Oak Ridge National Laboratory

Neutron Sciences

Managed by UT-Battelle for the U.S. Department of Energy

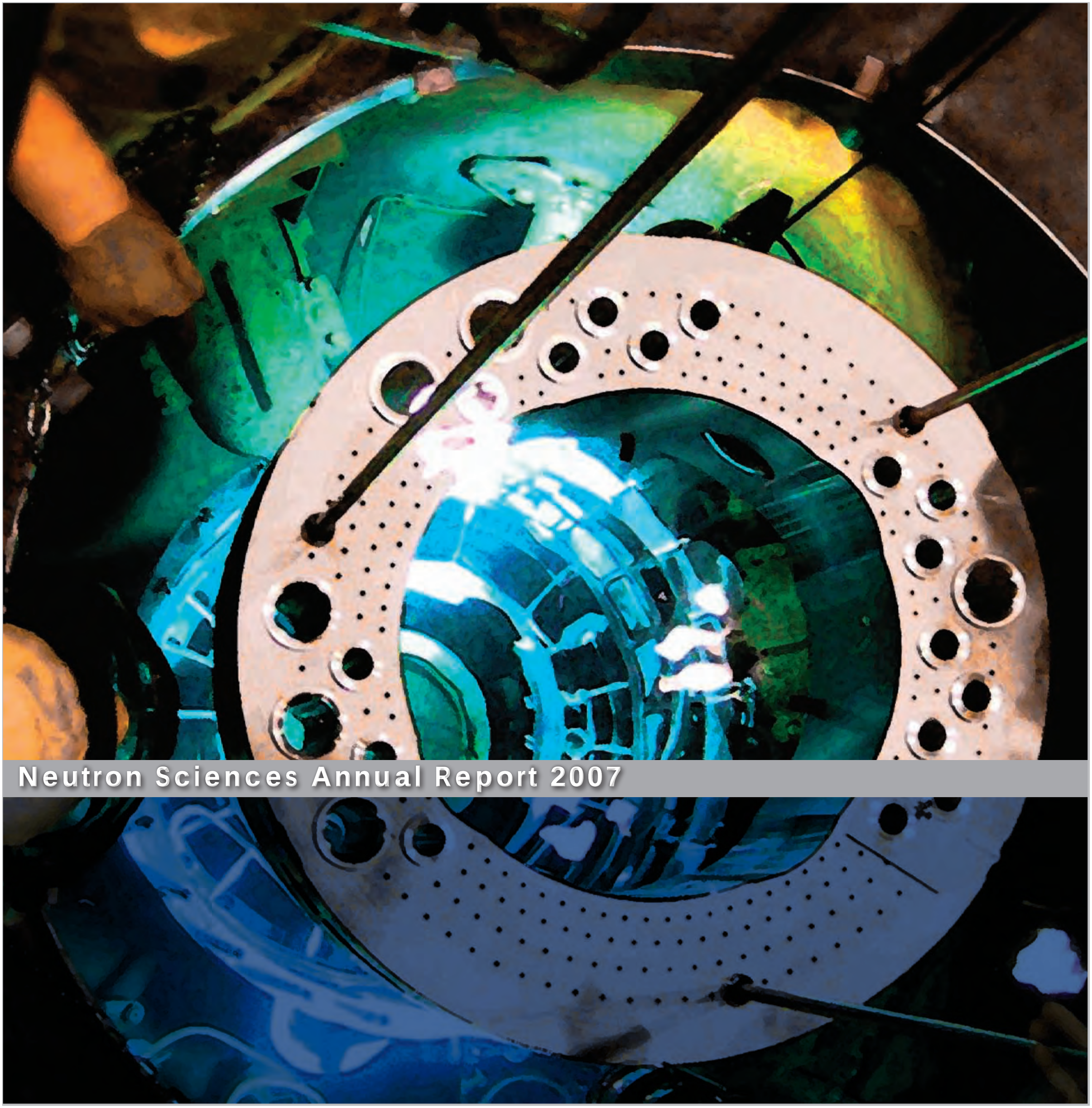
Annual Report 2007

This is the first annual report of the Oak Ridge National Laboratory Neutron Sciences Directorate for calendar year 2007. It describes the neutron science facilities, current developments, and future plans; highlights of the year's activities and scientific research; and information on the user program. It also contains information about education and outreach activities and about the organization and staff.

The Neutron Sciences Directorate is responsible for operation of the High Flux Isotope Reactor and the Spallation Neutron Source.

This report was compiled by the Neutron Sciences Communications Group
neutronscience@ornl.gov

Technical Editor:	*Deborah Counce*
Coordinating Editor:	*Charlie Horak*
Technical Illustrators:	*Reneé Manning*
	Genevieve Martin
Photography:	*Curtis Boles*
	Charlie Brooks
	Jay Nave

