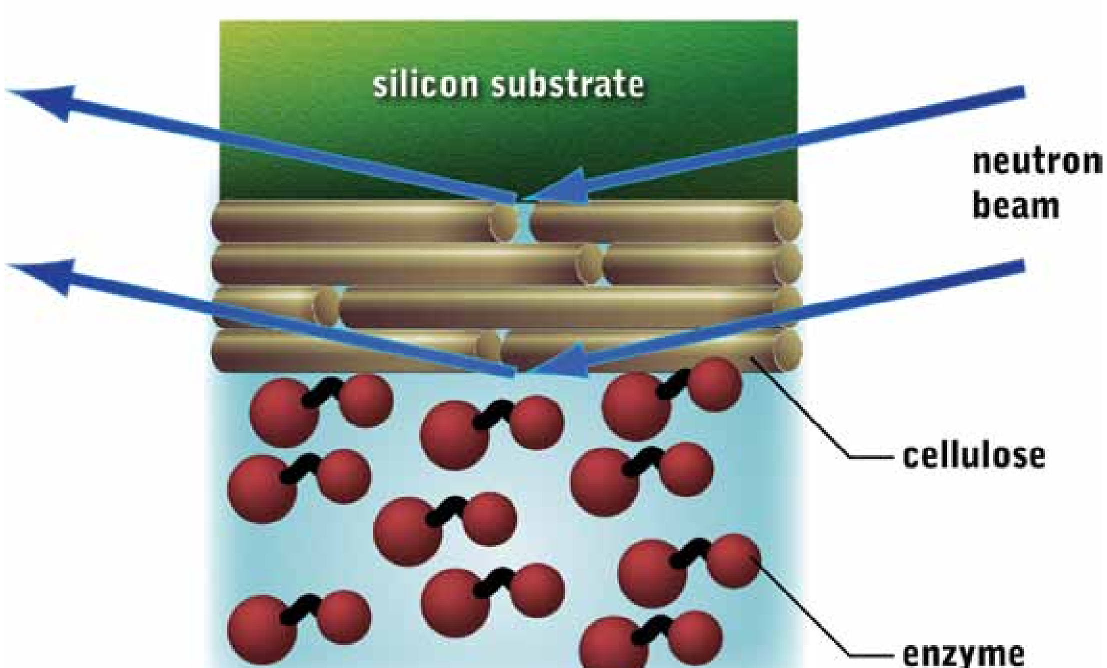
Jaclyn Murton produces the amorphous and crystalline films used in the study at Sandia (a JBEI partner). The films are sufficiently smooth to enable high-resolution study. The team then uses the SNS Liquids Reflectometer along with methods other than neutron scattering to probe the films. "We are using neutron reflection to resolve new details of the interaction between cellulase enzymes and amorphous and crystalline cellulose surfaces during digestion," Michael Kent explains. NR reveals changes in the cellulose films, such as the extent of water penetration into the films and the roughening of the solution-film interface, he said. NR could also be able to reveal some details of the conformation of the bound enzymes.

Enzymatic hydrolysis refers to the breaking down by catalysis of a chemical compound by reaction with water. The conversion of cellulosic materials into ethanol by adding specific enzymes is one example. "Typically, enzymatic hydrolysis proceeds to only a limited extent. High solution-to-solids ratios are required, and the rate of enzymatic hydrolysis typically decreases with time," Kent explains. "A range of mechanisms have been proposed to explain these phenomena, including denaturation of enzymes, nonproductive binding, product inhibition, differences in binding affinity, and activity for amorphous and crystalline cellulose." The current research is part of a broad program at JBEI to parse out the underlying mechanisms in the enzymatic digestion of cellulose, he said. The researchers hope that their study will help to distinguish among these mechanisms and to develop more efficient enzyme systems and pretreatments for the biofuels industry.

This research advances DOE's current programs in cellulosic biofuels. In October 2008, the U.S. Department of Agriculture and DOE released the National Biofuels Action Plan (NBAP), an interagency plan detailing the collaborative efforts of federal agencies to accelerate the development of a sustainable biofuels industry. The NBAP was developed to meet goals for cutting U.S. gasoline consumption by 20% over the next 10 years by investing in renewable and alternative fuel sources, increasing vehicle efficiency, and developing alternative-fuel vehicles. Mandatory funding of more than $1 billion followed, as loan guarantees for cellulosic ethanol projects as well as other renewable energy and energy-efficiency-related programs, a DOE news report said.

Under the strategy outlined, interagency working groups have been chartered to deliver key results such as the development of science-based sustainability criteria and indicators, 10-year research and development forecasts for research to develop cost-effective methods of producing cellulosic biofuels from nonfood-based feedstocks, advancement of these next-generation biofuels to commercialization, and recommendations on infrastructure issues. DOE has dedicated more than $1 billion to research, development, and demonstration of cellulosic biofuels technology through 2009. The current research is funded by DOE through JBEI.

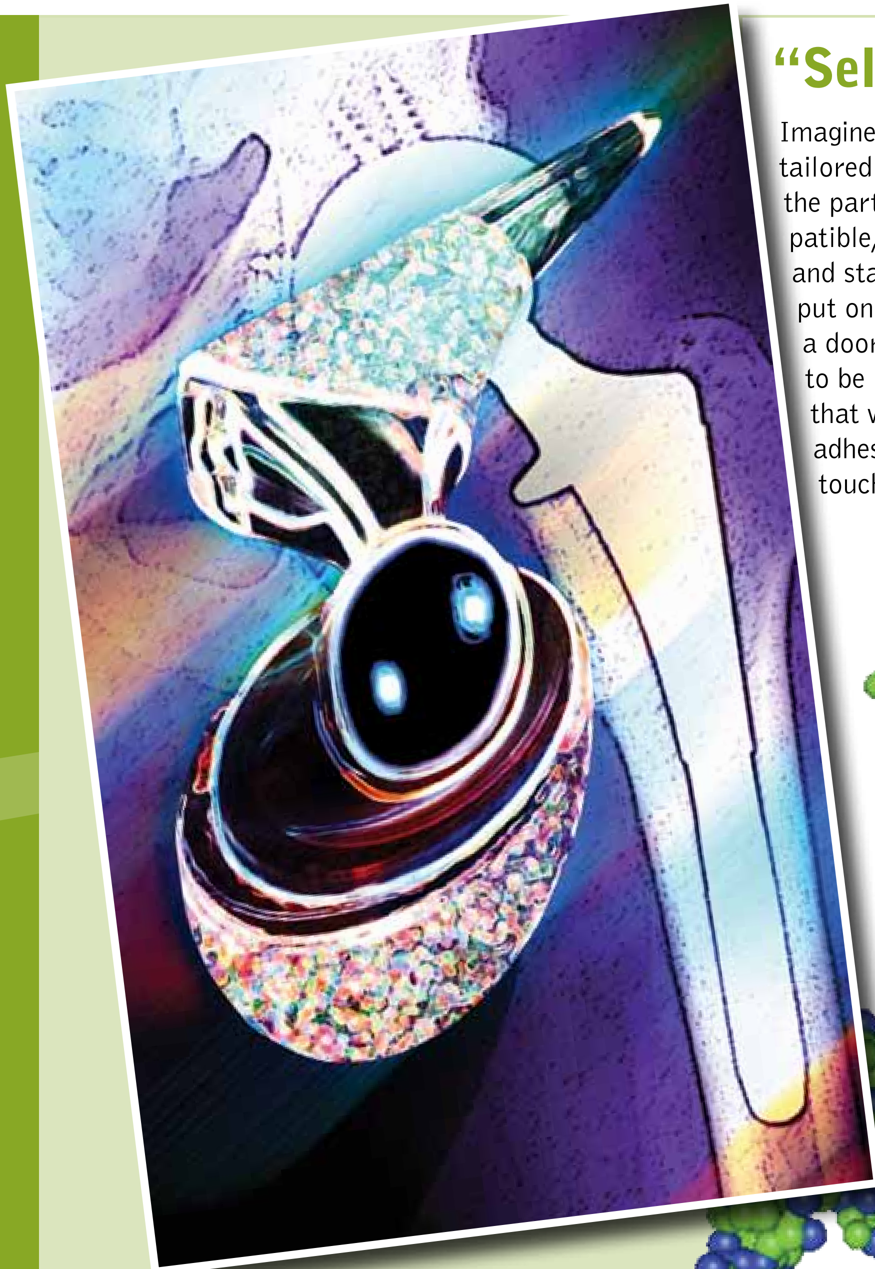
"Commercial enzyme products are cocktails that include many enzymes of different types that are believed to act synergistically," Kent observes. "Future work will involve individual, purified enzymes to better characterize their behavior alone and in concert with other enzymes."



Neutron reflection reveals details of enzymes in D_2O solution in contact with a cellulose film deposited onto a silicon substrate.

Candice Halbert, scientific associate for the Liquids Reflectometer.

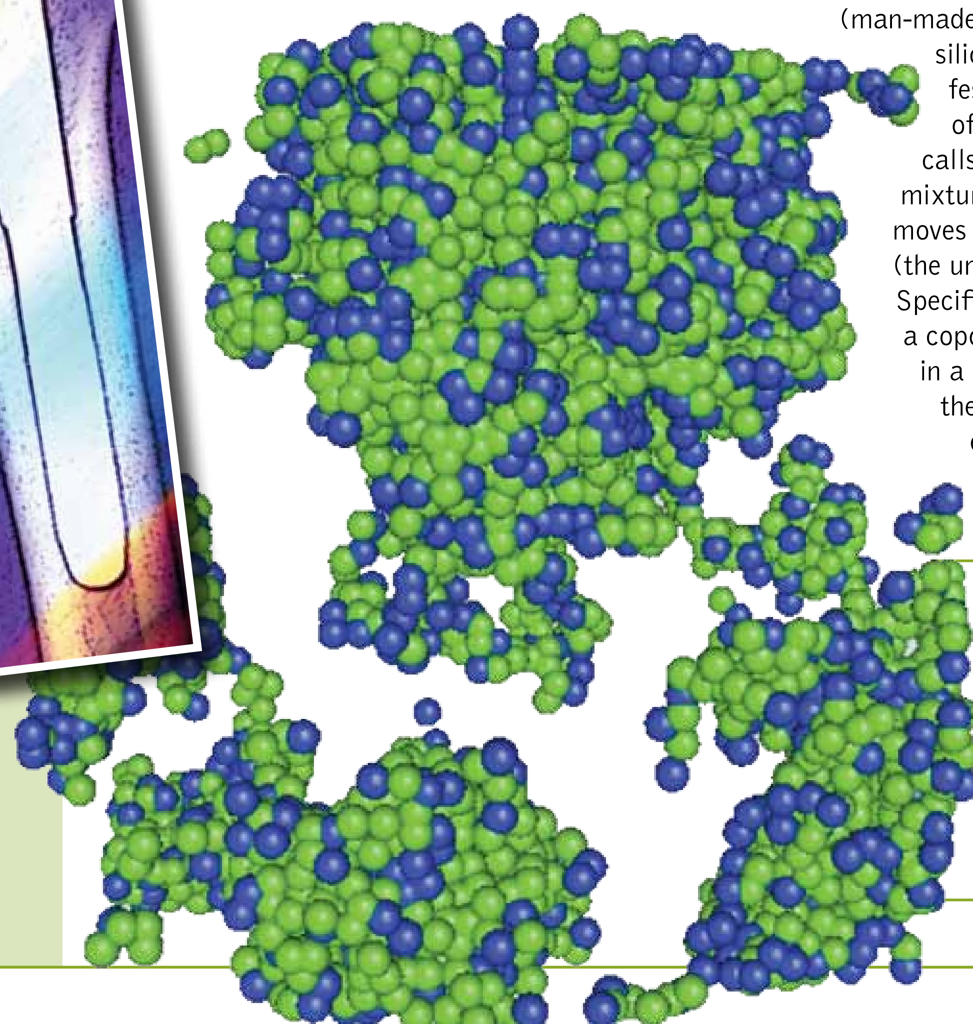
"Self-Healing" Polymers



Polymer studies will open up development of a whole new field of biologically dynamic materials that can be used for improved implants and antimicrobial agents.

Imagine a hip replacement made of materials so tailored that only a thin layer on the outer surface, the part that is in contact with the body, is biocompatible, while the rest of it is designed to be strong and stable to cope with any stress the body might put on it. Or imagine a material designed to coat a doorknob, in which the outer layer is designed to be microbially resistant, while the rest of it, that which holds it to the doorknob, is tailored for adhesive properties. When someone with a cold touches the doorknob, the antimicrobial agents immediately kill the bacteria, while the adhesive properties in the matrix material keep the coating in place. A collaboration of polymer scientists at ORNL is using the SNS Liquids Reflectometer to study the dynamics of polymer mixtures that hold promise for applications from biocompatible films for human implants to semiconductors, substrates for electronic displays, toys for children, and durable, self-repairing aircraft body materials.

Polymers in nature include cellulose, the main constituent of wood and paper. Some familiar synthetic (man-made) polymers include nylon, Teflon, and silicone. Mark Dadmun, a chemistry professor at UT and a joint faculty member of ORNL's CSD, is studying what he calls "self-healing materials," polymer mixtures in which one critical component moves quickly to the surface while the matrix (the understructure) gives structural rigidity. Specifically, he is looking at the dynamics of a copolymer (the targeted, surface material) in a matrix (the homopolymer, the bulk of the material). "We design it so that the copolymer comes to the surface and saturates the surface, and then we



Depiction of the aggregation of random copolymers in a homopolymer matrix as observed in Monte Carlo simulations. The presence of these aggregates impacts the dynamics of the copolymer in a homopolymer matrix and demonstrates the importance of thermodynamic interactions in understanding the dynamics of miscible polymer blends.

retain some in the matrix so that if we lose it at the surface, we can just force it to come to the surface again."

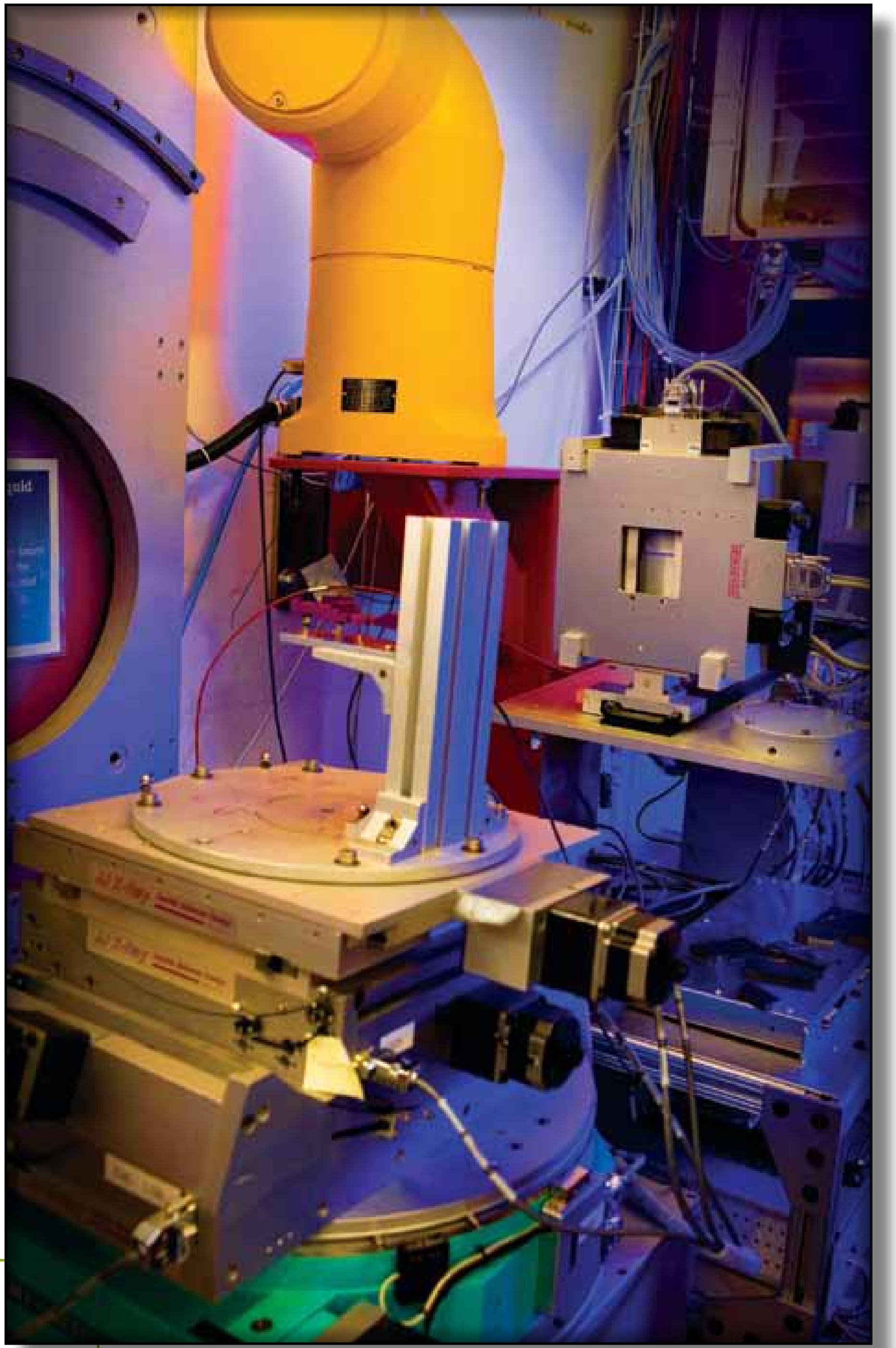
Dadmun works with instrument scientist John Ankner at SNS, materials scientist Joe Pickel at the Center for Nanophase Materials Sciences at ORNL, and UT and ORNL distinguished scientist Jimmy Mays. Pickel and Mays synthesized the polymer samples. In the self-healing materials, the key properties that are targeted include biocompatibility, microbial resistance, adhesion, and flammability, Dadmun says. Researchers can control these properties by preferential surface segregation of a single component.

"The idea is that we design a system where the majority of the component has the stability we need, the strength to be a suitable matrix. But we have another polymer we designed to bloom to the surface. And then it would potentially provide the surface-sensitive property that we are looking for. And even if it got washed off, because we started with a mixture and forced it to come to the surface, there would be a reservoir of this material that would continue to come to the surface."

Dadmun says that finding a copolymer that migrates to the surface is not difficult. What is difficult is finding one that gets there fast enough. This has to do with the thermodynamics of the material, how its structure reacts to a change in temperature. What they need to learn, he says, is how the specific structure of the copolymer affects how quickly it migrates to the surface.

In their experiments, the researchers begin with a silicon wafer, which they coat with a thin film that is a mixture of deuterated poly(methyl methacrylate) as the matrix polymer, and a branched copolymer of methyl methacrylate and ethylene oxide. As they heat this sample, allowing the mixture to approach thermal equilibrium, the graft copolymer (containing ethylene oxide) diffuses to the surface so that they can measure the water contact angle to verify that the copolymer segregates to the surface. "We can see that we're getting more ethylene oxide (from the copolymer in the mixture) at the surface then when we first started. But what we really want to do is extract information on how quickly it gets to the surface," Dadmun explains. This information is obtained using the Liquids Reflectometer at SNS.

"Neutrons are ideally suited to study the dynamics of the copolymer," Dadmun says, "because with neutrons we're able to selectively label the material." In Dadmun's samples, because of the different neutron scattering properties of the deuterated poly(methyl methacrylate) and the undeuterated poly(methyl methacrylate), they can observe the location and movement of the copolymer in the composite material as a function of the annealing time (i.e., heating and slow cooling).

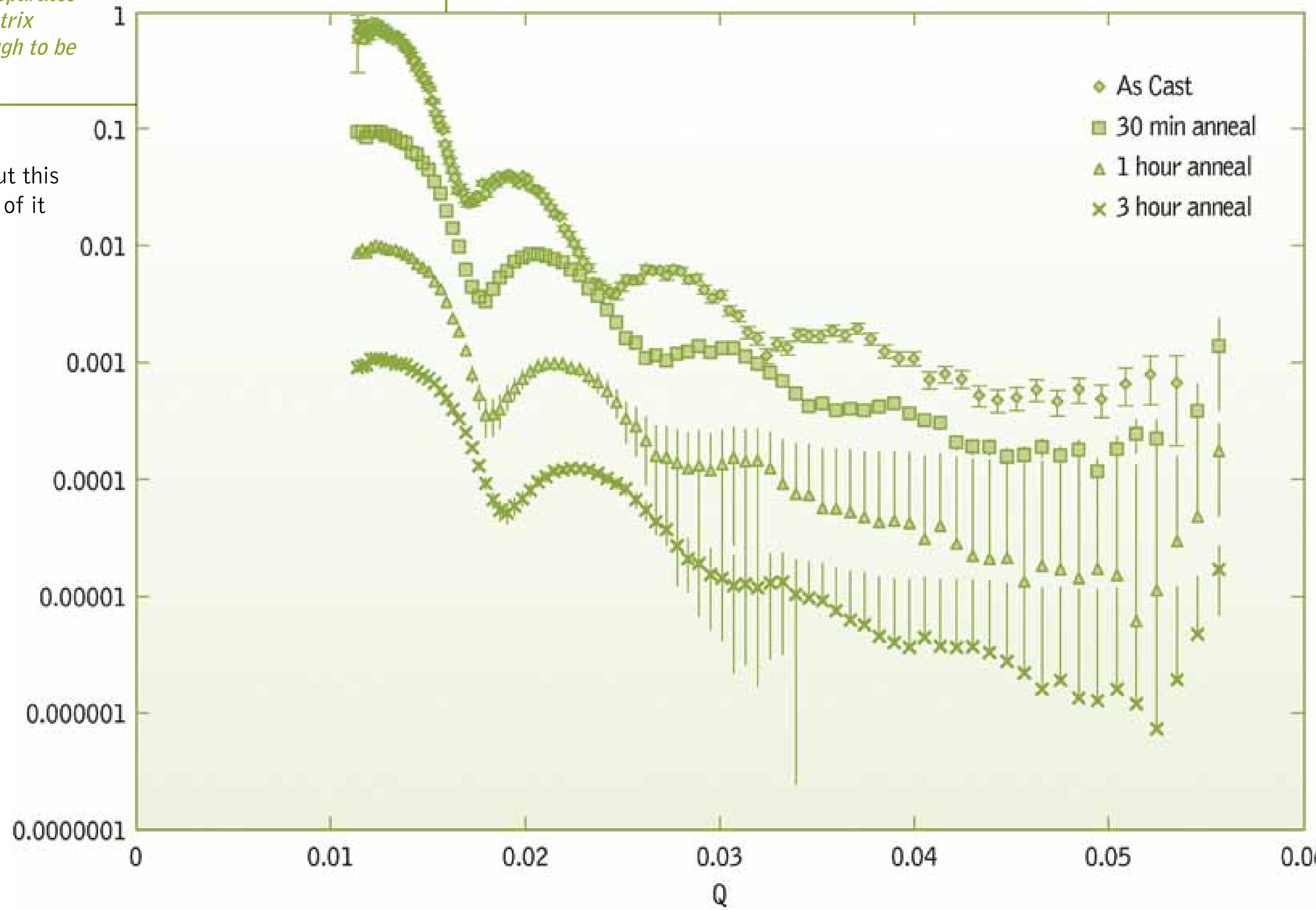


SNS Liquids Reflectometer.

SCIENCE HIGHLIGHTS

As it is heated, the copolymer tends to migrate to the surface. The experimenters observe the time dependence of the intensity of neutrons scattered from the copolymer near the surface, which can be analyzed to provide detailed dynamics of the copolymer diffusion process. "And so we can analyze that data to work out the diffusion coefficients, other precise dynamic information about this surface segregation process, how much of it gets there, and how quickly."

Reflectivity profiles of a miscible polymer blend of a linear and branched polymer as a function of annealing time. The curves represent changes in the structure of the material. The challenge in this research is finding a copolymer that separates from the matrix quickly enough to be useful.



Dadmun says they know from previous work that the polymer chain is actually collapsing. "It's changing its conformation away from its behavior in the homopolymer because of the repulsive interaction between the polymers. And that change in repulsive interaction—and change in conformation—alters the dynamics, which alters the properties. So it's that cascading effect which allows us to correlate the structure and thermodynamics of the copolymer to its dynamics.

"If you think of this polymer chain with the long arms, those long arms make it very difficult to move. But because of this repulsive interaction, they might actually be retracted in, and therefore could be moving faster ... we don't have evidence of this yet, but this is one of the things we're trying to find out."

How does Dadmun predict the future? Is he hopeful for these polymers? "Potentially, these are going to be too slow. All of the applications may not be commercially viable because it could take the copolymers too long to get to the surface. If they do make it to the surface, however, there will be a wide range of applications that we can utilize this concept for. That's why we do the research—to figure out what works and what doesn't."

FACILITY DEVELOPMENT

Instruments

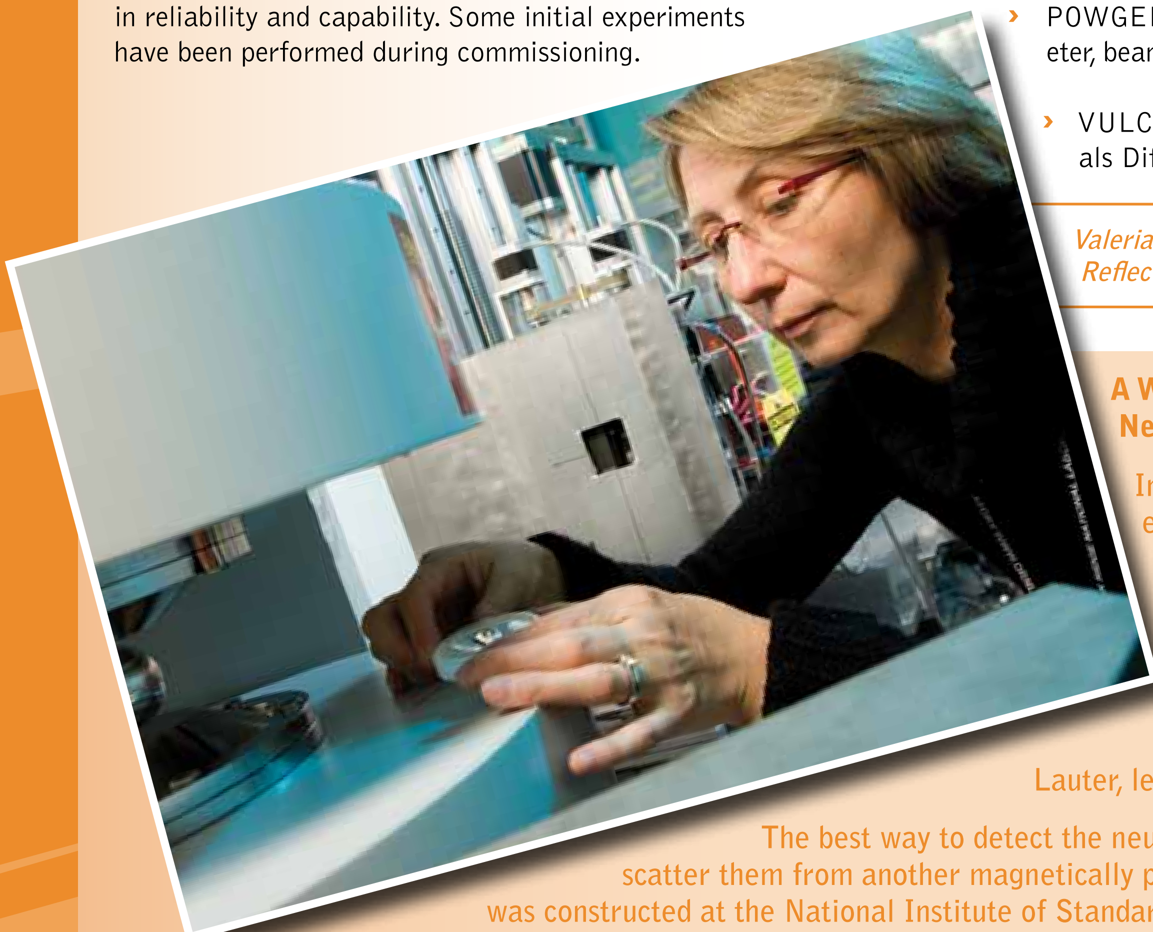
Spallation Neutron Source

Four new instruments were completed in 2008 and are now being commissioned: SNAP, CNCS, SEQUOIA, and FNPB. The new instruments are performing well and are expected to continue to expand in reliability and capability. Some initial experiments have been performed during commissioning.

SNS instrument development and construction continues at a fast pace, and progress is on schedule for five more instruments to be completed and begin commissioning during 2009:

- EQ-SANS: Extended Q-Range Small-Angle Neutron Scattering Diffractometer, beam line 6
- POWGEN: Powder Diffractometer, beam line 11A
- VULCAN: Engineering Materials Diffractometer, beam line 7
- TOPAZ: Single-Crystal Diffractometer, beam line 12
- NSE: Neutron Spin Echo Spectrometer, beam line 15

Two "SNS Instruments—Next Generation" (SING) projects will add seven more instruments to the SNS lineup between 2010 and 2014. SING I—a suite of five instruments—is more than 50% complete. The construction, commissioning, and schedule for the current SNS instrument suite is shown in the "Facts and Figures" section.



Valeria Lauter, SNS Magnetism Reflectometer.

A World's First: Magnetism Reflectometer Fitted With Helium Neutron Analyzer *with Online Pump-Up Polarization*

In July 2008, the experimental team of Hal Lee, Andre Parizzi, Richard Goyette, Hailemariam Ambaye, Lee Robertson, and Valeria Lauter successfully installed the world's first ^{3}He (helium isotope) neutron analyzer *with on-line pump-up polarization*. Neutrons have magnetic spin, and a device of this type allows researchers to detect the intensities and orientations of the individual spins (up or down) of scattered neutrons (i.e., polarization). "The data on the polarization of scattered neutrons provide unique information about the nature of magnetic interactions within a sample," said Valeria Lauter, lead instrument scientist for the Magnetism Reflectometer at SNS.

The best way to detect the neutrons' polarization after they have scattered from the sample is to again scatter them from another magnetically polarized substance. For this device, ^{3}He was used in the analyzer cell, which was constructed at the National Institute of Standards and Technology. During testing, the ORNL team was able to achieve an impressive 76% polarization (i.e., 76% of the ^{3}He atoms inside the analyzer were polarized one way—spin up or spin down). A trial study carried out with an iron-chromium multilayer demonstrated that the new analyzer performed well. "With future improvements and modifications, we anticipate that we will be able to carry out important studies of the magnetic properties of new nanoscale materials," Lauter said.

High Flux Isotope Reactor

The past year has been a productive one for instrument development at HFIR. Construction was completed for two new instruments, construction and upgrades continue on others, and major upgrades are in the works for others.

The Powder and Four-Circle diffractometers have been completed and are available for users. Installation of the monochromator drum and shielding was completed for the US/Japan Cold Triple-Axis Spectrometer. Depending on funding during the first half of fiscal year 2009, the instrument could be operational by October 2009. A project was initiated to provide major upgrades to the existing Wide-Angle Diffractometer (WAND), essentially making it a new instrument. The conceptual design of the new instrument has been completed, and detailed design, procurement, and installation are in progress. Finally, the conceptual design was completed for an image-plate, single-crystal diffractometer (IMAGINE).

In addition to instrument work, design of four cold test station beam lines was completed. These test stations will provide testing capabilities for imaging as well as for instrument concepts for both the HFIR and SNS beam lines. Both of these test stations will be operational during the summer of 2009.

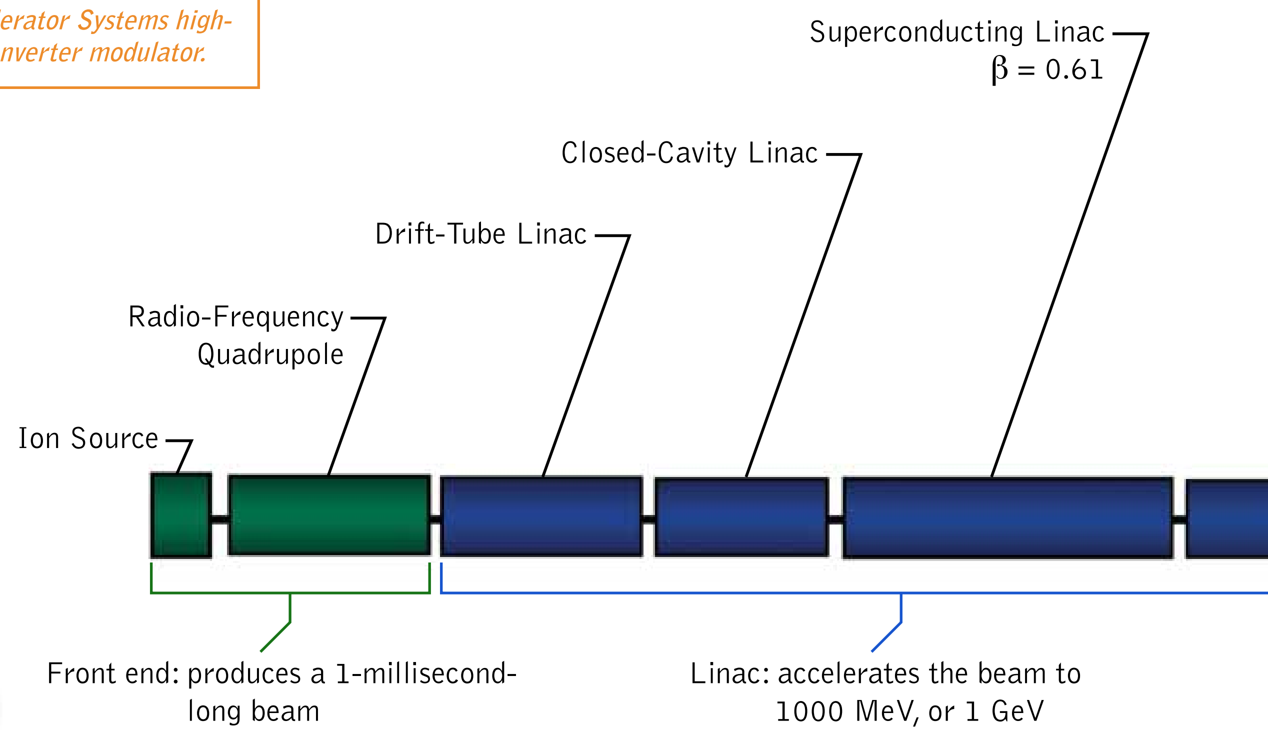
Other instrument projects being considered for HFIR include a neutron spin echo reflectometer and a second cold triple-axis spectrometer. Concepts for such instruments will be defined during the next year. The concepts will then be evaluated by an external advisory committee to determine their appropriateness for further world-class neutron scattering capabilities at HFIR.

Jaime Fernandez-Baca, lead instrument scientist for WAND.

Mark Loguillo, scientific associate for ARCS.

SNS Accelerator Systems

SNS Accelerator Systems high-voltage converter modulator.



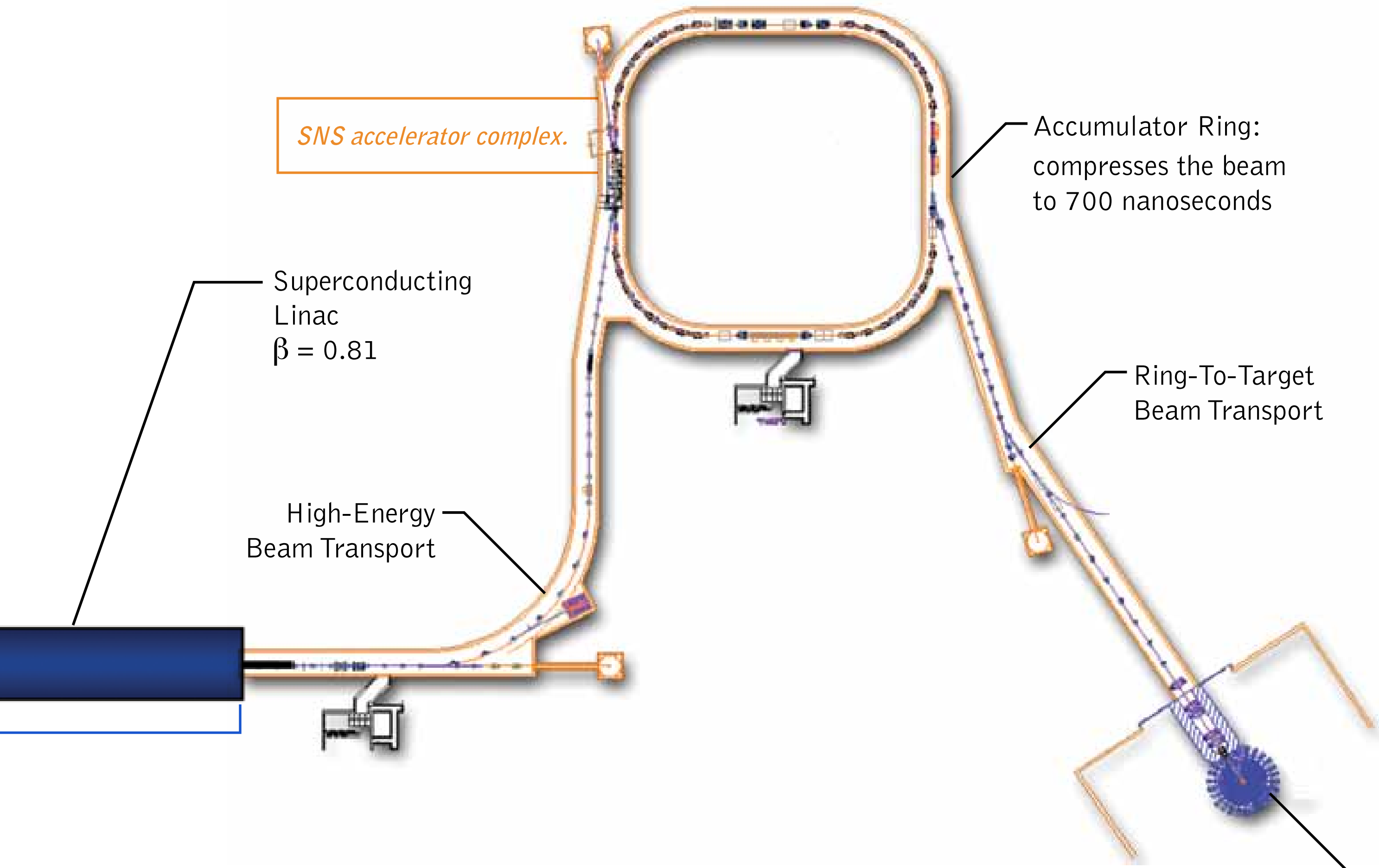
Front-End Systems

All aspects of SNS front-end systems performance were improved during 2008. The ion source team (Martin Stockli, Robert Welton, Baoxi Han, Syd Murray, and Terry Pennisi) boosted the SNS baseline source so that it operates at the peak 38 milliampere (mA) current specified in the SNS design. This improvement was made possible by use of the ion source test stand, a testing platform identical to that operating on the SNS front end. By modifying the source extraction geometry, improving the management and release of cesium (used to enhance surface electron emission), and exploring the operating parameters of the source, the team was able to increase peak current to the 38-mA design level by the end of 2008. In addition, lifetime tests performed on the platform showed that a single ion source could provide reliable operation for the 16-day neutron production run cycle initiated in 2008. (For information about future plans for the ion source, see "Booster Shot for SNS Ion Source" on p. 68.)