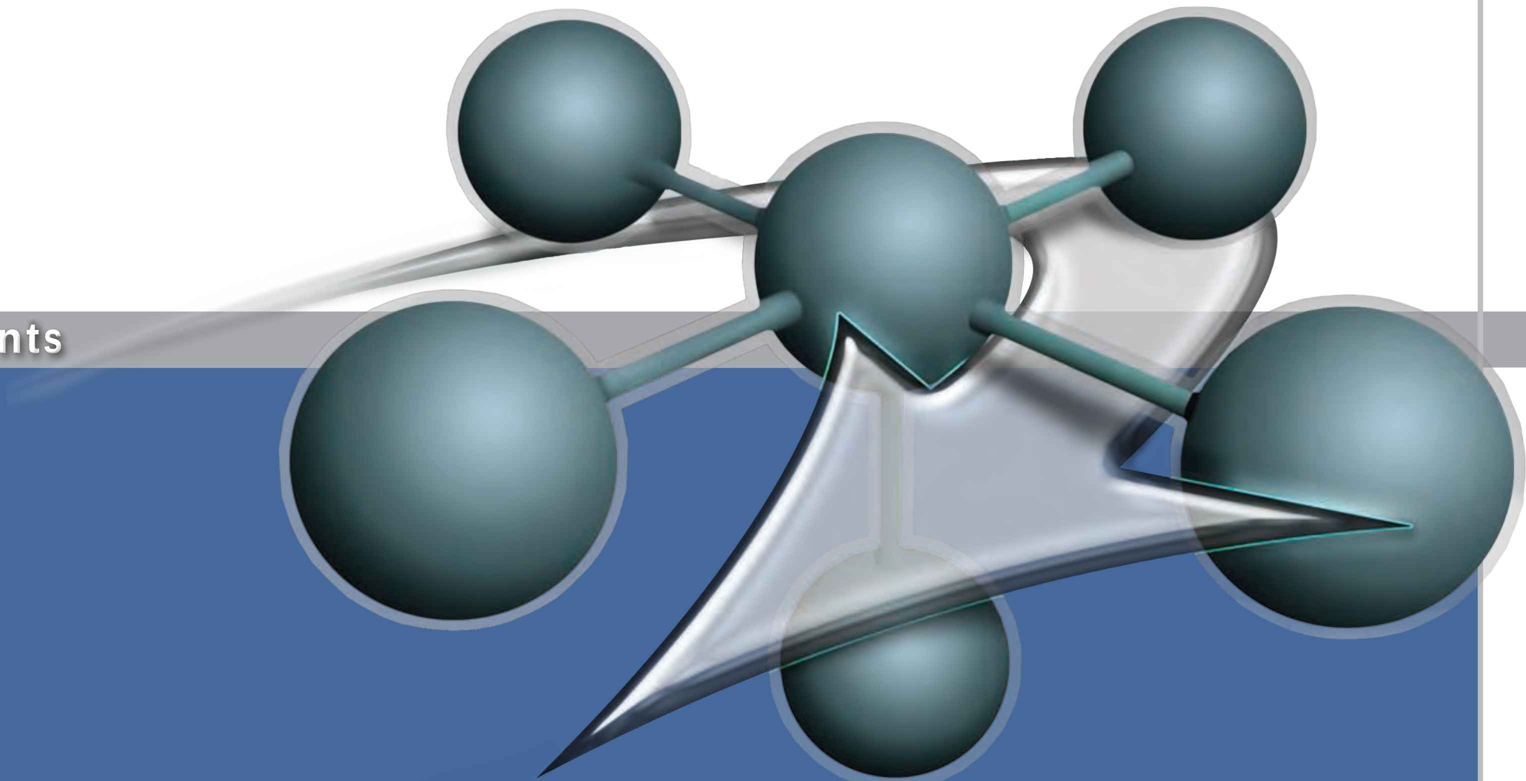


Neutron Sciences Annual Report 2007

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.



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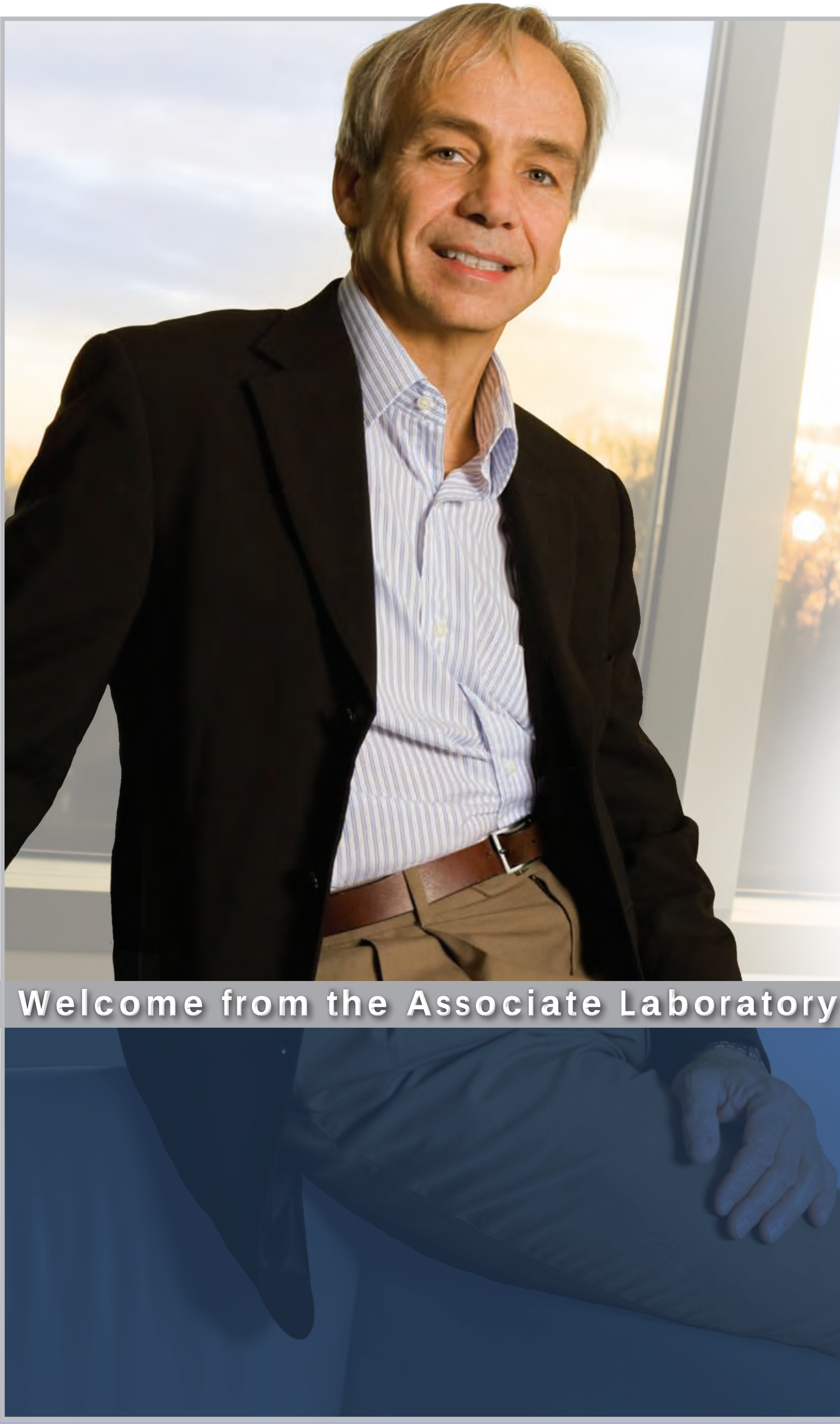


Ian Anderson

Associate Laboratory Director
for Neutron Sciences at
Oak Ridge National Laboratory
andersonian@ornl.gov

It is my pleasure to present you with the Oak Ridge National Laboratory Neutron Sciences Directorate's first annual report. This inaugural issue marks the restart of the High Flux Isotope Reactor, with its new cold source, and the first full year of operation of the Spallation Neutron Source, the world's most powerful pulsed spallation neutron source. With HFIR and SNS operating, ORNL now has two of the world's best neutron facilities and the opportunity to optimize the use of pulsed versus continuous sources, with the highest flux of both. This year also marks the beginning of my tenure as associate Laboratory director, and I am excited about the bright future for neutron sciences in Oak Ridge.