The front-end systems generate the negative hydrogen ion beam, form beam particles into individual packets of charge, remove one-third of the beam by chopping, and prepare the beam for injection into the linear accelerator (linac).

Superconducting Linac

The superconducting linac uses niobium radio-frequency resonators to accelerate the beam from 186 megaelectron volts (MeV) to the final output energy. At the beginning of 2008, the linac provided



SNS accelerator complex.

a beam energy of 860 MeV, substantially lower than the design energy of 1000 MeV, because some superconducting cavities were out of service and the superconducting resonators in the high-energy portion of the linac were operating at 15–20% below their design accelerating field. To correct these problems, repairs were completed to two cryomodules and associated superconducting cavities in the new SNS repair, maintenance, and testing facilities. The repairs will allow SNS to operate with 80 of 81 superconducting cavities, providing a linac output energy of about 930 MeV.

A potential superconducting cavity surface treatment process was conducted in which a radio-frequency plasma discharge was established in a superconducting cavity. The measured accelerating field after this "plasma cleaning" showed an increase of approximately 15% in cavity field, near the increase required to boost linac output energy to the design value of 1000 MeV. Next steps involve further development of this technique to enable in situ plasma cleaning of the installed superconducting cavities in the linac tunnel.

Modulators

The radio-frequency waves that power the linac's accelerating cavities are generated by klystrons, which in turn are driven by high-voltage converter modulators that provide 60 pulses of 10-megawatt power per second. These are state-of-the-art pulsed power devices with advanced solid-state, high-speed, high-power switches.

Since the modulator system accounts for the largest fraction of unscheduled down time, active efforts are in progress to improve its reliability. During 2008, the modulator systems were improved to allow operation at a full repetition rate of 60 pulses per second. Additional diagnostic and protection systems were built and installed to allow easier diagnosis and to protect equipment in the event of failure. A full replacement of problematic capacitors was initiated in late 2008, measurably improving reliability in the final month of 2008 operation.

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Sample Environment

The Sample Environment Group provides users with equipment and support for temperature, pressure, magnetic field, and controlled-atmosphere environments for experiments. Capabilities have grown substantially during the past year, making an increasing range of environments available to scientists at SNS and HFIR. Several workhorse temperature environments were commissioned this year, including four liquid helium cryostats and six closed-cycle refrigerator (CCR) systems. Many of these systems have undergone extensive in-house customization to optimize their performance. For example, low-background, sample-in-vacuum configurations have been implemented on the SNS ARCS, SEQUOIA, and CNCS spectrometers. "Hot exchange gas" CCRs have been developed to cover a wide temperature range (7 to 500 kelvin) while ensuring minimal temperature gradient along the sample. And specialized sample sticks have been designed with features such as sample rotation and gas loading.

In addition, the world's first self-shielded magnet for neutron scattering, a 5-Tesla vertical field system, was commissioned at SNS in May (see "Year in Review"), and a much stronger 16-Tesla system is scheduled for delivery in the summer. The magnetic field profile of these new shielded systems not only eliminates interference but also enhances the ability to use polarized neutron beam techniques. Meanwhile, older magnet systems are being updated and recommissioned. A 4.5-Tesla horizontal field magnet has been upgraded and dedicated to the HFIR GP-SANS instrument, and two vertical field magnets (5 and 6 Tesla) continue to serve as mainstays at HFIR.

We now have a substantial inventory of pressure-generating devices that includes large inert gas rigs (10 kilobars) and compact trolleys for liquids and gases ranging from 0.2 to 7 kilobars. Aluminum gas pressure cells rated to 4 kilobars have been purchased, and cells of various materials are under development through collaborative research and development. These include a single-crystal sapphire cell that is well suited for measurements on the SNS Backscattering Spectrometer and a titanium zirconium "null scattering" alloy cell for diffraction studies. Anvil pressure cells and related items have

Matthew Collins, Sample Environment Group, operates the crane in the SNS Target Building, lowering a sample environment to its needed beam line.

Andrew Church, left, and Saad Elorfi, right, of the Sample Environment Group change out a sample for ARCS.

been commissioned by the SNAP team. These include large-volume Paris-Edinburgh (P-E) presses, panoramic high-pressure cells with gem-anvils, a cryo-cooling system capable of cooling the massive P-E press, a graphite furnace heating system for the P-E press, and a laser heating system for the gem-anvil pressure cells.

The scope of the sample environment program is not limited to temperature, pressure, and magnetism however. Other developments include controlled gas atmosphere chambers, humidity cells, optical excitation probes, automatic sample changers and manipulators, and a variety of special sample cells. In addition, some users have exercised the option to supply their own specialized sample environments. Those experiments have gone smoothly thanks to the advance notification spelled out in the proposals and the subsequent interaction between the researchers and ORNL staff.

For the future, we aim to improve the standard equipment pool to achieve greater reliability and accuracy. We also hope to broaden our capabilities for extreme environments, such as 40-Tesla pulsed magnetic fields, containerless levitators operating at up to 3000°Celsius, and special environments to study disordered, surface, and reduced dimensional systems.

Our user community has been engaged in many of these development projects, resulting in a broad range of capability and in getting this young program off the ground. We look forward to another productive year of serving and collaborating with the user community.

A list of sample environment resources for each facility is available in the Facts and Figures section.

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HFIR: neutrons.ornl.gov/hfir_instrument_systems/hfir_sample.shtml

SNS: neutrons.ornl.gov/instrument_systems/sample/

Detector Systems

The Detector Group is responsible for developing, assembling, calibrating, installing, and commissioning neutron detectors for the HFIR and SNS beam lines. Detectors count the number of incoming neutrons and, more important, record the position and arrival time (i.e., energy) of each neutron seen by the detectors. Ongoing efforts are under way to count neutrons more efficiently, at higher rates, and at finer spatial resolution to increase the capacity and resolution of all the neutron scattering instruments. To assemble and calibrate detectors, the group maintains three detector laboratories, two 35-microgram ^{252}Cf neutron sources, three smaller check sources, and the interim HB-2DS Detector Test Station at HFIR.

In 2008 we continued to support the needs of operating instruments and to calibrate and install detector systems on new instruments. A major highlight of the year was achieving 1-millimeter resolution with the Anger camera system. The detector team focused on three areas to reach this goal: camera optics, enhanced calibration procedures, and lower-noise packaging. The camera housing was integrated with the electronics to reduce electronic noise and to ensure that the cameras could be mounted in spherical arrays.

Additional highlights were development of novel 8-pack packaging schemes and a new prototype for reflectometers called an incline detector. A technology transfer agreement for 8-pack production was established with GE Reuter Stokes (see "Year in Review").

Support for Operational Instruments

Continuing work on operational instruments has led to new developments and substantially improved operations. Efforts focused on increasing reliability and stability within all the detector systems, particularly the larger ones (ARCS has more than 900 detectors). Improving communications within detector arrays and fine tuning of power-up sequencing have significantly enhanced performance for all the operating instruments. At the beginning of the year, approximately 15% of the detectors had communication issues at any given time. By the end of the year, however, all systems were operating dependably.

Development of a "flat field correction" resulted in more uniform responses for some detectors. This improvement will increase the dynamic range of the experiments on the reflectometers and will improve the position resolution of the detectors for SNAP.

Bruce Hannan, Detector Group, inspects an optical sensor from the scintillator detector for VULCAN, an engineering materials diffractometer at SNS.

New Instrument Support

Detectors Group staff installed and tested literally thousands of new detector components and systems on instruments under construction or commissioning. Major efforts included installation of Anger cameras, linear position-sensitive detectors (LPSDs), wavelength shifting fiber detectors, and beam monitor systems.

Future Development

We are continually acquiring and developing equipment geared toward the needs of future instruments. For example, a 40-micron-resolution real-time imaging detector was obtained for radiography and very high-resolution crystallography. We are also participating in external development projects on scintillators, scattering detectors, and imaging detectors.

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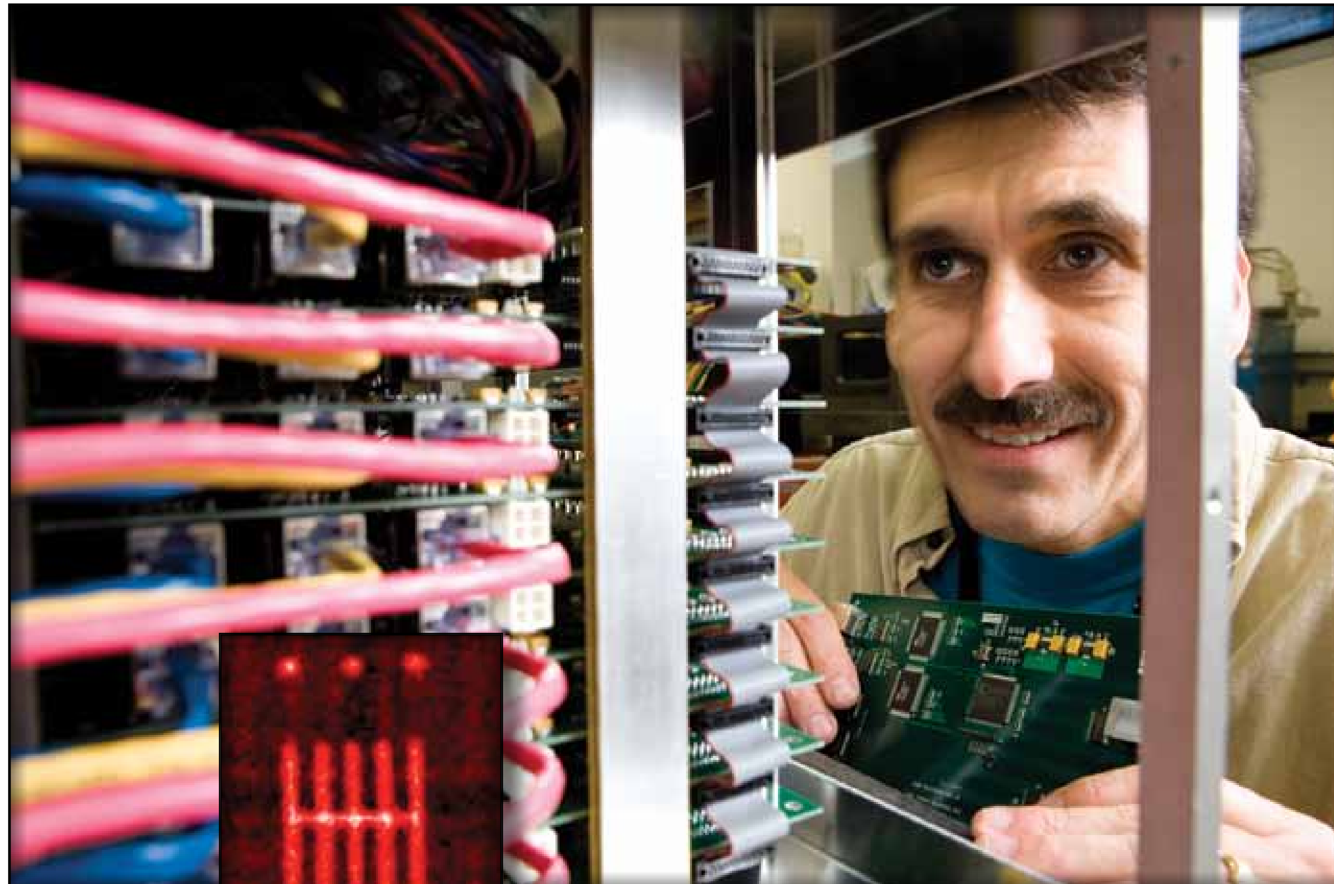
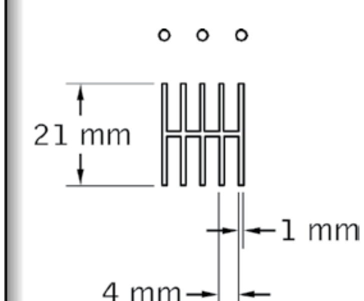
neutrons.ornl.gov/instrument_systems/components/detectors.shtml



Neil Donahue, Detectors Group, works on the Anger camera.

Neutron image of mask showing resolution is 1 mm



4H mask used for Topaz tests

Neutron image showing 1-millimeter Anger camera position resolution.

Array of LPSDs installed in the SEQUOIA tank at SNS.

Data Acquisition and Controls

Pam Morrison (left), Detectors Group, and Tara Thompson (right), Data Acquisition and Controls.

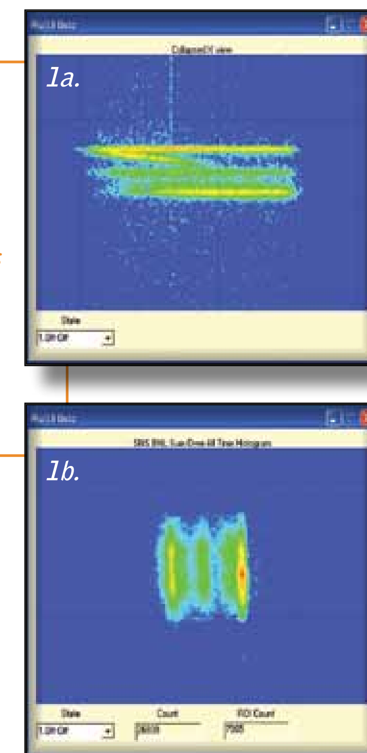
The Data Acquisition and Controls Group develops and tests software and electronics to meet the unique data collection and handling requirements of the instruments at SNS and HFIR. The data-related demands at these facilities will increase dramatically during the next few years, resulting in some of the fastest data rates and highest intensities anywhere.

In 2008, the group maintained and improved the capabilities of four operational instruments, while providing support for the commissioning of three new ones. Each of the three new instruments has its own particular challenges:

- SEQUOIA has more than 40 square meters of LPSDs;
- CNCS operates its detectors in an argon atmosphere; and
- SNAP has the largest-area Anger camera coverage in the world.

Each instrument required significant testing and validation of new state-of-the-art electronic designs. SNAP also required new software for calibration and detector setup.

In addition, flat field correction algorithms developed for the SNAP Anger camera detectors were extended for use at the Liquids and Magnetism reflectometers, providing better high Q performance and demonstrating how technology design for one detector system can positively affect the performance of other systems.

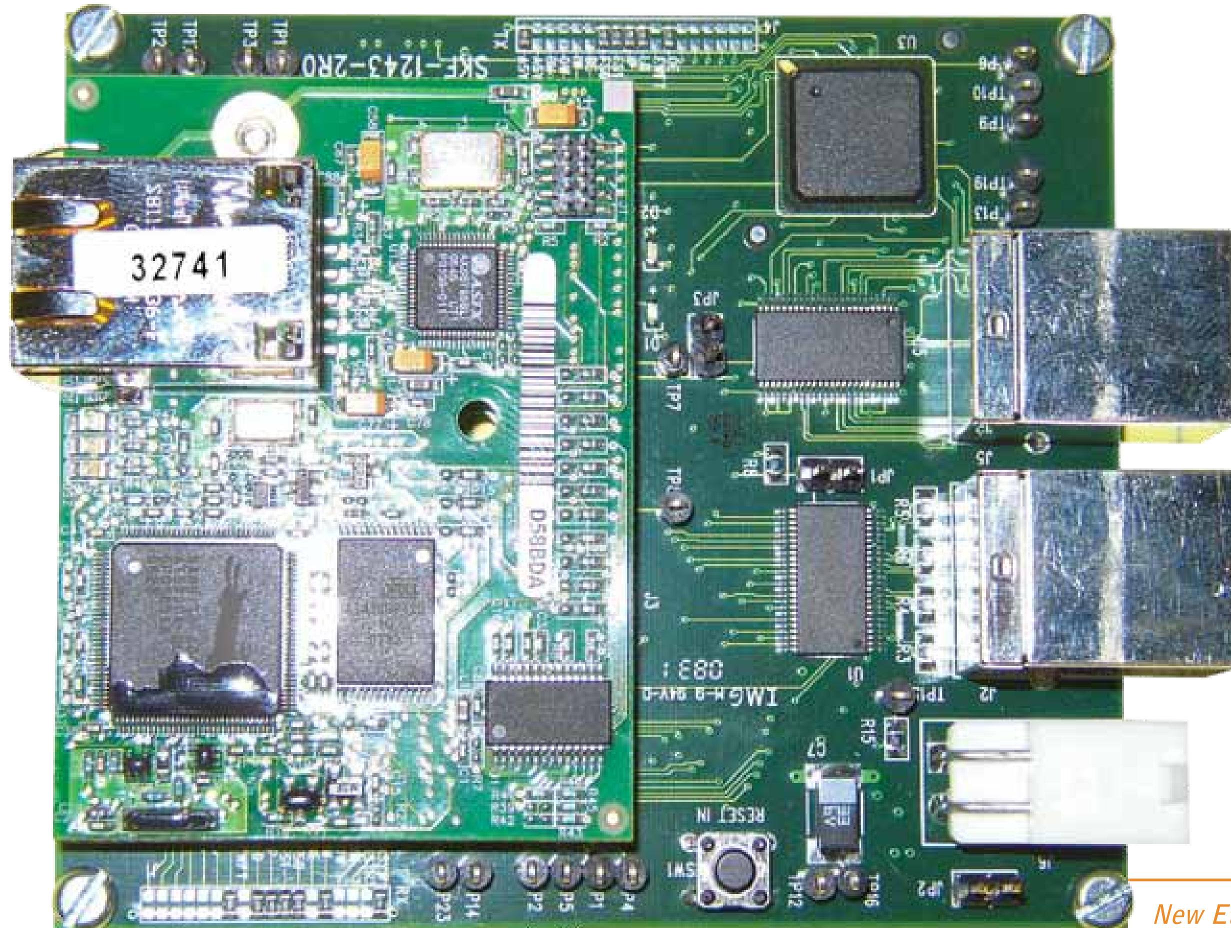


Simultaneous real-time views of data at the SNS Magnetism Reflectometer. Figure 1a shows the function int(x,y)dy on the y axis and time of flight on the x, while Figure 1b is int(x,y,t)dt. The polarizer/analyzer state is user selectable.

Software Development

As in previous years, software development was a top priority for our group. New control software for a variety of new sample environment setups, including magnetic environments and dual-zone temperature controllers, was used in a number of experiments. Motor software was extended to interface with a new robot sample changer for the Liquids Reflectometer and a sample positioning hexapod system for the Magnetism Reflectometer. Python scripting was expanded to allow more complex sequencing of multivariate experimental scans. The figure on p. 64 shows how additional real-time views of the scattering data were made available on user computers, providing users with more feedback on the progress of the experiment. New SPICE drivers were written to allow the use of SNS detector electronics at HFIR. The first of these upgraded systems, for the Four-Circle Diffractometer, is now in the commissioning phase.

The main highlight for the group was the technology transfer of the SNS LPSD detector electronics system, Pharos, to GE Reuter-Stokes (see "Year in Review"). This success allowed us to focus more efforts on new technologies. Two of these new design efforts are now in the testing phase. The first of these, a peripheral component interconnect express (PCI-e)–based data transfer card, allows the use of newer motherboard designs without the requirement of legacy PCI-x slots. The second, a new Ethernet-based interface card, will allow the use of our own detectors in lower-count-rate systems without the need of a PCI card.



New Ethernet interface board allowing greater flexibility in the use of neutron scattering detectors.

As we continue work on these technologies, we look forward to another year of developing the best new software and hardware to meet the needs of the neutron sciences users and staff.

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Data Analysis

Shelly Ren, software engineer for the Scientific Computing Group.

Scientific Computing

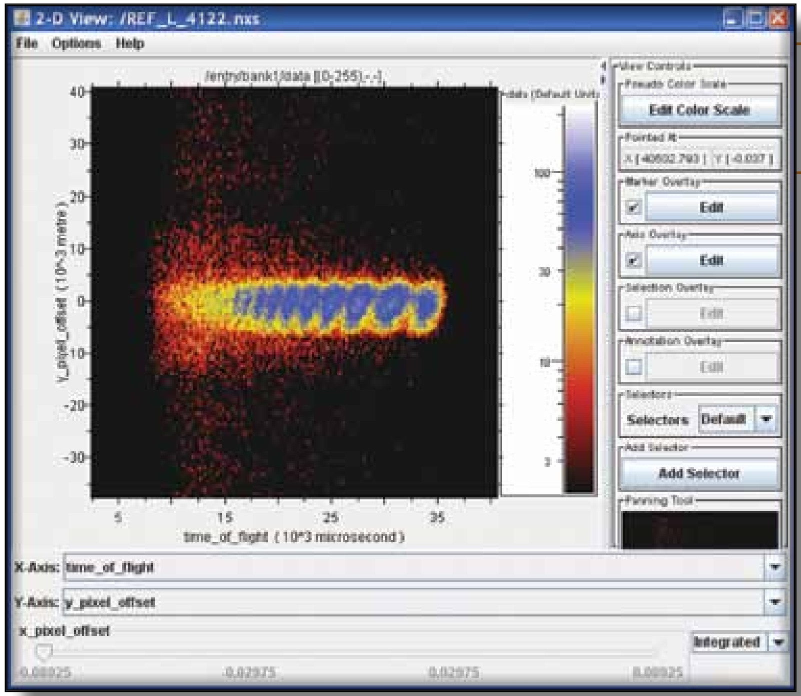
With more than two years of operation, the Neutron Scattering Data Portal provides users at SNS, HFIR, and now the Low Energy Neutron Source Facility at Indiana University with access to both data and computing resources. This past year the portal served more than 300 registered users, received more than one million "hits," and ran more than 115,000 jobs. With the closing of the Intense Pulse Neutron Source (IPNS) at Argonne National Laboratory early in 2008, the entire IPNS data repository is also now available via the portal. Data from the Lujan Neutron Scattering Center at Los Alamos National Laboratory are also available. The data are stored by facility/instrument/proposal, with access limited to proposal team members.

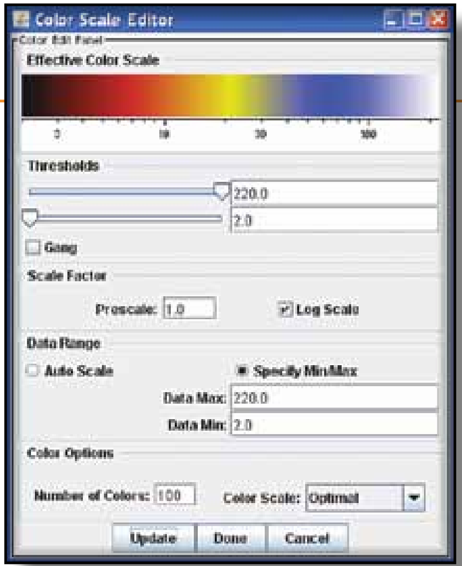
The portal provides a host of services, including data visualization, sample activation calculations, data reduction, and simulation. Improvements during the year include the following:

- A dashboard enabling users to observe status information and quality-of-service metrics such as latency and bandwidth.
- The ability to remotely access and reduce experiment data during an experiment.
- Integration with the SNS/HFIR proposal system to automatically associate experiment team members with their data.
- A new color tool that provides significantly more functionality in visualizing data, such as logarithmic scales and selection of multiple color scales. This feature is currently in beta testing (see the top images on p. 67).

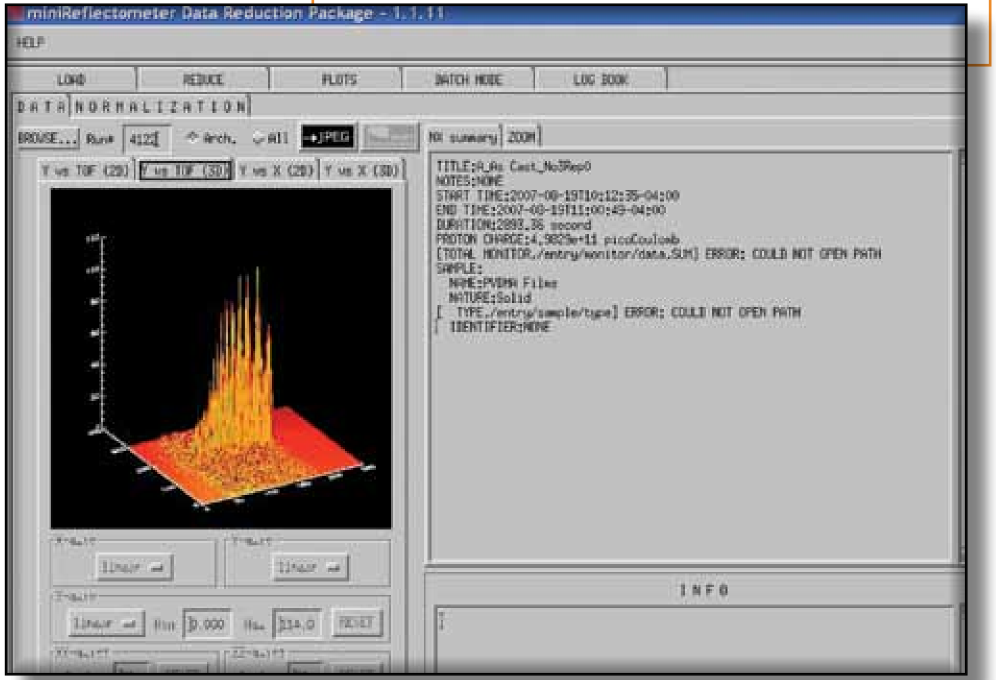
The portal home page, https://neutronsr.us.

The portal data repository currently contains more than 500,000 cataloged files and is ~2.5 terabytes. Experiment data are automatically managed by a process called "Live Cataloging," which transforms data into NeXus files and catalogs these along with the original raw data into the data management system. The NeXus files use the Hierarchical Data Format (HDF5) self-describing data file format, which is usable directly by such applications as IDL, Matlab, and Igor Pro. The histogram data within the NeXus files are





New ISAW visualization tool that can display in log scale.



Data reduction GUI for the Liquids Reflectometer at SNS. When used remotely, the application is displayed locally on a user's computer, while the data reside and processing occurs on computers at SNS. Remote applications are facilitated via a web browser running on a user's computer, which establishes an NX client "pipe" between the application displayed on the user's computer and the SNS servers where it is actually running remotely.

compressed upon file write and are automatically decompressed upon file read—a benefit of working with HDF5. Histograms may typically compress up to 95%, significantly reducing needed disk space.

The computing development team continues to spend significant effort producing and refining data reduction and diffraction software for both the instruments in the user program and those still in commissioning. The figure at right illustrates the Liquids Reflectometer reduction graphical user interface (GUI) as seen remotely via the portal; data and computing reside at SNS, while the GUI appears on the user's computer.

The development team has also been working closely with a number of external experts to improve our capabilities. One such collaboration is the Neutron TeraGrid Science Gateway team, headed by John Cobb. This team has integrated a McStas simulation application that is accessible via the portal while running via a community account on the National Science Foundation TeraGrid. We've also been working with Ruth and Dennis Mikkelson of the Integrated Spectral Analysis Workbench (ISAW) software development team. The Mikkelsons have been adapting ISAW to work with the SNS single-crystal instruments SNAP and TOPAZ.

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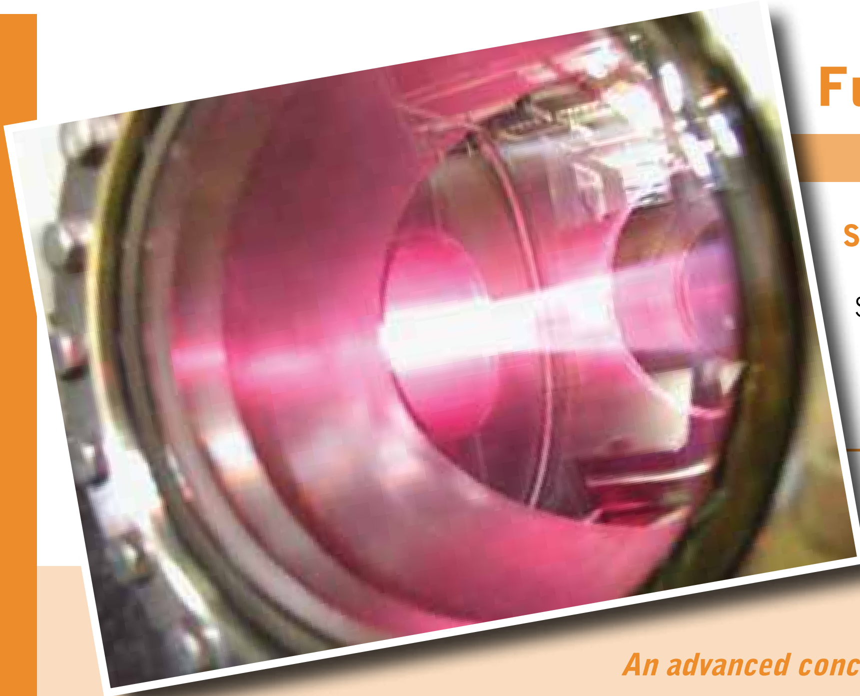
neutrons.ornl.gov/instrument_systems/computing



High-density hydrogen operation of the helicon ion source.

Future Initiatives

SNS Power Upgrade and Second Target Station

SNS was designed from the beginning to be upgraded in power and to accommodate a second target station to expand the science capabilities of the complex.

To improve the performance of the neutron source, a power upgrade project is in the works that will increase the beam energy by 30% from 1.0 to 1.3 gigaelectronvolt. The project is awaiting approval to begin planning and preliminary engineering. Construction is expected to start in 2012.

Booster Shot for SNS Ion Source

An advanced concept for space propulsion could help double the scientific capability of SNS.

When the beam power of the SNS linear accelerator reaches the design limit of 1.4 megawatts (MW), the beam current will be 38 milliamps. However, plans are to double the beam power to 3 MW by 2011 to help double the facility's scientific capability. To meet the requirements of a 3-MW neutron source, the ion beam current must be increased from 38 to 59 milliamps.

One approach to meeting this requirement is being pursued by a team of scientists from SNS and ORNL's Fusion Energy Division. The researchers are developing a new hybrid ion source based on a helicon plasma generator developed by the National Aeronautics and Space Administration (NASA) for the variable specific impulse magnetoplasma rocket (VASIMR), an advanced concept for electric space propulsion. NASA plans to test the technology on the International Space Station and possibly use it to propel manned spacecraft in the future.

By combining this high-efficiency plasma generator with the existing SNS ion source, developed by Lawrence Berkeley National Laboratory, the researchers hope to achieve higher beam currents than can be produced from conventional ion sources. The team has constructed a dedicated test facility capable of both plasma density and beam extraction measurements. Rob Welton, Rick Goulding, Dennis Sparks, Stan Forrester, and Danny Crisp delivered their first success early on. "We have already achieved much higher plasma densities than produced in typical radiofrequency-driven, negative hydrogen ion sources," Welton says. "As a starting point, we have recently extracted about 10 milliamps from this hybrid source by employing a modified magnetic configuration. Our main challenge now is to increase this beam current to the required 59 milliamps by adding cesium and reconfiguring the magnetic fields to best convert this record plasma density into usable beam."

This research promises to benefit fields beyond neutron scattering. "Because these characteristics are desirable in a generator used to create neutral beams for heating fusion plasma, the low power densities and neutral pressures present in the plasma generator could make the device of interest to the managers of the ITER [International Thermonuclear Experimental Reactor] fusion experiment," Goulding says. "Our findings are likely to advance the field of ion source development for advanced accelerators, ion implantation, and medical isotope production."

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A reference design concept for the second target station has been developed, and DOE has authorized SNS to proceed to a full conceptual design.

In the reference design, every third pulse from the accelerator will go to the second target station so that it operates at 20 pulses per second; the first target station will receive 40 pulses per second. The second target station would accept 1-millisecond-long proton pulses directly from the linac, increasing the power available. In this mode the facility could deliver 1.4 megawatts to the first target station and 1 megawatt to the second. The second target station will be optimized to provide the maximum flux of cold neutrons. Studies show that with this reference concept, the second station and associated instrumentation would improve performance by more than an order of magnitude for broad areas of forefront science and could open totally new areas to exploration.

SNS site on Chestnut Ridge. On the right is the projected location of the second target station.

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neutrons.ornl.gov/facilities/proposed_upgrades.shtml

Second Cold Source and Neutron Science Center at HFIR

As part of DOE's *Facilities for the Future: A Twenty-Year Outlook Plan*, HFIR is pursuing a second cold source and guide hall to support nine cold neutron guides with higher brightness than existing guides. In addition, to provide more permanent space and to satisfy future needs, layout and planning have started for the HFIR Neutron Science Center. This center would provide office and lab space and other user support facilities. Decisions to proceed with either or both of these projects are expected about 2012.

FACILITY DEVELOPMENT

Laser Removal of Electrons

When the ion beam in the SNS linear accelerator reaches the proton accumulator ring, the negatively charged ions undergo an identity change, becoming positively charged protons. The postage-stamp-size diamond foil that brings about this change has worked well and has lasted longer than a traditional carbon foil likely would.

There are concerns with the diamond foil technology, however. The design power of SNS is 1.4 megawatts; at 300 kilowatts the ion beam passing through the diamond foil produced a red glow at an estimated temperature of 2000 degrees. One concern is that a few protons—say, one out of every 10,000—will collide with carbon atoms in the diamond foil, making the surrounding hardware radioactive. Another concern is that the diamond foils could lose integrity when power reaches between 1 and 2 megawatts. Both occurrences could dramatically increase operating costs.

In a search for an alternative, Viatcheslav "Slava" Danilov and his accelerator physics team devised a successful laser stripping technology using an Nd:YAG (neodymium-doped yttrium aluminum garnet) lasing crystal. Danilov, who received an award from the European Physical Society for this work, describes this approach as a "paradigm shift." In the initial experiment, a laser beam with a pulse length of approximately 10 nanoseconds was directed at a negative ion beam, successfully removing electrons from the beam. The next step is to increase the electron-removal efficiency.

A larger, more expensive laser system that can operate more effectively for the full pulse length could be needed when the beam power reaches 1.4 megawatts. Nevertheless, laser-stripping technology could be one of the keys to ensuring that SNS can reach its full power potential.

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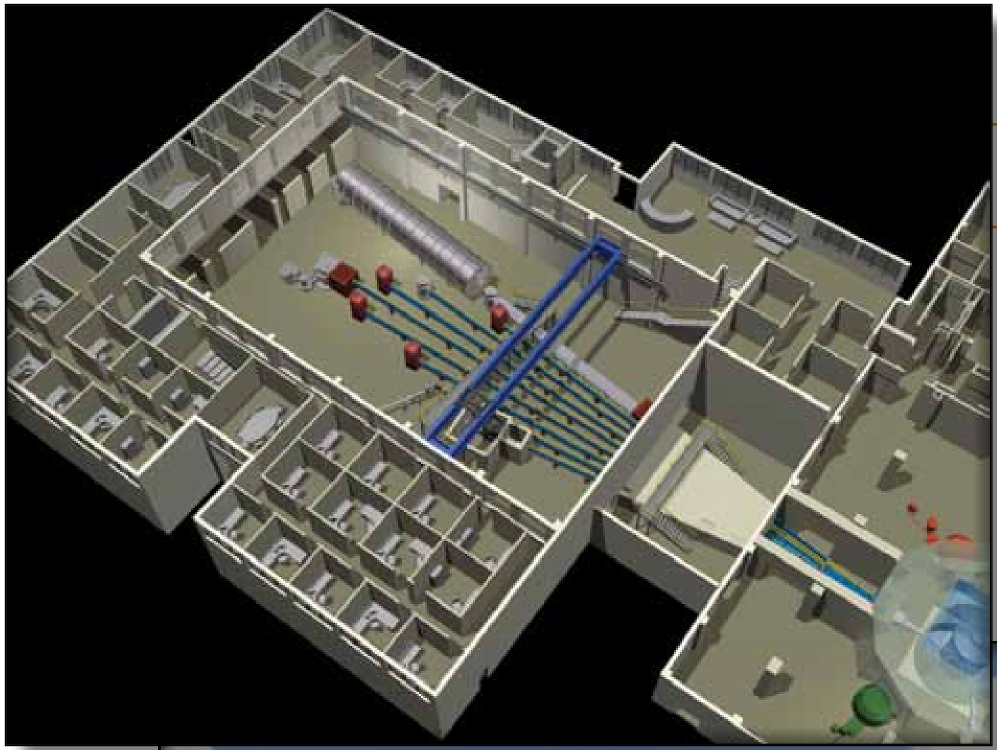


HFIR's proposed second cold source.

Artist rendition of HFIR's proposed Neutron Science Center.

USER PROGRAM

Igor Zaliznyak, SHUG Executive Committee Chair, left, with colleagues Alexei Tsvelik, middle, and Dmitri Kharzeev, right. All are research staff at Brookhaven National Laboratory.

From the SHUG chair

In August 2008, SNS reached ~40% of its planned operating power, and that number continues to climb. Operations at both SNS and HFIR are becoming more and more reliable, and the number of instruments available to users is increasing. Running a smooth user program on such a large scale, and within the tightly regulated environment of the national laboratories, is a complicated task that requires close cooperation with the user community. The SNS and HFIR User Group (SHUG) Executive Committee strives to provide a direct link between users and the facilities, lobbying for the interests of users by supplying facility managers with the user perspective on various choices and needs for future development.

ORNL Neutron Sciences continues to demonstrate its commitment to working with users in several ways. Funding has been provided for user support and education. Several research support programs are also in place, such as the Clifford Shull Fellowship and an extensive undergraduate summer research program. To support HFIR users, new office space has been set up, providing a pleasant and efficient work environment. In addition, the Web-based proposal management and submission system is running quite smoothly and provides users with a convenient interface for submitting their proposals. SHUG has provided input on the system throughout the development process and will continue to do so in the future.

As new instruments and capabilities are being developed, user participation is paramount, particularly in the area of software development. Neutron Sciences staff strongly encourage user engagement by providing multiple feedback methods, including postexperiment surveys, direct communication with instrument scientists and User Office representatives, as well as feedback through the Neutron Sciences Web site (neutrons.ornl.gov). As a core group of users, we SHUG members must take full advantage of these opportunities to contribute to the program. Our participation will help attract new users, which is vital for the continued success of neutron science at ORNL.

Wishing you success and a lot of fun in your experiments at SNS and HFIR,

Igor Zaliznyak
Brookhaven National Laboratory
SHUG Executive Committee Chair

User Eugene Motoyama of Stanford University analyzes results of his measurements on spin correlations at the Fixed-Incident-Energy Triple-Axis Spectrometer at HFIR.

HFIR and SNS Complete First Full Year of Joint Operation

In 2008, the big word was users! More than 400 users conducted research at SNS and HFIR. This number grew from fewer than 100 in 2007 (see graph on page 76). It was a year for tremendous development as well, with improvements being made in proposal management and user access and amenities.