The main highlights of 2007 were highly successful operation and instrument commissioning at both facilities. At HFIR, the year began with the reactor in shutdown mode and work on the new cold source progressing as planned. The restart on May 16, with the cold source operating, was a significant achievement. Furthermore, measurements of the cold source showed that the performance exceeded expectations, making it one of the world's most brilliant sources of cold neutrons. HFIR finished the year having completed five run cycles and 5,880 MWd of operation. At SNS, the year began with 20 kW of beam power on target; and thanks to a highly motivated staff, we reached a record-breaking power level of 183 kW by the end of the year. Integrated beam power delivered to the target was 160 MWh. Although this is a substantial accomplishment, the next year will bring the challenge of increasing the integrated beam power delivered to 887 MWh as we chart our path toward 5,350 MWh by 2011.

This year also saw the beginning of our combined user program at both facilities. At HFIR, users took advantage of the Neutron Residual Stress Facility and the three operating triple-axis instruments. Some notable experiments were also performed on the Wide-Angle Neutron Diffractometer, sponsored by the United States and Japan. Perhaps most noteworthy was the commissioning of the two new small-angle neutron scattering instruments, which have already starting producing excellent results and are now available to users. At SNS, three instruments were available to users: the Magnetism and Liquids Reflectometers and the Backscattering Spectrometer. During the 2007 fiscal year (October 2006 to September 2007), 96 users performed 63 experiments between the two facilities.

Another noteworthy accomplishment was the launching of our Integrated Proposal Management System. The system is used to process user proposals and was put into production in the summer. Users will soon be able to use this one system to submit proposals to four ORNL facilities—HFIR, SNS, the Center for Nanophase Materials Sciences, and the Shared Research Equipment User Facility.

As safety to our staff and users is paramount, I am proud to report that while staff at both HFIR and SNS worked hard to meet goals, they also did so with an outstanding safety record. Staff and contractors working at both facilities finished 2007 with no lost workday cases.

As we look to the future, several significant enhancements are under way for both facilities. In addition to commissioning of new instruments that take full advantage of the new cold source at HFIR, long-term plans include the possibility of a second cold source and establishment of the HFIR Neutron Science Center. At SNS, the number of SNS instruments available to users will more than double, and approval has been granted for a power upgrade that will increase proton energy by 30% and beam current by 60%. Work is also proceeding to obtain funding for a second, long-wavelength target station that will double the number of available instruments as well as the scientific capabilities of the facility.

The vision for Neutron Sciences at ORNL has been and will continue to be developed in collaboration with the scientific community. Through workshops and meetings, particularly with the user community, we continually seek input from outside the Neutron Sciences Directorate and ORNL. This communication is essential to meet the needs of the scientific community. Another key to continuing to develop an effective program is our partnerships with users at universities and other neutron sources.

ORNL is uniquely placed to enable forefront research using neutrons, and in this report you will find selected highlights of the initial research conducted during the past year. The scientific results achieved thus far promise exciting work to come. You can find out more about the user program and our education and outreach activities. You can also read about recent facility developments and the support capabilities in place for a wide variety of experiments in almost any discipline. Finally, we've included information about the people in Neutron Sciences—the foundation for all of our successes.

Neutron Primer

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

1. 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.

2. 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.

3. 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.

4. 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.

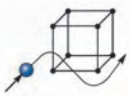
Neutron Properties

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

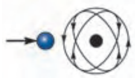
Neutrons have a MAGNETIC moment. They can be used to
- *study microscopic magnetic structure,*
- *study magnetic fluctuations, and*
- *develop magnetic materials.*

Neutrons have SPIN. They can be
- *formed into polarized neutron beams,*
- *used to study nuclear (atomic) orientation, and*
- *used for 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} cm 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.*

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—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.

ORNL
Neutron Sciences

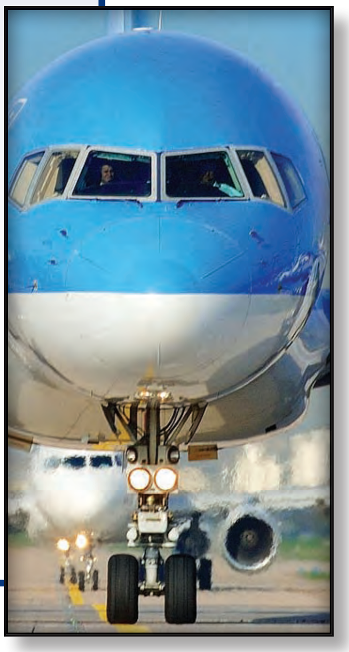
ORNL is home to two of the most advanced neutron scattering research facilities in the world, the High Flux Isotope Reactor and the Spallation Neutron Source. Scientists from all over the world come to conduct basic research at these facilities. Studies conducted at SNS and HFIR go beyond basic research and development, leading to technological advances that benefit the scientific, business, and industrial communities.

ORNL's Neutron Sciences Directorate manages neutron science activities at both facilities, which are funded by the U.S. Department of Energy Office of Basic Energy Sciences. The directorate was formed in 2006—when SNS was just coming on line and a major upgrade of HFIR was being completed. The new organization was charged with realizing ORNL's goal of becoming the world's foremost center for neutron science, providing researchers with unmatched capabilities for understanding the structure and properties of materials, macromolecular and biological systems, and the fundamental physics of the neutron.

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.

The main goal for the directorate is achieving 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've set up a common user program and have structured operations to facilitate scientific integration between the two facilities. 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.

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 co-recipient 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.



Much of the Boeing 757 airplane is made of lightweight plastic. Neutron studies could lead to stronger, safer, more energy-efficient aircraft.

High Flux Isotope Reactor and Spallation Neutron Source

For some research, having neutrons available in a continuous beam is advantageous; for other research, a pulsed beam is better. The availability of both types of neutron sources at one facility gives scientists unprecedented opportunities to work with some of the most advanced technology in the world. In addition, neutron scattering can provide information about the structure and properties of materials that can't be obtained from other techniques such as X rays or electron microscopes.

The 85-MW 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 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 15 instruments planned or in operation. A new cold neutron source installed during a HFIR refurbishment in 2006–2007 greatly enhances the reactor's research capabilities, particularly in the biological sciences.

SNS is a recently completed 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.

Year in Review: *Highlights*

The many exciting events of 2007 make it difficult to cover them all in detail. For the Year in Review, we present a few of the most significant events for neutron sciences at ORNL:

- SNS becomes the world's most powerful pulsed spallation neutron source.
- HFIR is restarted, with a newly installed cold source.
- The fourth SNS instrument—the Wide Angular-Range Chopper Spectrometer—begins commissioning.
- Two new small-angle neutron scattering (SANS) instruments, designed for use with cold neutrons, are commissioned at HFIR.