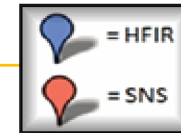
Proposal Management

This was also the first full year of operation for the Integrated Proposal Tracking System (IPTS). The number of external proposal

U.S. institutions represented by users at HFIR and SNS.

reviewers has more than doubled from 103 to over 235. This growth has greatly enhanced the selection process for accepting proposals. In addition, based on feedback from both users and ORNL staff, many changes were implemented as the system matured.

An IPTS Advisory Group was formed to provide advice on development of IPTS, test enhancements, and communicate with users and other stakeholders. Group membership includes users and staff who use the system. The group developed new web pages and tested reorganization of existing pages to improve information flow.



Institutions throughout the world represented by users at SNS and HFIR.

A Happy User

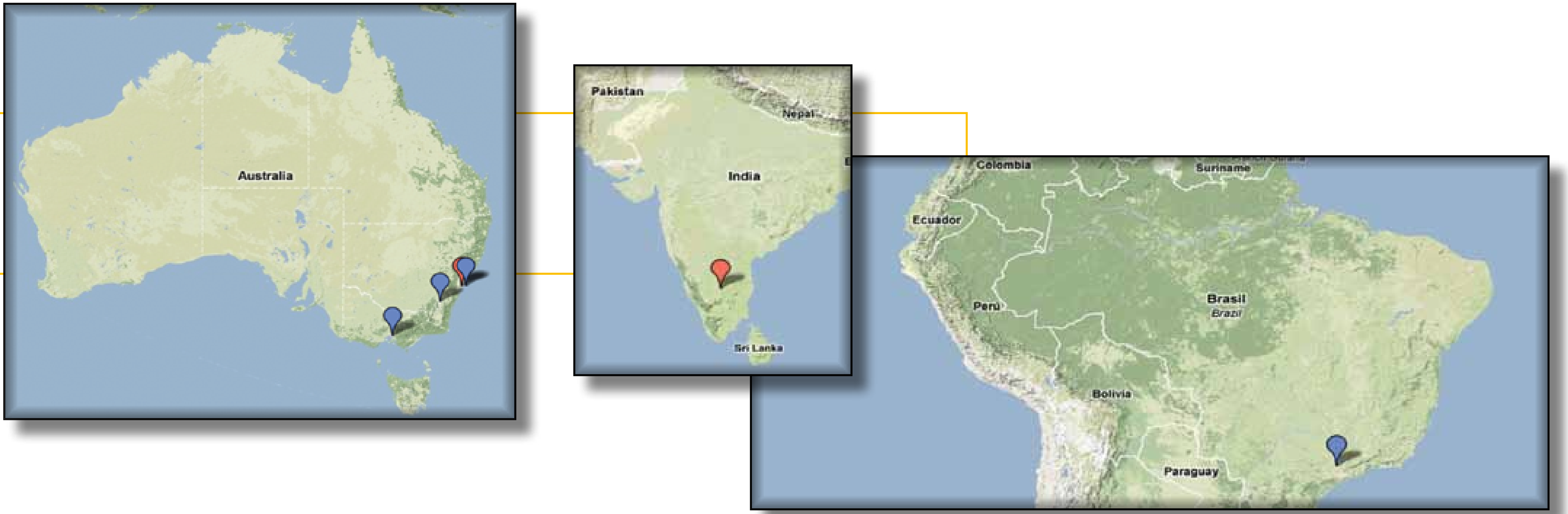
Dvora Perahia, second from left, with her Clemson University graduate students.

In the summer of 2008, Dvora Perahia, associate professor of chemistry at Clemson University in South Carolina, and her graduate students carried out neutron scattering experiments at both HFIR and SNS. Perahia and the graduate students have been using neutron tools at various U.S. facilities to investigate the structure and dynamics of polymers. Their research addresses important scientific and technological challenges.

"We hope to identify new materials that will enhance the efficiency of fuel cells to provide clean energy, and we are exploring the use of thin polymer films and nanocomposites as responsive materials," says Perahia. She explains that responsiveness is the ability of certain materials to change following external triggers such as rising temperature, presence of a solvent, and exposure to light. The structure and motions of molecules, as revealed by neutron techniques, guide researchers in designing better responsive materials. Applications of responsive materials could range from drug delivery to self-healing coatings for electronic and optical components.

Perahia characterized her user experience at Oak Ridge as "very exciting because the newly built instruments with the high flux of neutrons from HFIR and SNS open up new research possibilities in the United States. The success of an experiment depends on multiple factors, including an effective collaboration between the user and the national lab team."

On the administrative side, Kay Carter in the User Office has been priceless, Perahia says, because she "not only coordinates all the details of our visits, but also makes us feel welcome.



Each instrument at HFIR and the SNS is managed by a scientist in the Neutron Sciences organization. The scientific teams we had the pleasure to work with included Ken Littrell and Yuri Melnichenko at HFIR's GP-SANS beam line and John Ankner, Jim Browning, and Candice Halbert at the SNS Liquids Reflectometer. They provided outstanding support that contributed to the success of our work. Helpful advice from Greg Smith facilitated effective navigation of the proposal system."

A native of Israel, Perahia grew up in Rehovot, home of the distinguished Weizmann Institute of Science. This international center of scientific research and graduate studies triggered her imagination at a very early age.

"My parents took with a stride one of my first experiments–disassembling our most precious radio to find the 'people' with whom 38,000 were talking," she recalls. Her educational environment placed a significant emphasis on science teaching. "I was fortunate to participate in the Weizmann Institute's mathematics outreach program as early as the third grade," she says. "Later on, our high school chemistry teacher inspired most of our class to choose science as our career path."

Perahia received her undergraduate degree in chemistry from Hebrew University in Jerusalem. She then returned to her home town to earn a graduate degree in chemistry at the Weizmann Institute of Science, fulfilling a childhood dream. Perahia's postdoctoral advisers, Sunnil Sinha, currently at the University of California at San Diego, and John Huang, a former Exxon Research and Engineering Laboratory scientist like Perahia, introduced her to the unique contributions of neutron scattering to the understanding of materials.

She admits that being a woman in science is not always easy. "It certainly was a challenge to carry out my doctorate studies with two young children" she says. "I would have never made it without a very supportive husband." Among obstacles to surmount has been both open and disguised prejudice regarding women in science. "Education and focusing on scientific goals are the keys to overcoming these challenges," she observes.

Perahia plans to continue her scientific research. "At some stage, I would like to incorporate a science management component in my work," Perahia says. She is looking forward to returning to ORNL to carry out more experiments with her graduate students.

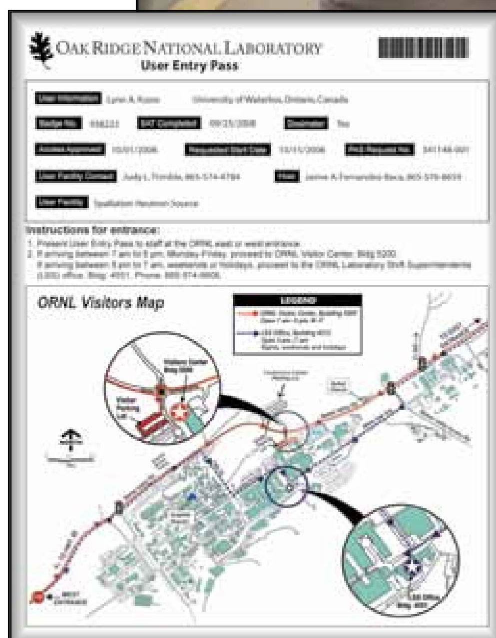
Other enhancements include an improved log-in system and a feedback tool that makes it easy for users to submit suggestions. The preexperiment process for approved proposals has been improved to enable principle investigators (PIs) to confirm team members, and experimenters can more easily identify laboratory capabilities for their experiments.

User Administration

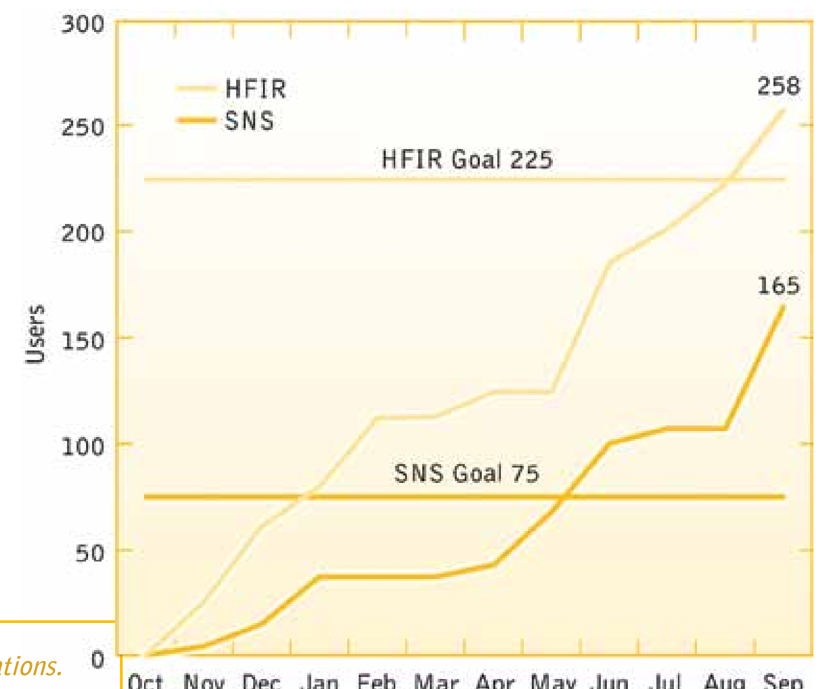
As the number of users grows, it is becoming increasing important to improve not only the facilities but also the processes for user access. Neutron Sciences staff serve on the ORNL User Facility Process Improvement Team, and the User Office volunteered to pilot a user entry pass (similar to an airline boarding pass). The capability to arrange for team member access has been added to the proposal system, and this is used by about 35% of the PIs. Computer accounts are now provided pre-arrival, enabling data analysis as soon as data are taken. Finally, in response to user requests, around-the-clock site access is now available.

User amenities have also improved at both facilities. Orientation and training programs have been revamped to better fit users at each site. User cubicles have been fully equipped at both SNS and HFIR. Lounge, meeting, and outdoor gathering areas are available at both sites. Improved vending services, food preparation capabilities, and evening meal service are being pursued.

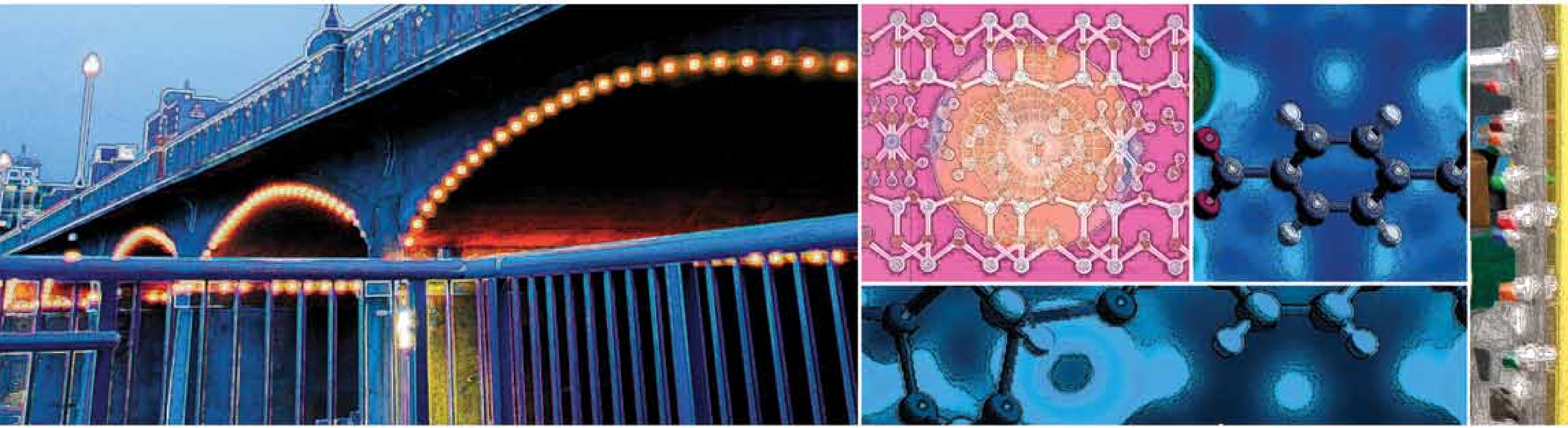
Jun Zhao (University of Tennessee) and Clarina de la Cruz (joint University of Tennessee–ORNL postdoc) discuss the results of their measurements on an iron aresenide superconductor at the Polarized Triple-Axis Spectrometer at HFIR.



Prototype of ORNL user entry pass.



Neutron Sciences users in fiscal year 2008 far exceeded expectations.



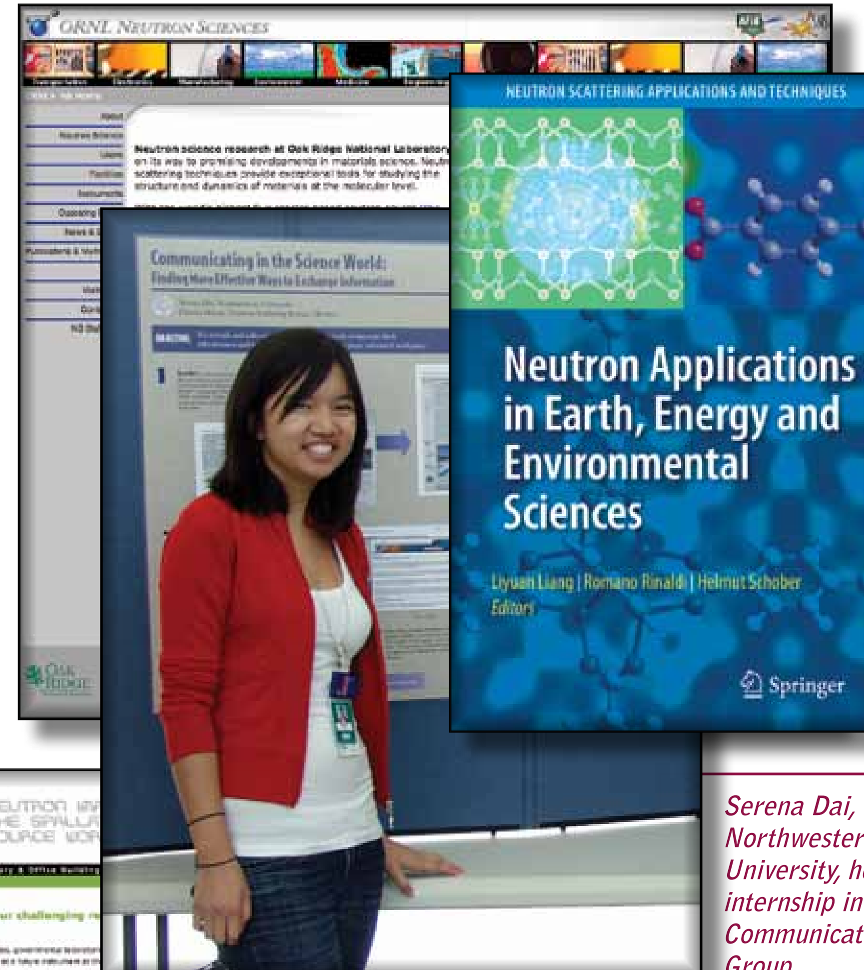
EDUCATION AND OUTREACH

Education and Outreach

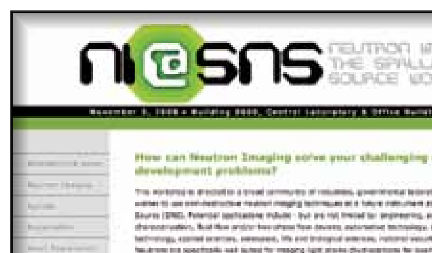
A top priority for the Neutron Sciences organization is to educate scientists, students, and the general public about both the advances from past neutron scattering research and the limitless possibilities for the future. We hope to attract members of the science and engineering community to learn more about the capabilities of neutron scattering in general and about the available resources at HFIR and SNS in particular.

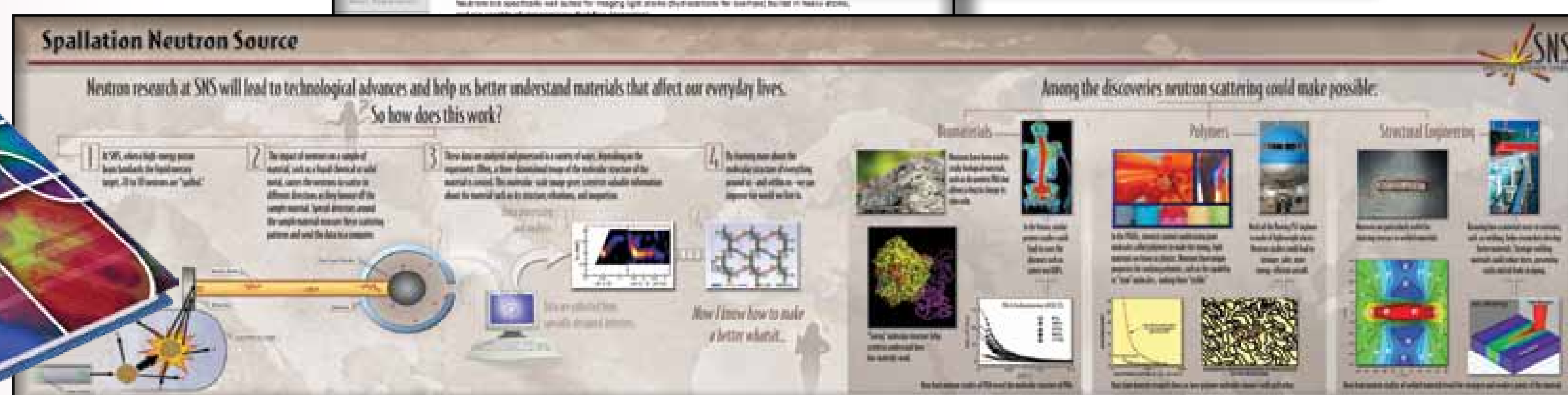
To achieve these goals, our staff actively participate in the scientific community by taking part in or hosting conferences and workshops, by presenting educational information at local community meetings and events, and through many other activities. During the past year, our main educational and outreach activities included organizing (in conjunction with Argonne National Laboratory) the first National School on Neutron and X-Ray Scattering at SNS and HFIR, funding 5 postdoctoral fellowships, hosting 42 interns, and hosting or supporting 10 workshops. Other ongoing efforts include the following:

- Work with the Joint Institute for Neutron Sciences
- Presentations at local universities, public schools, and civic meetings
- Facility tours for special groups and the general public
- Outreach materials such as publications, displays, and multimedia
- The Neutron Sciences public Web site



Serena Dai, Northwestern University, held an internship in the Communications Group.





Meetings and Workshops

Planning and coordinating meetings and workshops is one of our most vital outreach activities. As usual, 2008 was a very busy year.

Neutron Scattering Education Workshop

Education efforts were highlighted by the workshop "Building a Network for Neutron Scattering Education," held in March 2008. The goal of this workshop was to define and design a roadmap for a comprehensive neutron scattering education program in the United States. The workshop report is available at neutrons.ornl.gov/workshops/nse2008/WorkshopReport.pdf.

Workshop participants developed recommendations for three audiences: the general public, scientists who do not currently use neutron scattering, and scientists who already use neutron scattering. For each audience, the participants developed goals, metrics, a description of the current status, gaps, and proposed actions. The proposed actions were partitioned into those that should be initiated now, those that should be initiated within a year, and those that are long term. Four primary actions were identified that have the highest priority for implementation: developing a neutronsources.org Web site, enhancing university-based teaching, expanding neutron schools, and providing advanced software and virtual tools.

Workshop activity for fiscal year 2008 (October 2007–September 2008)

Workshop	Attendees	Date	Location
Residual Stress Summit 2007	100	October 2–4, 2007	Oak Ridge, Tennessee
SNS-HFIR User Group Meeting	250	October 8–10, 2007	Oak Ridge, Tennessee
ORNL Users Week	367	October 8–11, 2007	Oak Ridge, Tennessee
Materials Research Society 2007 Fall Meeting	5000	November 26–30, 2007	Boston, Massachusetts
Building a Network for Neutron Scattering Education	47	March 27–28, 2007	Chantilly, Virginia
SNAP/COMPRES 2008: Spallation Neutrons and Pressure 5th Annual Meeting	60	April 13–15, 2007	Oak Ridge, Tennessee
2008 American Conference on Neutron Scattering	350	May 11–15, 2008	Santa Fe, New Mexico
Diagnosis and Treatment of Problem Structures: A Bruker Workshop on Single Crystal X-Ray Diffraction	40	May 30, 2008	Knoxville, Tennessee
American Crystallographic Association Annual Meeting	600	May 31–June 5, 2008	Knoxville, Tennessee
Applications of Neutron Scattering in Geochemistry and Mineralogy (session 20i) V M Goldschmidt Conference		July 13–18, 2008	Vancouver, British Columbia, Canada
National School on Neutron and X-Ray Scattering	46	September 24–October 11, 2008	Oak Ridge, Tennessee, and Argonne, Illinois

National School on Neutrons and X-Ray Scattering

Jim Browning, far left, with students from the National School on Neutrons and X-Ray Scattering.

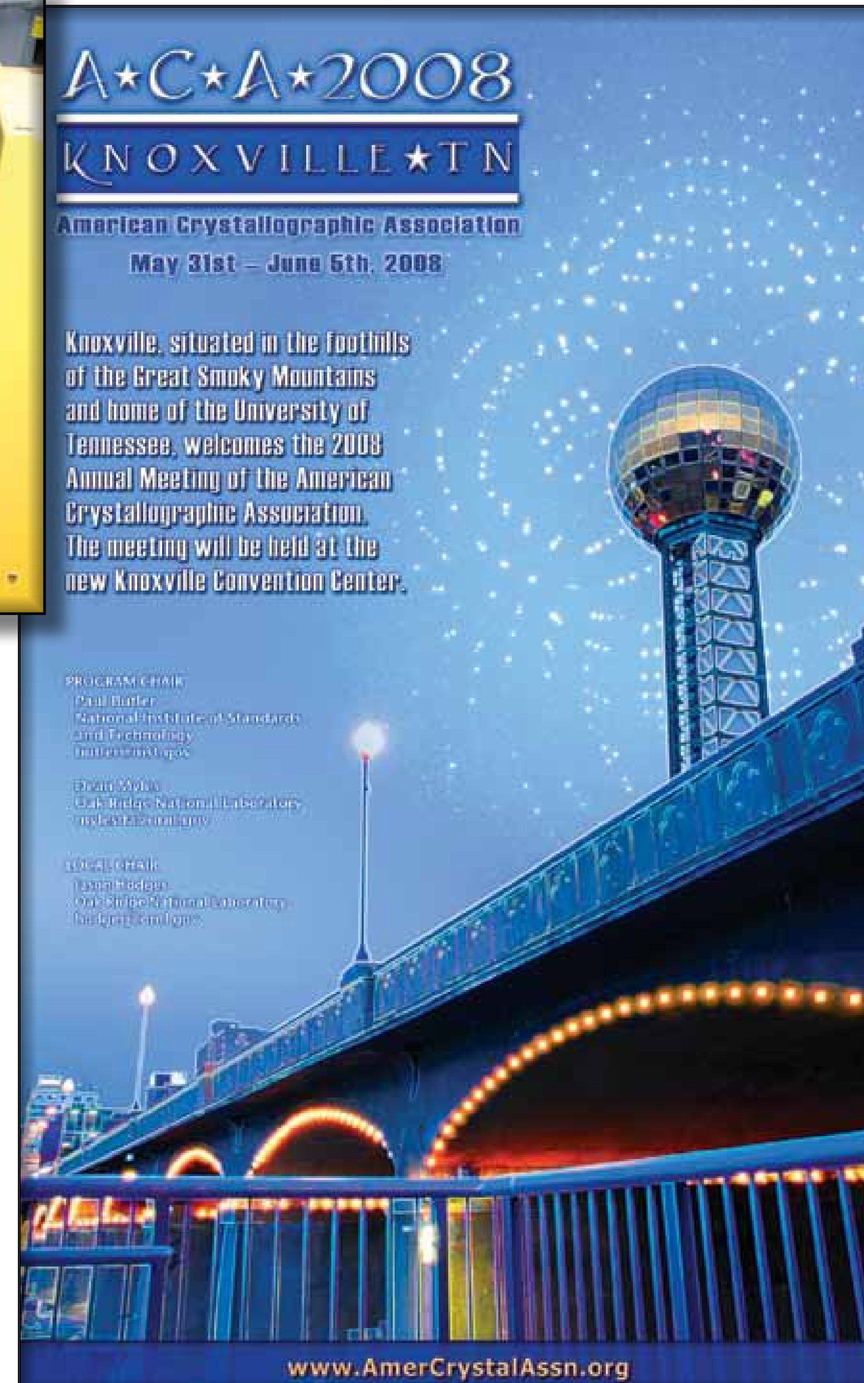
This year the tenth National School on Neutron and X-Ray Scattering was held as a collaboration between ORNL and Argonne National Laboratory. Previous schools had been hosted by Argonne only. The target audience was graduate students attending U.S. universities and majoring in physics, chemistry, materials science, or related fields. With 166 applicants for 46 positions, competition was stiff. The selected students came from 34 universities in the United States and one international academic institution. Funded by DOE, expenses for travel, lodging, and food were paid for most attendees.

The main purpose of this school is to teach students how to make the best use of major neutron and x-ray facilities. Students spent time at both Argonne and Oak Ridge National Laboratories, providing them with access to both world-class facilities. Lectures presented by researchers from academia, industry, and national laboratories included basic tutorials on the principles of scattering theory and the characteristics of the sources, as well as seminars on the application of scattering methods to a variety of scientific subjects. At Argonne, the students performed two experiments at the Advanced Photon Source. At Oak Ridge, they conducted two experiments at HFIR and one at SNS.

The Oak Ridge portion of the 2009 school will be held May 30 to June 5.

American Crystallographic Association Meeting

Neutron Sciences staff were heavily involved in hosting and organizing the American Crystallographic Association Annual Meeting. Neutron Scattering Science Division Director Dean Myles served as chair of the program committee, and Jason Hodges, lead instrument scientist for the SNS Powder Diffractometer, served as local organizing committee chair. In addition, many dozens of staff helped organize technical sessions, social events, and an SNS tour for more than 250 attendees.



Fellowships and Internships

Shull fellows Christopher Stanley (top left), Sylvia McLain (top middle), Wei-Ren Chen (top right), Andrew Christianson (bottom left), and Olivier Delaire (bottom right).

Clifford G. Shull Fellowship

The Shull Fellowship was established in 2005, with the first appointments in 2006. Corecipient of the 1994 Nobel Prize in Physics, Shull began his work in 1946 at what is now ORNL. He is often called the "Father of Neutron Scattering," and this fellowship was established in recognition of his pioneering work in this field. The goal of this fellowship is to attract new scientific talent to ORNL for development of its neutron science program. We look for candidates with exceptional ability who are capable of developing innovative research programs and who show the promise of outstanding leadership. Appointments are for two to three years. To date, five Shull fellows have been appointed.

Olivier Delaire was appointed a Shull fellow in 2008. He received his PhD in materials science from the California Institute of Technology. His current work involves investigations of the microscopic structure and dynamics of materials for energy applications with neutron scattering and computer simulations.

Sylvia McLain (University of Oxford and ISIS) and Christopher Stanley (National Institute of Standards and Technology and the National Research Council) were appointed as Shull fellows in 2007. Chris received his PhD in polymer science and engineering from the University of Massachusetts, Amherst. He is currently working on protein structure and aggregation related to neurological disorders using small-angle neutron scattering. Sylvia received her PhD in chemistry from the University of Tennessee. Recent research included studies of the atomic structure of amino acids in solution. Sylvia is now continuing her research in the UK.

The first two Shull fellowships were awarded in 2006 to Andrew Christianson and Wei-Ren Chen. Andy received his PhD in physics in 2003 from Colorado State University. Recent work includes studies of new superconducting materials and the structure and dynamics of magnetic nanoparticles. Wei-Ren received his PhD in nuclear science and engineering in 2004 from the Massachusetts Institute of Technology. Recent work includes studies of the structure and dynamics of synthetic macromolecules.

Summer student Meaghan Riemer presents a poster at the Neutron Sciences student poster session.

Student Internships

Every year the Neutron Sciences sponsors internships for high school and college students. In 2008, we hosted a record 42 students. Applications from each student are reviewed, an interview is conducted, and selected students are assigned to areas best suited to their paths of study and interest. Each student is assigned a mentor, who is responsible for overseeing the student's work and for providing opportunities for the student to learn and grow from the experience.

Postdoctoral appointments are also made throughout the year. During the past year, five postdoc assignments were made.

Contact: Bob Martin (martinrg@ornl.gov)

neutrons.ornl.gov/jobs

Summer Student Amazed by Neutron Scattering Results

If a pin is rotated against a metallic alloy 10 times at pressures perhaps 10 to 100 thousand times the ambient pressure range, this rubbing effect can cause severe plastic deformation, compressing the microstructure beneath the pin to a nanostructure that can be measured using SANS. This new method of metal grain refinement, called high-pressure torsion (HPT), can reduce metal grains, ranging in size from 20 to 200 micrometers, to as tiny as 20 nanometers—or 1,000 to 10,000 times smaller than the initial grain size.

Meaghan Riemer, a summer student from Clemson University, collaborated with Xun-Li Wang, Sheng Cheng, Ken Littrell, and Ducu Stoica, all of the Neutron Scattering Science Division, to answer this question: if nanometer-sized grains of different nickel alloys are subjected to HPT, how will the microstructure change? To determine the answer, the team conducted SANS experiments at HFIR.

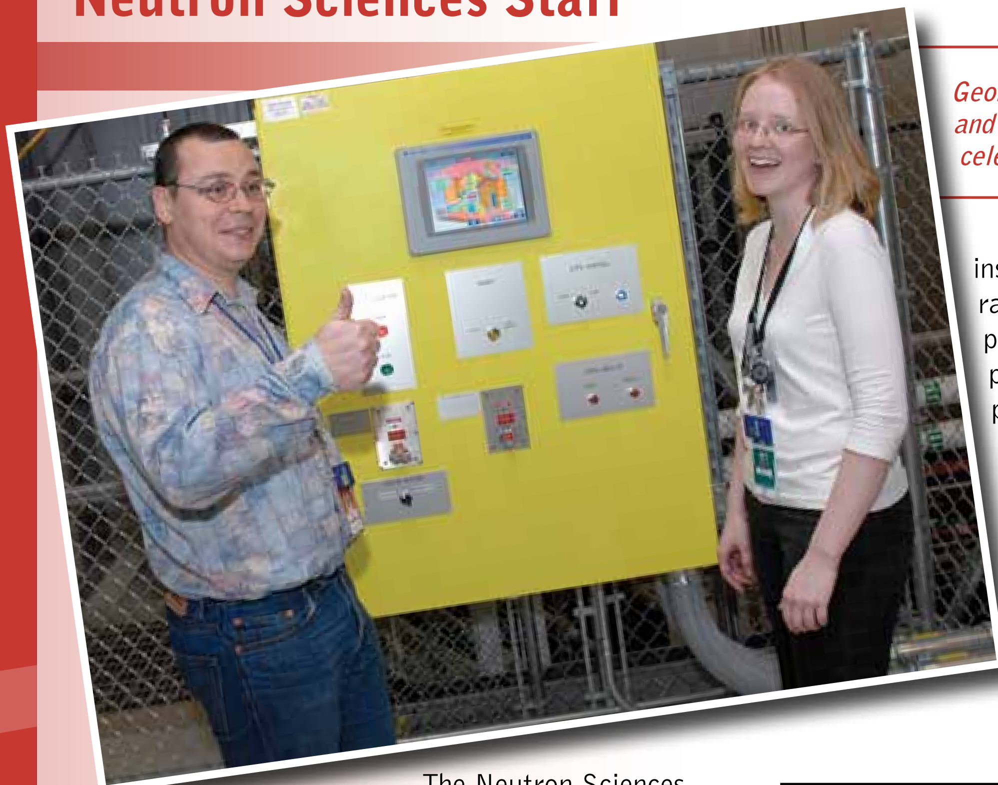
"We experimentally addressed questions about different alloy samples with different grain sizes to determine how their internal structure changed after high-pressure torsion," says Littrell, the instrument scientist for the General-Purpose SANS instrument at HFIR. "Within a few HPT cycles, the microstructures of all the samples, which initially had different grain sizes, looked identical."

"The upshot of this study is that there appears to be an optimum grain size in a metal or alloy subjected to high-pressure torsion, regardless of the material's initial microstructure," says Xun-Li Wang, a materials scientist at SNS. "It appears that HPT crushes large grains to smaller sizes. When the grain size is too small—in the nanometer range, for example—the grains are unstable and tend to grow under deformation." He added that more experiments are needed to get a complete picture.

Reached at Clemson University, Meaghan Riemer said, "I'm really impressed with the capabilities of the SANS instrument at HFIR to capture the effects on metal grain sizes of high-pressure torsion. More experiments may uncover some interesting applications of HPT in the material sciences, such as improving metal strength. I found it exciting to observe the flexibility of SANS for doing different experiments. I hope to return to participate in additional experiments using SANS. My summer at ORNL was truly an enriching experience."

People

Neutron Sciences Staff



Georg Ehlers, lead instrument scientist, and Jennifer Niedziela, scientific associate, celebrate the start of the CNCS at SNS.

The Neutron Sciences Directorate is composed of four groups, each focused on a specific mission:

- Neutron Facilities Development Division (NFDD)
- Neutron Scattering Science Division (NSSD)
- Research Accelerator Division (RAD)
- Research Reactors Division (RRD)

With a staff of about 600, Neutron Sciences is one of the largest science groups at ORNL. HFIR and SNS personnel work with staff from other ORNL research organizations, the Joint Institute for Neutron Sciences, universities, industry, and other research institutes. The goals of these collaborations are to broaden the range and productivity of science programs, promote educational and outreach programs, and ensure the optimum use of ORNL's world-leading neutron facilities.

Neutron Sciences hired 100 new staff members in 2008 and hosted 42 students throughout the year. The students were associated with programs such as the Oak Ridge Associated Universities Higher Education Research Experiences Program, the DOE National Science Foundation Faculty–Student Teams Program, ORNL's Nuclear Engineering Science Laboratory Synthesis Program, and DOE–Office of Science Undergraduate Laboratory internships.

Neutron Sciences staff are actively involved in the community and donate their time, money, and energy to organizations such as the United Way, Habitat for Humanity, and others too numerous to mention.

Neutron Sciences
Building the Future
Habitat for Humanity

Left: Lori Lane of the Neutron Sciences Directorate Office assists another volunteer during a Habitat for Humanity project.
Top: Neutron Sciences staff participate in the Angel Tree program, which benefits struggling families within the community.

Hahn Choo

VULCAN

Joint Appointments

One joint appointment was awarded to Hahn Choo, who joined ORNL as a member of the Power Diffraction Group at SNS. He is also an associate professor at the University of Tennessee College of Engineering. He is currently working on VULCAN, the engineering diffractometer under construction at SNS.

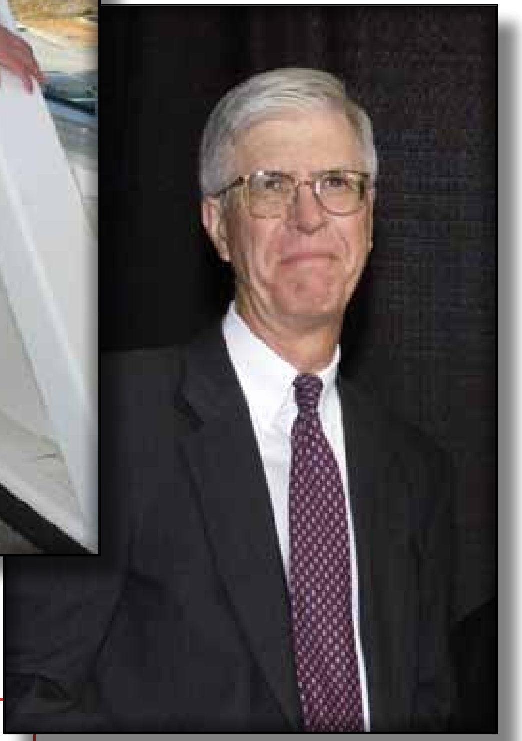
Honors and Awards

Herb Mook, a senior corporate fellow in NSSD was named winner of the 2008 Jesse W. Beams Award from the Southeastern Section of the American Physical Society. Herb was cited for "groundbreaking research in magnetism and superconductivity and leadership in bringing world-leading neutron scattering capabilities to North America." Each year, the society awards three prizes for contributions to the field. Herb started his neutron science research at ORNL in 1965 after receiving his doctorate at Harvard University. He was appointed a corporate fellow in 1987 and a senior corporate fellow in 1995.

RAD physicist Slava Danilov received a European Physical Society Accelerator Group 2008 Achievement Prize. Slava was recognized "for numerous contributions to accelerator physics, in particular for the proposal, calculation, design, construction, and demonstration of efficient laser H- stripping" (see "Facility Development, Future Initiatives"). One of three prizes awarded biennally by the society, this award is for an individual in the early part of his or her career, who has made a recent significant, original contribution to the accelerator field.

Slava joined the SNS project in 1998 and is part of the Accelerator Physics Group. His research interests include self-consistent distributions of intense beam, collective effects, nonlinear dynamics and integrable systems, and quantum physics of beams.

Slava Danilov



Herb Mook

NSSD's Ashfia Huq was awarded the Mary Lyon Award by the Alumnae Association of Mount Holyoke College. The award, named after the college's 1837 founder, Mary Lyon, is presented to an outstanding young alumna who has been out of college 15 years or less.

Ashfia is an instrument scientist with POWGEN, a third-generation powder diffractometer at SNS. Her area of expertise is high-resolution neutron and x-ray powder diffraction of condensed matter systems. Her scientific interests include hydrogen storage materials, catalysis, magnetic and structural properties of strongly correlated electron systems, and ab initio structure solutions from powder data.

Ashfia Huq

Neutron scientist Bryan Chakoumakos was recently elected a fellow of the Mineralogical Society of America. The society was founded in 1919 and, among other goals, encourages fundamental research on natural materials and supports education through its publications, educational grants, and courses.

Bryan Chakoumakos

A member of NSSD, Bryan leads the Single-Crystal Diffraction Group. His areas of expertise include structure property relationships in technological and natural materials and the synthesis, crystal growth, and characterization of novel materials. He employs crystallography, mineralogy, and single-crystal and powder diffraction methods.

Dave Anderson of RAD received an Appreciation Award from Secretary of Energy Samuel Bodman for his contributions to the Electrical Safety Improvement Project Team. In a letter congratulating him, Laboratory Director Thom Mason said that Dave's work has "had a direct and positive impact on our safety at Oak Ridge National Laboratory." The team's efforts led to a substantial revision of the *DOE Electrical Safety Handbook* and have led to significant improvements in electrical safety performance across the DOE complex.