HFIR Restart

The restart of HFIR on May 16, 2007, after a 16-month outage for upgrades and the addition of new instruments, was a milestone for neutron science at ORNL. The restart began the 40-year-old HFIR's 408th run cycle. The reactor was taken to 10% power initially for confirmation of safety parameters and then was quickly increased to its peak power level of 85 MW.

Major additions to HFIR are the new guide hall facility for cold source instruments, two new cold source instruments, and the liquid hydrogen cold source itself. Installation of the cold source was especially significant to prospective HFIR users. In September, the neutron flux and brightness of the cold neutron beams were tested using time-of-flight methods. Tests revealed the brightness to be significantly greater than was predicted by earlier

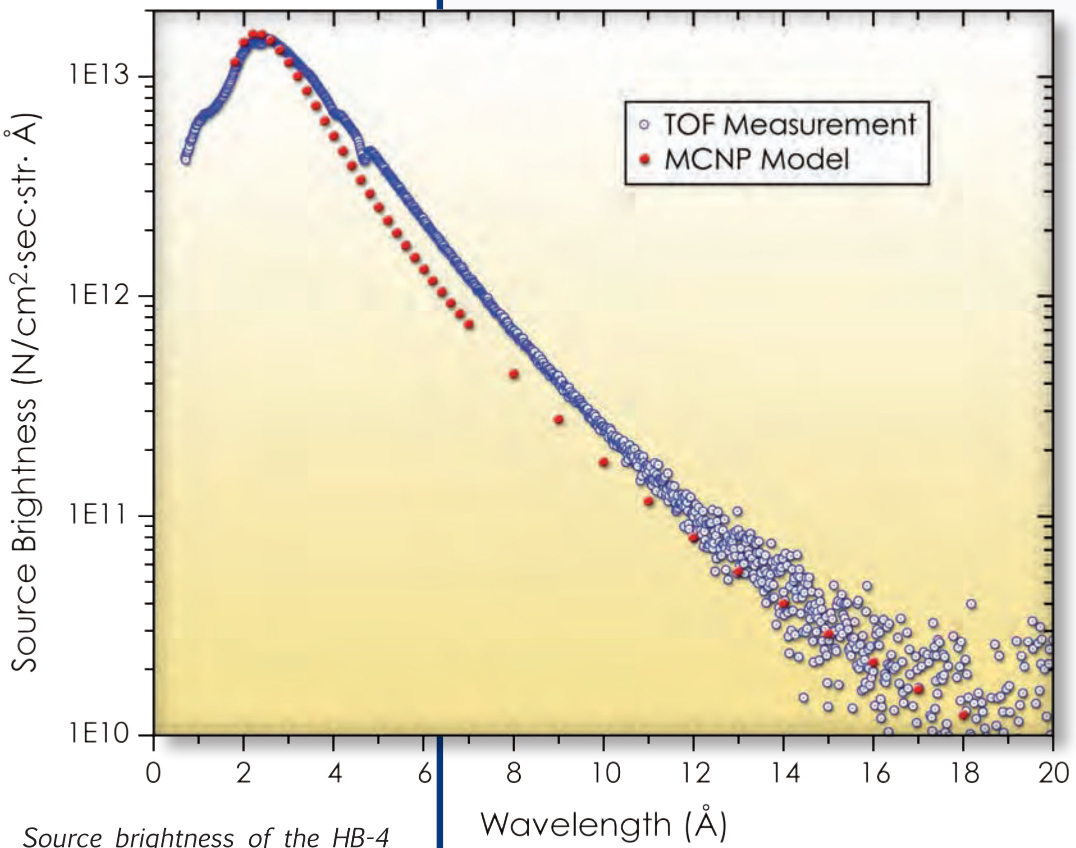
HFIR employees at the restart celebration on May 24, 2007.

computer simulations in the highly valued 4 to 12 Å range. This achievement confirms HFIR's performance as one of the highest-flux reactor-based sources of cold neutrons in the world.

Why Cold Neutrons?

For neutron scattering experiments, it is ideal to match the wavelength and energy of the neutron to the length and energy scales, respectively, of the materials under investigation. Therefore, neutrons with long wavelengths and low energies—cold neutrons—are the best for studying large-scale structures (e.g., molecular organization, nanopore-size distributions, and aggregate size and shape) and low-energy excitations (e.g., excitations in frustrated systems and various problems in magnetism, superconductivity, and correlated electron systems).

The thermal (room temperature) neutron spectrum of a reactor produces neutrons with wavelengths on the order of a few tenths of a nanometer, well matched to investigating atomic length scales and lattice vibrational energies. When thermal neutrons are passed through a container of low-temperature liquid hydrogen, they are slowed by collisions with the hydrogen. This process produces slower neutrons better suited for studies of soft matter. Because they reflect well from surfaces, cold neutrons can be transported over long distances with little loss.

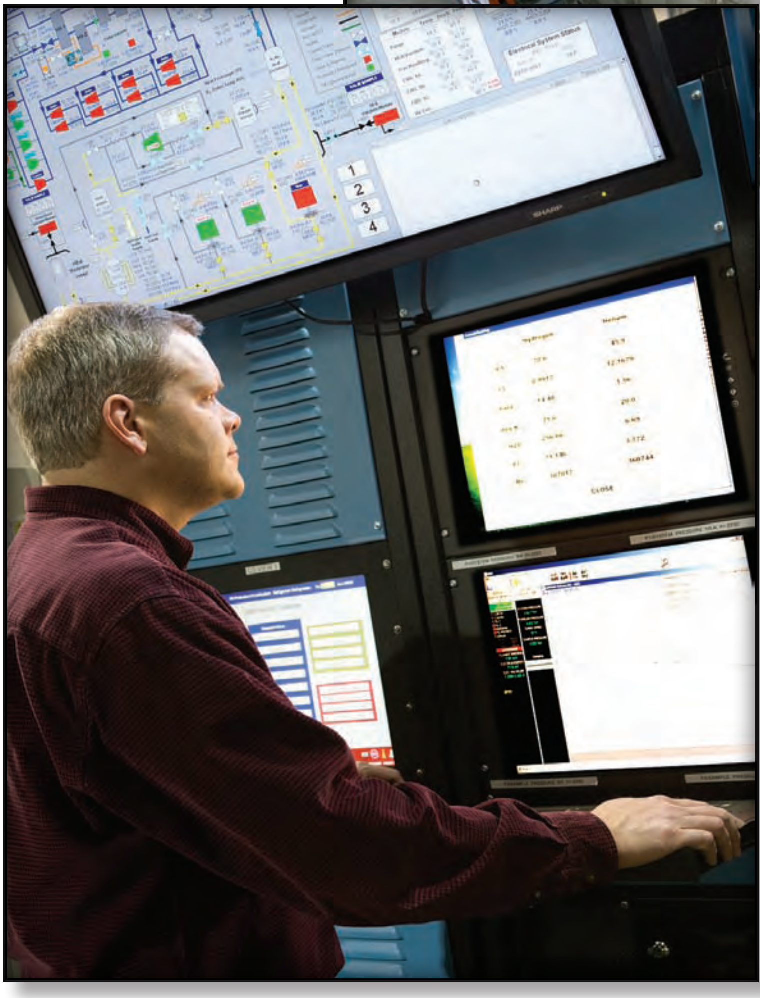


Source brightness of the HB-4 cold source at reactor power of 85 MW and moderator temperature of 22.5 K.