Several Neutron Sciences staff were recognized as outstanding mentors at ORNL and within the community—from NSSD: Al Ekkebus, Jamie Fernandez-Baca, Christina Hoffmann, Chrissi Schnell, and Lakeisha Walker; from RAD: Willem Blokland and Jeff Holmes.

Eighteen staff contributed to the engineering design project, "Spallation Neutron Source Target Hot Cell," which received a 2008 Grand Award from the American Council of Engineering Companies Annual Engineering Excellence Awards program. The team was honored for its design of the hot cell facility, which protects staff and users while allowing maintenance of target and experimental equipment.

Dave Anderson

Recognition of outstanding mentors at ORNL.

PEOPLE

Advisory Committees

Several review committees and advisory teams provide advice and support to the Neutron Sciences organization. The committees are made up primarily of members of the scientific community outside ORNL, as well as some ORNL staff.

Neutron Sciences Advisory Board

Chair, Gregory Boebinger, Florida State University

This committee reports to the ORNL director and advises the associate Laboratory director for Neutron Sciences on all aspects of ORNL's neutron facilities. The goal of the committee is to maximize the scientific impact and benefit of these facilities to ORNL, DOE, and the national and international scientific communities. The committee identifies and brings to the attention of Laboratory management any issues the resolution of which is critical to the technical and scientific success of ORNL neutron facilities, including meeting performance, cost, and schedule goals. The committee is made up of members of the scientific communities that are fundamentally involved with HFIR and SNS, as well as individuals with experience managing major science facilities, particularly materials research facilities.

Neutron Scattering Science Advisory Committee

Chair, Susan Krueger, National Institute of Standards and Technology

This committee reports to the associate Laboratory director for Neutron Sciences and advises the NSSD and the NFDD directors on the directorate's science programs and instrument development. Primarily, the committee provides advice on the types of instruments required to effectively meet the requirements of a multidisciplinary scientific community. The committee also counsels the NSSD director on outreach programs and interaction with the neutron user community. Committee members consist mainly of members from the scientific community who are experts in the instrumentation at HFIR and SNS, potential users, and managers with experience in the effective operation of user programs.

SNS Accelerator Advisory Committee

Chair, Gerry Dugan, Cornell University

This committee reports to the associate Laboratory director for Neutron Sciences and advises the RAD and NFDD directors on the operations and performance of the SNS accelerator complex. Committee members are appointed by the Neutron Sciences associate Laboratory director in consultation with the RAD and NFDD directors.

Instrument Advisory and Development Teams

Instrument advisory teams work with the ORNL staff to design and construct instruments funded by ORNL Neutron Sciences. These instruments are made available to the user community through a peer reviewed proposal system. Instrument development teams (IDTs) build, and sometimes operate, instruments funded from other sources. A portion of beam time on these instruments is allotted for the scientific program of the IDT, with the balance available for general users. At least 75% of the beam time for these instruments is devoted to the general user program. Policies and guidelines regarding instrument development and use are available at neutrons.ornl.gov/users/policies.shtml.

FACTS AND FIGURES

Technical Parameters–SNS

Primary Parameters

Proton beam power on target	1.4 MW
Proton beam kinetic energy on target	1.0 GeV
Average beam current on target	1.4 mA
Pulse repetition rate	60 Hz
Protons per pulse on target	1.5 x 10^{14} protons
Charge per pulse on target	24 μc
Energy per pulse on target	24 kJ
Proton pulse length on target	695 ns
Ion type (Front-end, Linac[a], HEBT[b])	H minus
Average linac macropulse H- current	26 mA
Linac beam macropulse duty factor	6%
Front-end length	7.5 m
Linac length	331 m
HEBT length	170 m
Ring circumference	248 m
RTBT[c] length	150 m
Ion type (Ring, RTBT, Target)	Proton
Ring filling time	1.0 ms
Ring revolution frequency	1.058 MHz
Number of injected turns	1060
Ring filling fraction	250 ns
Maximum uncontrolled beam loss	1 W/m
Target material	Hg
Number of ambient/cold moderators	1/3
Number of neutron beam shutters	18
Initial number of instruments	5

[a]Linear accelerator. [b]High-energy beam transport (system).
[c]Ring-to-target beam transport (system).

Beam Line Allocation

Beam Line	Position[a]	Moderator	Instrument
1A	TU	Hydrogen decoupled	Ultra-Small-Angle Neutron Scattering Instrument (USANS)[b]
1B	TU	Hydrogen decoupled	Nanoscale-Ordered Materials Diffractometer (NOMAD)[b]
2	TU	Hydrogen decoupled	Backscattering Spectrometer (BASIS)
3	TU	Hydrogen decoupled	Spallation Neutrons and Pressure Diffractometer (SNAP)
4A	TU	Hydrogen coupled	Magnetism Reflectometer
4B	TU	Hydrogen coupled	Liquids Reflectometer
5	TU	Hydrogen coupled	Cold Neutron Chopper Spectrometer (CNCS)
6	TU	Hydrogen coupled	Extended Q-Range Small-Angle Neutron Scattering Diffractometer (EQ-SANS)
7	BD	Water	Engineering Materials Diffractometer (VULCAN)[b]
8A	BD	Water	Future development
8B	BD	Water	Future development
9	BD	Water	Elastic Diffuse Scattering Spectrometer (CORELLI)[b]
10	TU	Hydrogen decoupled	Future development
11A	TU	Hydrogen decoupled	Powder Diffractometer (POWGEN)
11B	TU	Hydrogen decoupled	Macromolecular Diffractometer (MaNDi)[b]
12	TU	Hydrogen decoupled	Single-Crystal Diffractometer (TOPAZ)[b]
13	BD	Hydrogen coupled	Fundamental Neutron Physics Beam Line
14A	BD	Hydrogen coupled	Future development
14B	BD	Hydrogen coupled	Hybrid Spectrometer (HYSPEC)[b]
15	BD	Hydrogen coupled	Neutron Spin Echo Spectrometer (NSE)[b]
16A	BD	Water	Future development
16B	BD	Water	Chemical Spectrometer (VISION)[b]
17	BD	Water	Fine-Resolution Fermi Chopper Spectrometer (SEQUOIA)
18	BD	Water	Wide Angular-Range Chopper Spectrometer (ARCS)

[a] T=Top, U=Upstream, D=Downstream, B=Bottom.
[b] Under development.

Technical Parameters–HFIR

Reactor Design Parameters

Core Geometry and Dimensions	
Type of core	Cylindrical annulus, flux trap
Type of fuel elements	Cylindrical annuli (2); Involute 6061-Al fuel plates assembled in 6061-Al side plates
Number of plates (inner element)	171
Number of plates (outer element)	369
Fuel plate thickness	0.050 in.
Fuel plate spacing (coolant channel)	0.050 in.
Fuel plate length	24 in.
Length of active fuel	20 in.
Inner fuel element (inside diameter)	5.067 in.
Inner fuel element (outer diameter)	10.590 in.
Outer fuel element (inside diameter)	11.250 in.
Outer fuel element (outer diameter)	17.134 in.
Active fuel volume	50.59 L
Heat transfer surface area	428.8 ft^2
Reactor Core Materials	
Fuel	U_3O_8 (93% U_{235}) dispersed in aluminum
Total fuel loading • Inner fuel element fuel loading • Outer fuel element fuel loading	9.4 kg 2.6 kg 6.8 kg
Burnable poison (inner element only) • Inner fuel element poison loading	B_4C dispersed in aluminum 2.8 g
Reflector	Beryllium
Moderator	H_2O

Operating Parameters

Reactor Power	
Rated power level	85 MW thermal
Average reactor power density	1.64 MW/L
Typical Operating Cycle	
Normal operation	Steady-state, 85 MW thermal
Length (dependent on core loading)	22–25 days
Maximum Unperturbed Thermal Flux Density in Reflector (Beam Tube Source)	
Beginning of cycle	9.35E+14 n/cm^2 s
End of cycle	1.36E+15 n/cm^2 s
Unperturbed Thermal Flux Density at Reflector Outer Diameter	
Beginning of cycle	1.19E+14 n/cm^2 s
End of cycle	1.45E+14 n/cm^2 s
Peak Thermal Flux Density	
Measured thermal flux in target region	2.5E+15 n/cm^2 s
Reactor Coolant Parameters	
Coolant/moderator	H_2O
Inlet temperature	120°
Outlet temperature	156°
Fuel coolant volumetric flow rate	13,000 gal/min
Total coolant volumetric flow rate	16,000 gal/min
Inlet pressure	468 psig
Fuel clad surface temperature	327°
Average heat flux	0.66E+05 Btu/h ft^2
Hot spot heat flux	2.15E+06 Btu/h ft^2

Neutron Beam Allocation

Horizontal Beam Tube HB-1: Thermal Neutron Beam—Tangential to Core	
HB-1	Polarized Triple-Axis Spectrometer
HB-1A	Fixed-Incident-Energy Triple-Axis Spectrometer
Horizontal Beam Tube HB-2: Thermal Neutron Beam—Radial to Core	
HB-2A	Neutron Powder Diffractometer
HB-2B	Neutron Residual Stress Mapping Facility
HB-2C	US/Japan Wide-Angle Neutron Diffractometer (WAND)
HB-2D	Future development
Horizontal Beam Tube HB-3: Thermal Neutron Beam—Tangential to Core	
HB-3	Triple-Axis Spectrometer
HB-3A	Four-Circle Diffractometer
Horizontal Beam Tube HB-4: Cold Neutron Beam—Tangential to Core	
CG-1	Future development
CG-2	General-Purpose Small-Angle Neutron Scattering Diffractometer (GP-SANS)
CG-3	Biological Small-Angle Neutron Scattering Instrument (Bio-SANS)
CG-4A	Future development
CG-4B	Future development
CG-4C	US/Japan Cold Neutron Triple-Axis Spectrometer (under development)
CG-4D	Future development

SNS Sample Environment Inventory

Liquid Helium Cryostats					
Device ID	Description	Temperature Range (K)	Sample Space	Options	Availability
CRYO 01	JANIS cryo/furnace	1.6-600	D[a] = 58 mm, H_2[b] = 50 mm	^{3}He insert 300 mK	Shared (all BL)
CRYO 02	Continuous flow JANIS "SuperTran"	4-300	D = 50 mm, H_2 = 50 mm		Shared
CRYO 03	Orange cryostat 70 mm	1.5-300	D = 70 mm, H_2 = 50 mm		Shared
CRYO 04	Orange cryostat 50 mm	1.5-300	D = 50 mm		On order
CRYO 05	Orange cryostat 50 mm	1.5-300	D = 100 mm		On order

Closed-Cycle Refrigerators					
Device ID	Description	Temperature Range (K)	Sample Space	Options	Availability
CCR 03	FERNS[c] auto changer	7-300	Custom: 4, 6, or 8 mm V cans	Holds 24 samples	POWGEN-3 dedicated
CCR 04	Sumitomo bottom loader	4-450	D = 55 mm*, H_2 = 100 mm	*Alternate shield for larger samples	Shared
CCR 05	ARS "Split Head" top loader	10-300	D = 47 mm, H_2 = 45 mm		Shared
CCR 06	SNS top load interface with DE-210 cold head	8-475	D = 60 mm, H_2 = 75 mm	Rotating sample stick	Shared
CCR 07	ARCS cryo-goniometer	20-300	Large bottom load space	Sample tilt and rotation	ARCS dedicated
CCR 08	Displex with Joule-Thomason 3rd stage	1.7-300	Bottom load, D = 55 mm, H1[d] + H2 = 100 mm, H1: 13 to 88 mm	Thimble rig with vertical height adjustment	Shared
CCR 09	ICEoxford 1K-pot system	2-300	D = 34 mm	Dil-fridge compatible	On order
CCR 10	ARS DE-204 bottom load configuration	4-300	Large bottom load space		CNCS
CCR 11	ARS DE-204 on horizontal rotation axis	4-300	Custom sample holder	1.5 Tesla electromagnet	Magnetism Reflectometer
CCR 12	ARCS thimble rog	4-300	Large bottom load space		ARCS dedicated, under development
CCR 13	SEQUOIA rotating cold head	4-300	Large bottom load space		SEQUOIA
CCR 14	P-E cell chiller	<50 K	Anvil pressure cell	Used to cool Paris-Edinburg cell	SNAP
CCR 15	SNS sapphire top loader	7-500	D = 60 mm, H_2 = 75 mm	Hot/cold sample in exchange gas	Shared
CCR 16	JANIS 100 mm ARCS	4-800			On order
CCR 17	JANIS 100 mm shared	4-800			On order
CCR 18	JANIS for BASIS	4-800			On order

Furnaces

Device ID	Description	Temperature Range (K)	Sample Space	Options	Availability
HOT-01	ILL niobium foil vacuum furnace	Ambient to 1600	D = 40 mm	Gas flow insert (see HOT-03)	Shared
HOT-02	Controlled atmosphere furnace	Ambient to 1073	Special sample holders – consult SE team	Controlled gas atmosphere	Shared SNS and HFIR
HOT-03	Gas flow insert	Ambient to 1073	Special sample holders – consult SE team	Controlled gas atmosphere	Under development
HOT-04	"Sapphire" vertical tube furnace	Ambient to 1073	D = 90, H_2 = 110	Gas/liquid pressure cells	BASIS
HOT-05	Cal-Tech low-background furnace	Ambient to 950	Special sample holder – consult SE team		ARCS
HOT-06	ILL niobium foil vacuum furnace	Ambient to 1600			On order

Magnet Systems

Device ID	Field Strength [Tesla] and Orientation	Temperature Range (K)	Sample Space	Options	Availability
MAG-01	5-T vertical field actively shielded "Slim SAM"	1.5-300	M^e = 1/4-28 stud, D = 34 mm, H1 = 51 mm, H2 = 81 mm	Dil-fridge insert (on order)	Shared
MAG-02	16-T vertical field Swiss collaboration shielded magnet	1.5-300	D = 34 mm	Dil-fridge insert	Summer 2009
MAG-03	2-T vertical field Bruker electromagnet	5 to 300 w/CCR-11	Custom sample holder – consult beam line		Magnetism Reflectometer
MAG-04	7-T vertical field IPNS magnet				POWGEN—modification under way
MAG-05	10-T vertical field				Solicitation under development

Ultra-Low Temperature Devices					
Device ID	Description	Base T (mK)	Sample Space	Options	Availability
ULT-01	JANIS helium-3 insert for CRYO-01	300	M = 1-in. B.C. 4 X 4-40 tapped D = 35 mm, H1 = 19 mm, H2 = 47 mm	Spacer available to increase H1	Shared
ULT-02	IceOxford dil insert	25	D=28 mm	Dil-fridge insert	On order
ULT-03	ILL dil insert for MAG-02	25			On order

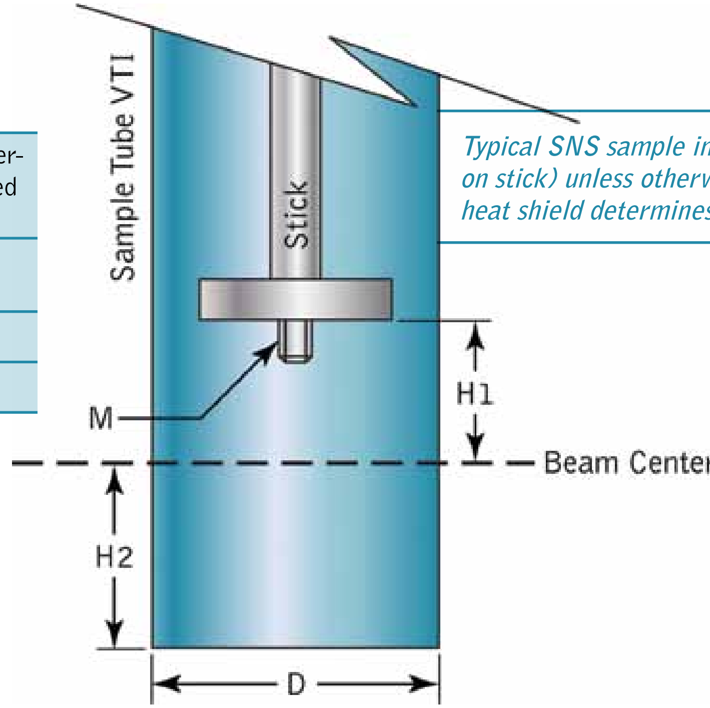
High-Pressure Cells and Equipment					
Device ID	Description	Pressure (kBar)	Cell Size	Options	Availability
GASCELL 01	Titanium-zirconium null scattering alloy gas pressure cell	1	0.25 in. ID 4 in. long		Shared
GASCELL 02	Sapphire gas/liquid cell	Proof tests pending	5.0 mm ID 80 mm length		BASIS
GASCELL 03	TZM cell (TiZrMo alloy)	Proof tests pending			BASIS
GASCELL 03-07	Aluminum cells Carnegie Institute design Harwood fab			Coming soon	Shared
ANVIL	The SNAP beam line has 12 small gem anvil pressure cells and 8 large-volume Paris-Edinburg cells. Seek assistance from SNAP and/or SE team.				

Other Special Environments	
Description	Availability
Langmuir trough for studying thin layers of surfactants or other materials on the surfaces of liquids, such as cell-membrane analogs	Liquids Reflectometer
Controlled humidity cell	Liquids Reflectometer

[a]D = Diameter limit of sample.
[b]H2 = Height below beam.
[c]FERNS = Fast Exchange Refrigerator for Neutron Science.
[d]H1 = Height of mounting surface above beam. Adjustable unless otherwise noted.
[e]M = Mounting stud 5/16-18 UNC (unless otherwise noted). Sample cell has center-tapped 5/16-18 hole.

Legend

M	Mounting stud 5/16-18 UNC (unless otherwise noted). Sample cell has center-tapped 5/16-18 hole.
H1	Height of mounting surface above beam. Adjustable unless otherwise stated.
H2	Height below beam.
D	Diameter limit of sample.



Typical SNS sample interface. Devices are top loading (sample on stick) unless otherwise stated. For bottom loaders, the inner heat shield determines size restriction.