New SANS Instruments

Two of the four cold source guides provide beams to the now operational SANS instruments, which are among the most advanced in the world. One of these is a general-purpose SANS instrument, designed for experimentation on hard and soft condensed matter and magnetic systems. The other, the Bio-SANS, is designed especially for studying the structure and function of biological materials and complexes, including biomacromolecules such as proteins and viruses, membranes, and biomimetic systems. Commissioning of the instruments with cold neutrons began in mid-2007 and was completed in December.

Detector tanks for the new SANS instruments. On the right is the general-purpose, high-resolution instrument; on the left is the Bio-SANS instrument, constructed specifically for biological research.

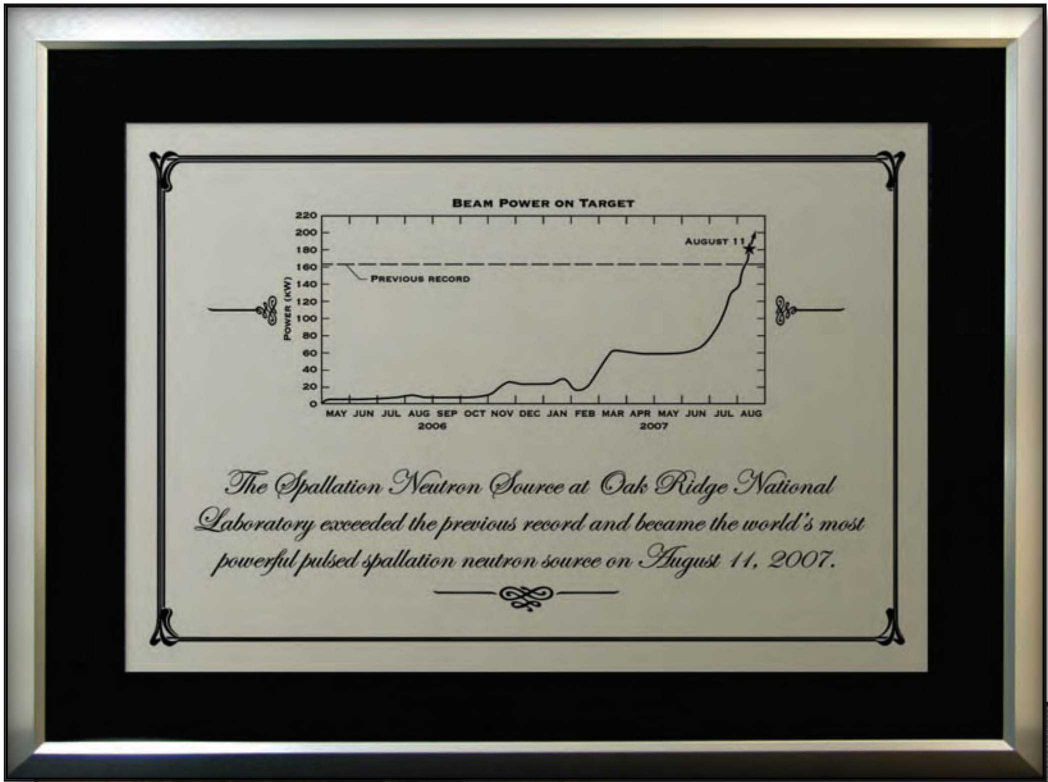


Research Reactors Division Director, Ron Crone, reviews cold source data.

Other improvements at HFIR include an overhauled reactor, upgraded instruments, and new control systems. In addition, laboratories are being equipped for users, and plans are in place to continue improving the overall facilities. When fully instrumented, HFIR will include 15 of the most advanced neutron scattering instruments in the world, 7 of which will be designed exclusively for cold neutron experiments. With the successful commissioning of the cold source and more than $70 million in renovations, HFIR regained its status as a world-class facility.

SNS Becomes the World's Most Powerful Pulsed Spallation Neutron Source

On August 11, 2007, SNS set a new technological record and became the world's most powerful pulsed spallation neutron source by maintaining continuous operations at 183 kW. Throughout the next several months, operational and neutron production goals were reached and often exceeded. In addition to offering the research community neutron beams more intense than ever before available, SNS demonstrated that it could also provide those neutrons with high reliability. After 1.4 billion dollars and five years of construction, these highly successful operations confirmed that not only could SNS operate as planned but also that it could perform above and beyond expectations, opening a new realm of possibilities to scientists all over the globe.



Plaque posted in the SNS Central Control Room commemorating SNS becoming the world's most powerful pulsed spallation neutron source. An official recognition ceremony was held on August 29 and was attended by U.S. Senator Lamar Alexander and U.S. Representatives Zach Wamp and Bart Gordon.

SNS staff outside the Central Laboratory and Office Building, August 11, 2007.

Wide Angular-Range Chopper Spectrometer

In September, commissioning began for the SNS Wide Angular-Range Chopper Spectrometer (ARCS). ARCS is optimized to provide a high neutron flux at the sample and a large solid angle of detector coverage for inelastic scattering. The spectrometer is capable of selecting incident energies over the full energy spectrum of neutrons, making it useful for studies of excitations from a few to several hundred millielectron volts. An elliptically shaped supermirror guide in the incident flight path boosts the performance at the lower end of this range. The sample and detector vacuum chambers provide a window-free final flight path and incorporate a large gate valve to allow rapid sample change-

September 2007 Commissioning of ARCS in the SNS Target Building. On the left, ARCS lead instrument scientist Doug Abernathy holds the shutter key just before opening the shutter for the first time. Beside him is ARCS lead engineer Kevin Shaw. In the background is David Vandergriff, lead engineer for the SNS Fine-Resolution Fermi Chopper Spectrometer (SEQUOIA).

out. A new T-zero neutron chopper is being developed not only to block the prompt radiation from the source but also to eliminate unwanted high-energy neutrons from the incident beam line.

To date, inelastic neutron scattering experiments have been constrained by low neutron flux, forcing experimental compromises in energy resolution, momentum resolution, and the number of spectra that can be measured. With its high detection efficiency, ARCS will free experimenters from many restrictions caused by low flux. The ARCS team worked hard to ensure that the most robust, highly advanced hardware and software were incorporated into ARCS, enabling new experiments with a sophistication not previously achieved with chopper spectrometers. Compared with current instruments, the increased sensitivity of ARCS offers new opportunities for scientific studies in lattice dynamics, magnetic dynamics, and chemical physics.

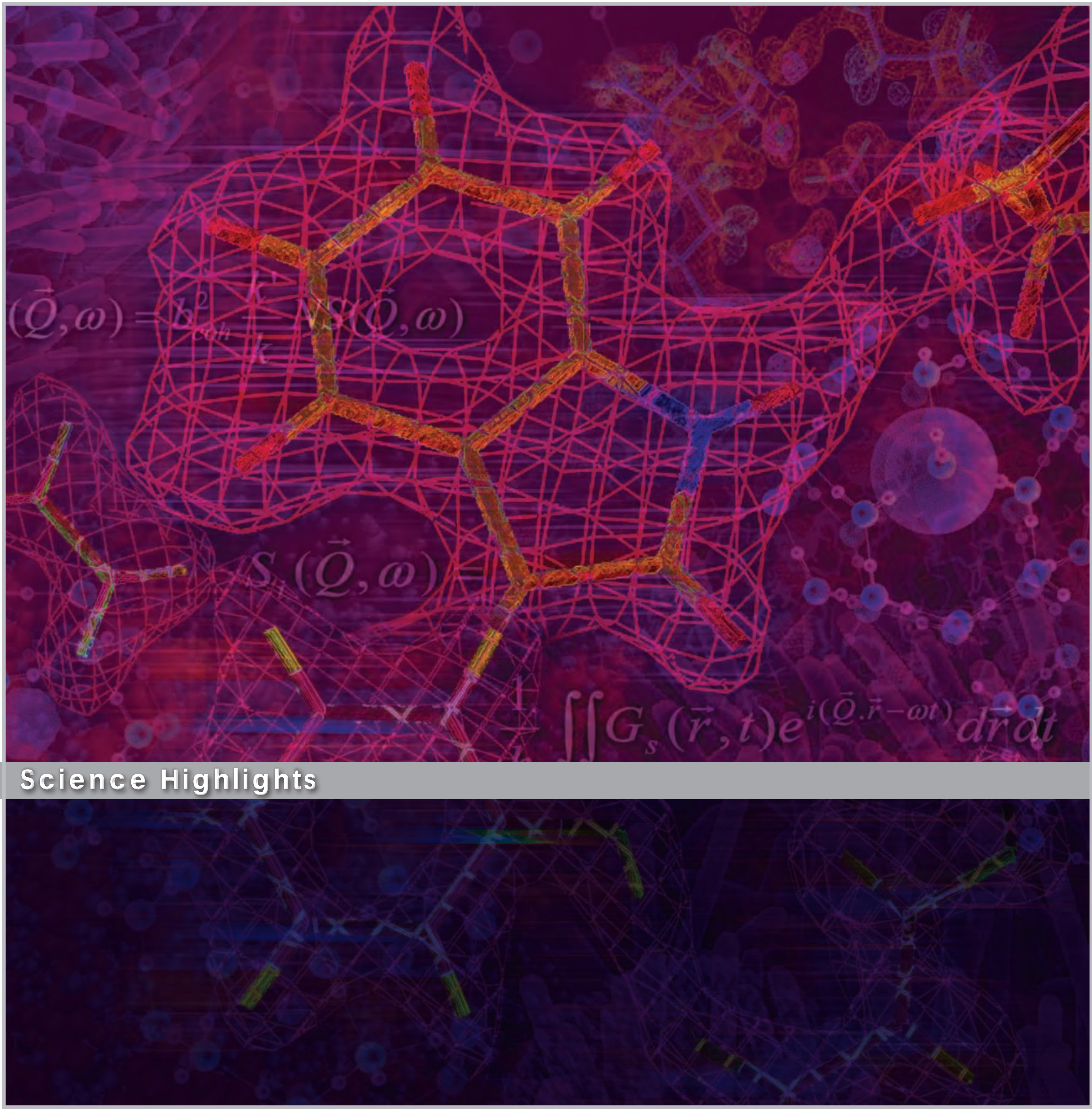
More information about ARCS is available in the Facts and Figures section.

Contact: Doug Abernathy (abernathydl@ornl.gov)

neutrons.ornl.gov/instrument_systems/beamline_18_arcs/

Top: Doug Abernathy (left) and Bill McHargue (SNS instrument support) in the ARCS control room. Left: Installation of detector tubes in the ARCS instrument.

Science Highlights



from the Neutron Scattering Chief Scientist

It is a great pleasure to introduce the “Science Highlights” section of the first annual progress report for the ORNL Neutron Sciences Directorate. ORNL has a long tradition of excellence in neutron-related research, starting with the pioneering development of neutron diffraction by Ernest Wollan, Clifford Shull, and their colleagues. Even by these standards, the past year has been very special. HFIR has returned to operation after a long hiatus, initiating a new era of research with cold neutrons at ORNL. SNS has officially arrived as a world-class pulsed neutron source, and neutron scattering experiments have begun on the first three instruments to enter the user program.

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

This year’s selected science highlights offer a glimpse into a future full of robust and diverse forefront research. These are just the first baby steps for science in the new directorate, under conditions of limited beam availability and instruments still in commissioning. Even so the results are exciting. At SNS, the dynamics of molecules tethered to a porous silica surface have been investigated using the Backscattering Spectrometer, BASIS. The results clearly illustrate this instrument’s unprecedented combination of excellent energy resolution and large signal-to–background ratio. Some of the early measurements with the Liquids Reflectometer have shed light on the environmentally triggered behavior of polyelectrolyte multilayers, materials with possible widespread applications as “smart” coatings. These measurements have resulted in the first peer-reviewed publication of data from SNS.