HFIR Sample Environment Inventory

Closed-Cycle Refrigerators—Bottom Loading						
Description	Temperature Range (K)	Bore Size (mm)	Interface Connection	Distance from Interface to Beam Center (in.)	Stick Distance to Beam Center (in.)	Special Features/Comments
High-temp displex-1AF	5-800	N/A	0.25-in. Hole	2	N/A	
Displex-1A	11-300	N/A	1/4-28 Female	2.325	N/A	For use with standard sample can
Displex-A	4-300	N/A	1/4-28 Female	2.325	N/A	
Displex-B	6.5-300	N/A	1/4-28 Female	2.325	N/A	
Displex-H	8-300	N/A	1/4-28 Female	2.325	N/A	Optional saphire window for SANS
Displex-I	8-300	N/A	1/4-28 Female	2.325	N/A	Turbo-1 hour RT to base temp
Displex-M	14-300	N/A	1/4-28 Female	2.325	N/A	High capacity for use with high-pressure cells
Closed-Cycle Refrigerators—Top Loading, Sample in Exchange Gas						
Omniplex-0	6-300	50	1/4-28 Female	1.5 w/ +/-2 adj.	19-7/8	Top-loading displex
Omniplex-02	5-300	50	1/4-28 Female	1.5 w/ +/-2 adj.	19-7/8	Top-loading displex
JANIS	4-300	Recent addition				

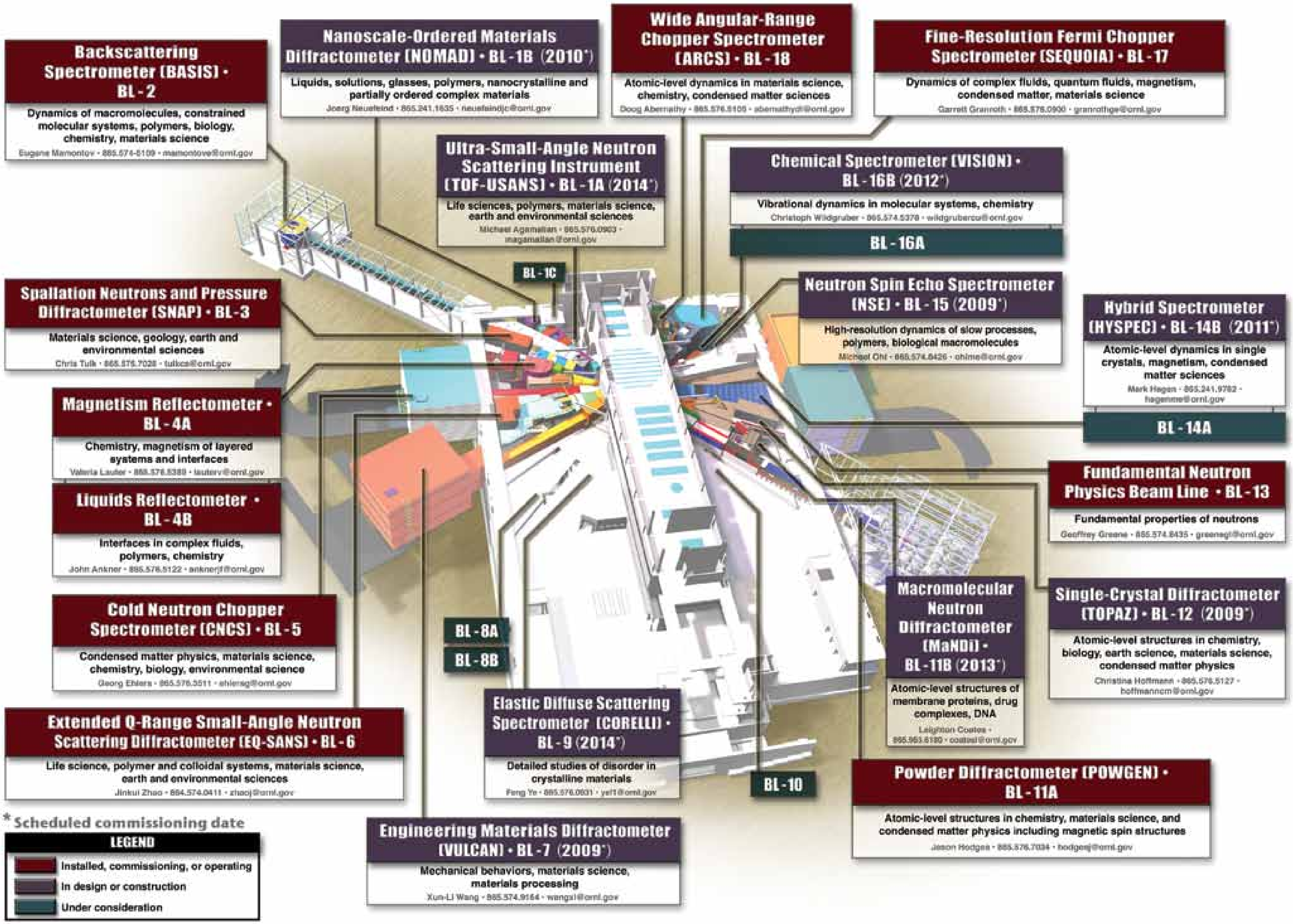
Furnaces						
Description	Temperature Range (K)	Bore Size (mm)	Sample Space	Distance from Interface to Beam Center (in.)	Stick Distance to Beam Center	Special Features/Comments
ILL niobium foil vacuum furnace	Ambient to 1600	40	D = 40 mm	1.5 w/ +/-2 adj.		
HOT-O_2 controlled atmosphere furnace	Ambient to 1073	40	Special sample holders – consult SE team	1.5 w/ +/-2 adj.		Controlled gas atmosphere

Magnet Systems						
Description	Temperature Range (K)	Bore Size (mm)	Interface Connection	Distance from Interface to Beam Center	Stick Distance to Beam Center	Special Features/Comments
4.5-Tesla horizontal field magnet	1.8-300	40	M6 Male	2.325 in./59 mm	44.325 in./1125 mm	Access for SANS use only
5-Tesla vertical field magnet	2-300	50	Custom	1.97 in./50 mm	33.75 in./857 mm +/-15 mm	WAND mount capable
7-Tesla vertical field magnet	2-300	25	M6 Male	Nominal 1.5 in.	46 in.	Field limited to 5.5 T at HB-1A

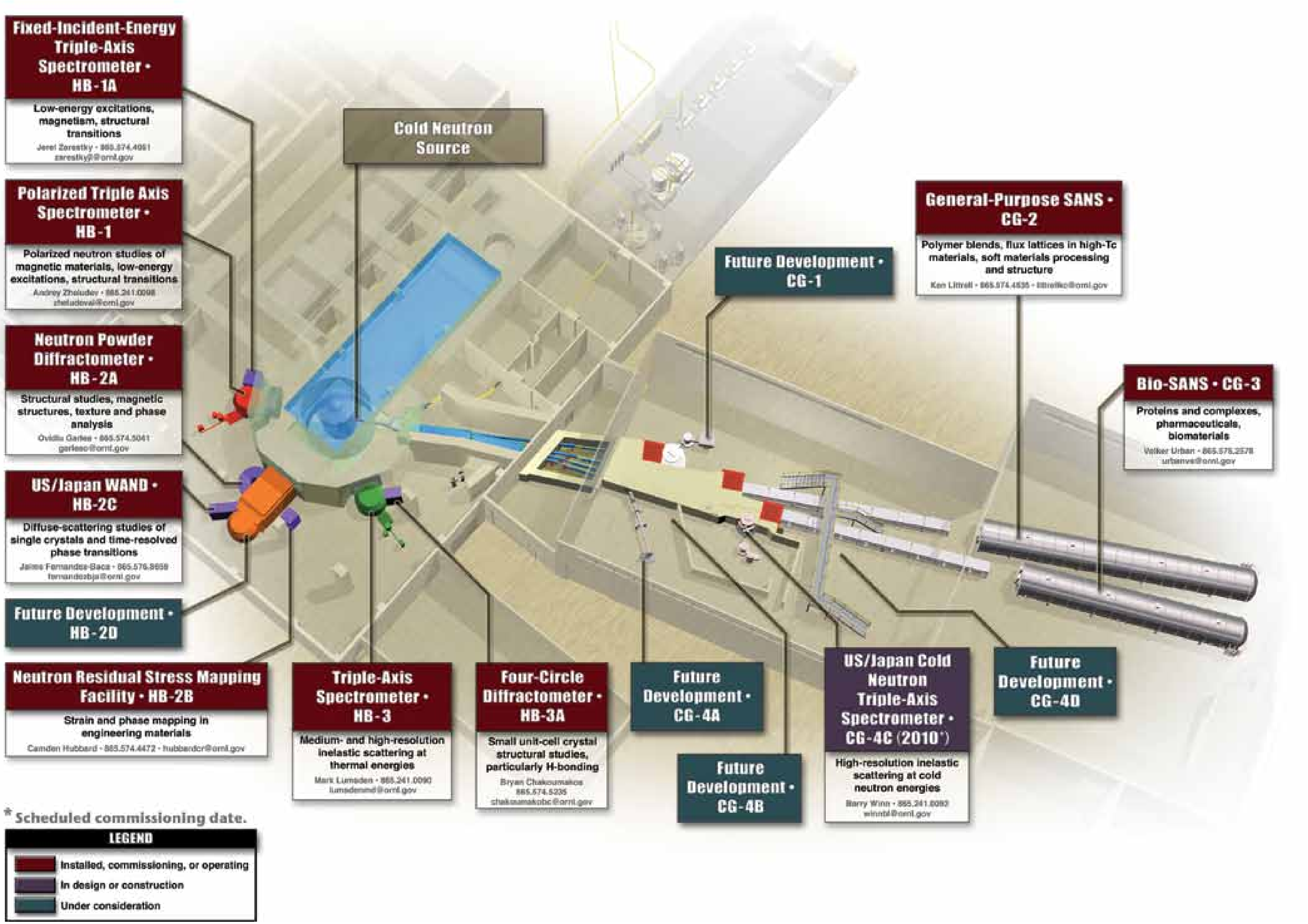
Liquid Helium Cryostats						
Description	Temperature Range (K)	Bore Size (mm)	Interface Connection	Distance from Interface to Beam Center	Stick Distance to Beam Center	Special Features/Comments
Helium cryostat—Variox 1	1.5-300	50	M8 Female	Nominal 1.5 in.	46 in.	
Helium cryostat—Old blue	Variable	50	Custom	N/A	N/A	For use with high-pressure cells
Helium Cryostat—ILL-01	1.5-300	50	M8 Female	2.5 in.	37.25 in.	
Furnace—HOT-02	300-1900	50	Custom	N/A	N/A	

[a] T=Top, U=Upstream, D=Downstream, B=Bottom, [b] Under development.

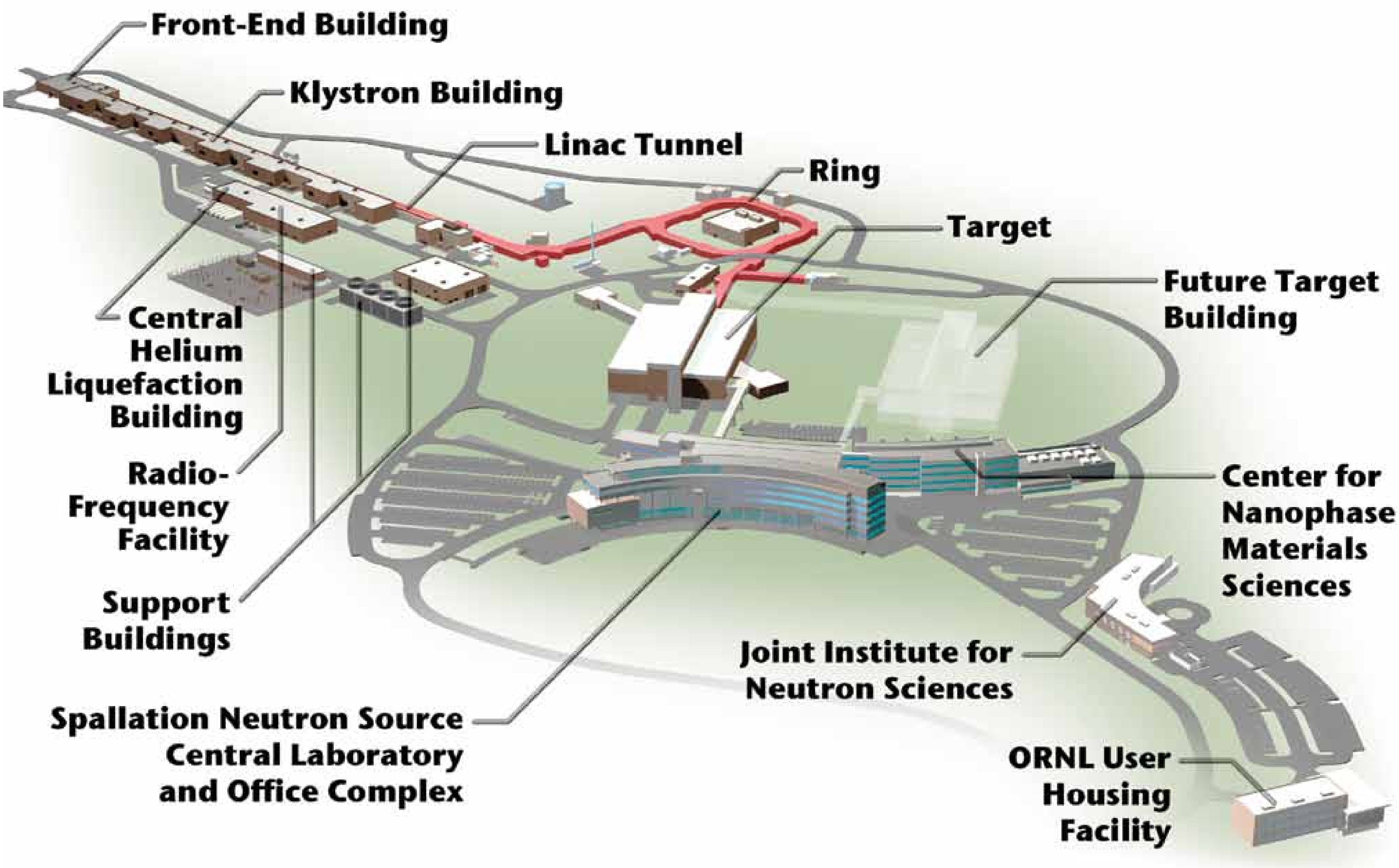
Instrument Layout–SNS

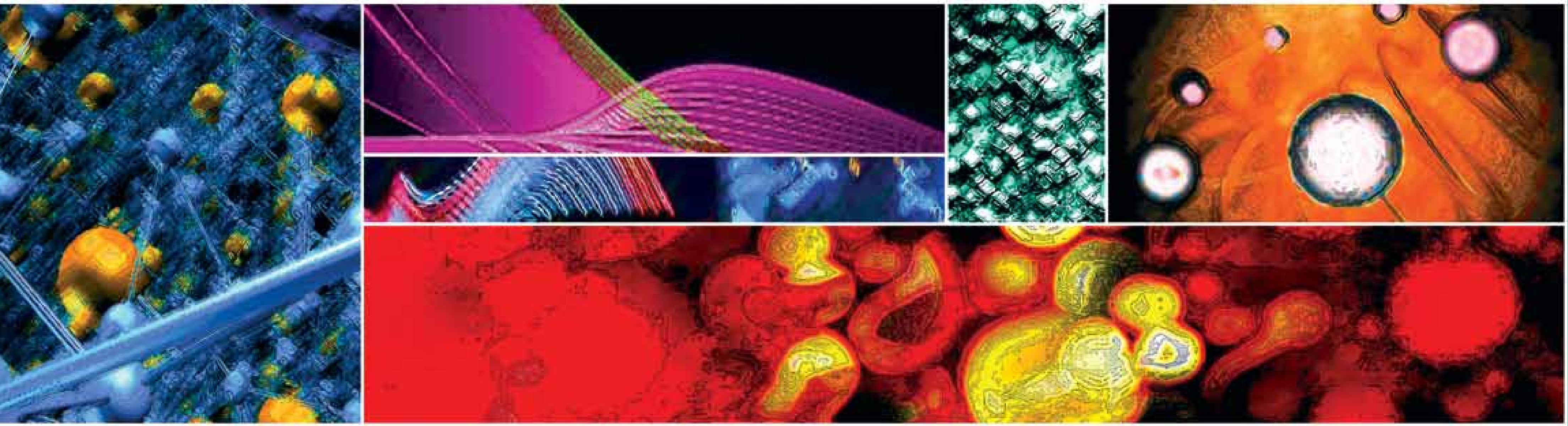


Instrument Layout–HFIR



Conceptual Drawing–SNS





PUBLICATIONS

During the past year, users came to ORNL from institutions all over the world and produced an impressive array of research results. More than 140 publications were authored or coauthored by users and Neutron Sciences staff during 2008. The following publications document the results of studies enabled in part or completely by use of SNS and HFIR.

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Acronyms

ARCS Wide Angular-Range Chopper Spectrometer

BASIS Backscattering Spectrometer
BESC BioEnergy Science Center

CCR closed-cycle refrigerator
CNCS Cold Neutron Chopper Spectrometer
CNMS Center for Nanophase Materials Sciences
CORELLI Elastic Diffuse Scattering Spectrometer
CREB CAMP response element binding
CSD Chemical Sciences Division
CSMB Center for Structural Molecular Biology

DOE U.S. Department of Energy

EQ-SANS Extended Q-Range Small-Angle Neutron Scattering Diffractometer

FNPB Fundamental Neutron Physics Beam Line

GFP green fluorescent protein
GUI graphical user interface

HD Huntington's disease
HDF hierarchical data format
HFIR High Flux Isotope Reactor
HPT high-pressure torsion
HTML High Temperature Materials Laboratory
HTS high-temperature superconductors
HYSPEC Hybrid Spectrometer

IMAGINE Image-Plate, Single-Crystal Diffractometer
IPNS Intense Pulse Neutron Source
IPTS Integrated Proposal Tracking System
ISAW Integrated Spectral Analysis Workbench

JBEI Joint BioEnergy Institute

LCF Leadership Computing Facility
LHC light harvesting complex
LPSD linear position-sensitive detectors

MaNDi Macromolecular Diffractometer

NASA National Aeronautics and Space Administration
NBAP National Biofuels Action Plan
NCCS National Center for Computational Sciences
NFDD Neutron Facilities Development Division
NOMAD Nanoscale-Ordered Materials Diffractometer
NSSD Neutron Scattering Science Division
NSE Neutron Spin Echo Spectrometer

PCI-e peripheral component interconnect express
P-E Paris-Edinburgh
POWGEN Powder Diffractometer

RAD Research Accelerator Division
RRD Research Reactors Division

SEQUOIA Fine-Resolution Fermi Chopper Spectrometer
SHaRE Shared Research Equipment User Facility
SHUG SNS and HFIR User Group
Slim SAM shielded asymmetric magnet at SNS
SNAP Spallation Neutrons and Pressure Diffractometer
SNS Spallation Neutron Source

T_c critical temperature
TEM transmission electron microscopy
TOPAZ Single-Crystal Diffractometer

USANS Ultra-Small-Angle Neutron Scattering Instrument
UT University of Tennessee

VASIMR variable specific impulse magnetoplasma rocket
VDMA vinyldimethylazlactone
VISION Chemical Spectrometer
VULCAN Engineering Materials Diffractometer

WAND Wide-Angle Diffractometer

Units

Btu	British thermal unit
cm	centimeter
ft	foot
gal/min	gallons per minute
GeV	gigaelectronvolt
h	hour
Hz	hertz
in.	inch
K	kelvin
kJ	kilojoule
kW	kilowatt
linac	linear accelerator
m	meter
mA	milliampere
MeV	megaelectronvolt
mm	millimeter
μm	micrometer
MW	megawatt
nm	nanometer
ns	nanosecond
psig	pounds per square inch

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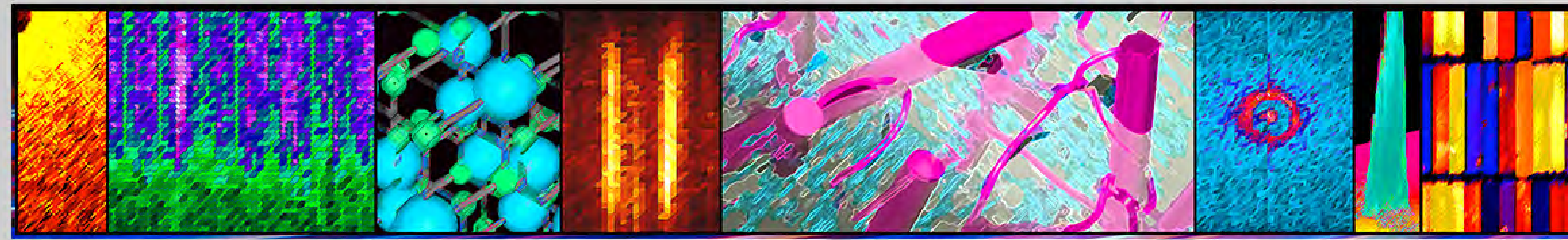

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