At HFIR, the use of thermal beams for inelastic neutron spectroscopy has resumed and is represented here by an experiment on lattice dynamics in a colossal-magnetoresistive oxide material. The thermal beams have also been used to explore magnetic structures: neutron diffraction has been used to elucidate subtle magnetic correlations present in a fascinating new multiferroic material. New directions in in situ applied research are adumbrated by time-resolved diffraction measurements of iron-carbon alloys, simulating real-life processing in the presence of magnetic fields. Engineering applications of neutron diffraction are represented by a report on cracks induced by metal fatigue, a topic of great interest to the airline industry, among others. Finally, the first data have been taken using the new small-angle neutron scattering machines in the cold neutron guide hall. A fascinating study on the role of defects in high-performance ceramic materials is reported here: look for exciting highlights from these instruments in the near future!

As neutron sciences activity builds up over the next several years, we anticipate that highlights of some amazing science will appear in these pages. I hope that you, the reader, will be able to participate in the voyage of discovery that lies ahead.

Environmental Triggers for Smart Multilayer Coatings

Polyelectrolyte multilayer (PEM) coatings have great potential for use in biosensors, drug delivery systems, antifogging or antireflection surfaces, devices for controlling nanochemical reactions, and regulators for the flow of solutions through microchannels. They will be even more valuable if researchers can develop "smart" PEM coatings that can respond to variations in the environment around them, such as temperature or pH changes. Designing PEMs with predictable, controllable responses is not yet possible, though, because the fundamental mechanisms of such environmental triggers are not fully understood. A more precise understanding of the fundamental mechanisms by which environmental changes trigger responses in PEMs could enable researchers to design PEMs whose responses can be manipulated for various applications.

Candice Halbert, scientific associate for the Liquids Reflectometer, fills a Langmuir trough with water. The trough is essentially a Teflon pool used to form a flat surface for water. Neutrons are reflected from molecules spread on the surface.

In a bid to expand understanding of how PEM coatings react to environmental changes, the Liquids Reflectometer at SNS is being used to study the effects of changes in the pH in the environment surrounding a PEM coating. The team—Eugenia Kharlampieva and Svetlana A. Sukhishvili of Stevens Institute of Technology, John Ankner of ORNL, and Michael Rubinstein of the University of North Carolina–Chapel Hill—is investigating the process by which polymer molecules in a coating are released and reabsorbed as the pH of a surrounding solution is increased and decreased. The results of this work are presented in the March 25, 2008, issue of *Physical Review Letters.*

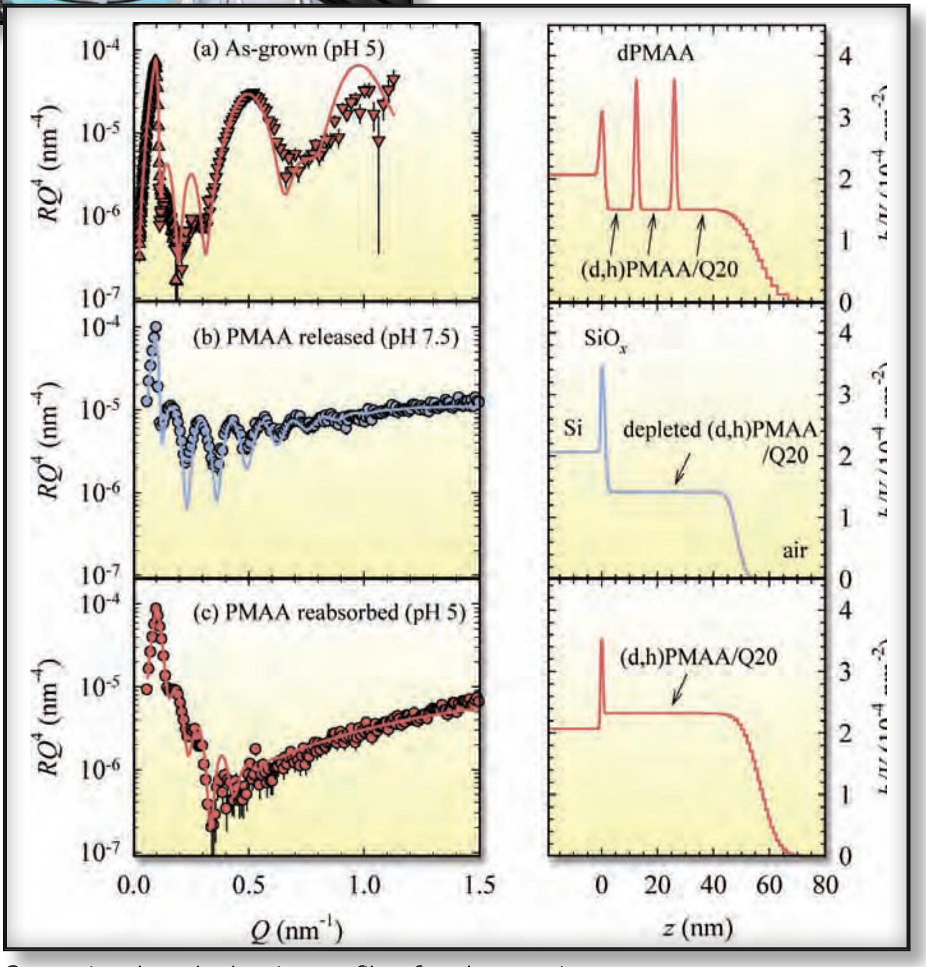
PEM coatings can be prepared simply by immersing a substrate—such as a silicon wafer, glass slide, or plastic sheet—alternately in positively and then negatively charged polyelectrolyte solutions. Weak PEM coatings respond to pH variation via an induced accumulation of excess charge within them. Consider that a molecule, or a functional group within a molecule, may lose or gain a proton when the molecule is placed in solution. The exact probability of this happening depends on the equilibrium constant for that reaction (the ratio of reactants to product) and the pH of the solution. If the pH of the solution changes while a weak polyacid or a polybase component of the multilayer coating is near its equilibrium constant, positive or negative charge is created within the PEM. This charge can be used to control the PEM, for example, to bind and release dyes or drugs or to fabricate novel, metal-containing inorganic nanocomposite materials.

As a result of pH-induced electrostatic stress within the coating, PEM coatings swell and change shape in a discontinuous, or stepwise, manner. The pH-induced variation of charge within PEM coatings also underlies the use of such coatings to control electroosmotic flow in microchannels (electroosmotic flow is a flow of ions in a solution through very narrow channels, caused by applying a voltage across the channels). Porous coatings can be produced from PEMs by varying the ionic strength and pH of the solution environment to which they are exposed. Recently, environmentally triggered changes in the morphologies of PEMs were used to produce coatings with controlled porosity for antireflection coatings.

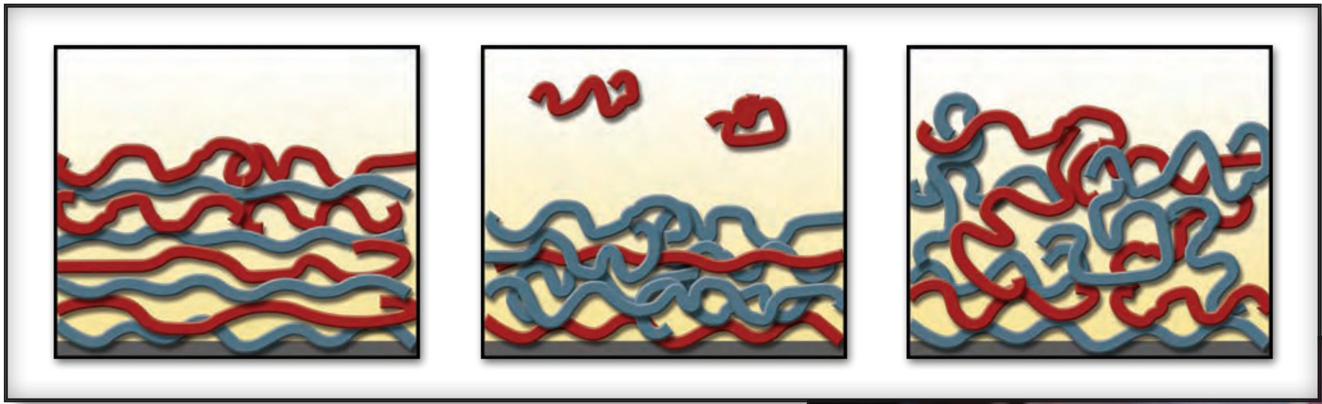
Most other studies have considered situations in which pH variations do not result in the removal of material from the coatings, and the coatings remain compositionally stable. This research presents a different scenario in which coatings respond to pH variations by changing composition. The effort addresses the mechanism by which macromolecules in PEM coatings are released and reabsorbed in response to pH changes, with the emphasis on changes in the composition of the coating. Neutron reflectometry is used, which is the method of choice for elucidating the structure and function of such multilayer coatings.

One question the researchers are exploring is whether the polymer chains released by changes in pH are reabsorbed by the coating when the pH is returned to the initial value used during the self-assembly of the coating. The experiments show that the coating reabsorbs a large fraction of the polyacid released at high pH when the pH is lowered to its initial value. However, the amount of PMAA (polymethacrylic acid) reabsorbed is 20% smaller than the amount released when the pH changes. This incomplete reversibility is likely a result of sluggish kinetics due to the atomic reorganization required within the coating to accommodate the absorption of the polymer component.

Liquids Reflectometer.



Scattering length density profiles for dry coatings.



Visualization representing neutron reflectivity data obtained experimentally for dry coatings.

Emptying the Langmuir trough.

Finally, scientists want to know whether the pH-triggered release of polymer chains affects the overall multilayer coating structure. The model coating consisted of 20 bilayers of PMAA and poly-4 vinyl-pyridine (Q20) modified so that 20% of the monomers are positively charged in solution. Every fifth PMAA layer was deuterated (i.e., the hydrogen atoms were replaced by deuterium atoms to tailor the scattering contrast). Three samples were deposited under identical conditions and then dried for neutron measurements in air using the SNS Liquids Reflectometer and the NG-7 instrument at the National Institute of Standards and Technology. All three samples were deposited on silicon substrates with 1 to 2 nm thick native oxide layers.

The data show that the regular multilayer structure completely disappears after a pH-induced release of PMAA. An absence of diffraction peaks in the reflectivity profile reveals complete mixing of the Q20 and PMAA layers, and the reduced thickness of the polymer layer implies that 38% of the PMAA originally present in the as-deposited coating is released. After the pH returns to its original value of 5, the coating reabsorbs all of the PMAA. The constant scattering-length-density profile of the coating after reabsorption implies that the PMAA is distributed uniformly; and the coating recovers its original thickness, implying that all of the PMAA is reabsorbed from solution. The reabsorbed material does not reconstitute the original arrangement of deuterated and protonated layers, so we cannot be certain of the organization of the reabsorbed layers. Most likely they form lamellar domains (thin plates) distributed randomly on the surface.

Both as-deposited and reabsorbed coatings exhibit rough surfaces; the released coating has a much smoother surface. The change from rough as-deposited surface, to smooth released surface, back to rough reabsorbed surface implies that surface roughness is controlled by electrostatic interactions intrinsic to the polymers themselves, rather than being irreversible surface damage.

Eugenia Kharlampieva, John F. Ankner, Michael Rubinstein, and Svetlana A. Sukhishvili, "pH-Induced Release of Polyanions from Multilayer Films," *Physical Review Letters* **85** (March 25, 2008).

Contact: John Ankner (anknerjf@ornl.gov)

Dynamics of Molecules Tethered to the Pore Surface of Porous Silica

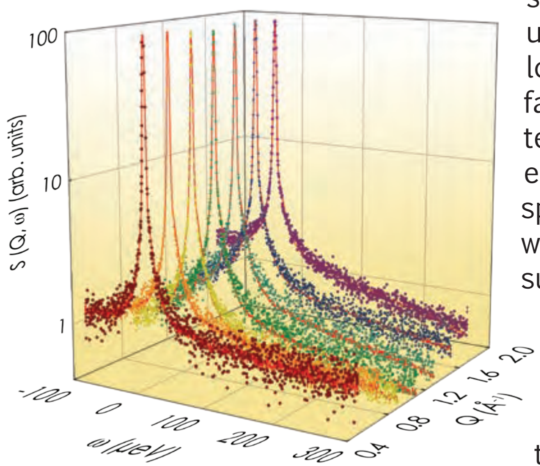
Inside the backscattering tank you can see the analyzer crystals (hexagonal Si(111) wafers)–the "heart" of BASIS. Pictured is BASIS scientific associate Stephanie Hammons.

The interactions and transformations of organic molecules in the vicinity of solid interfaces form the foundation of many key technologies and fields of scientific inquiry, including catalysis, chemical sensing, and chemical separations. Investigation of the structure and dynamics at the organic-inorganic interface on the nanoscale is required to understand the physical basis of observable macroscopic phenomena such as reaction kinetics and product selectivity. A previous study reported the impact of pore confinement on both reaction kinetics and product selectivity during pyrolysis (heating in the absence of oxygen) for molecules of 1,3-diphenylpropane (DPP) immobilized by grafting to the interior pore surface of a porous silica, MCM-41. The focus of this study was to determine the influence of hydrogen bonding on molecular motion at this interface by comparing the dynamics of DPP and of phenethyl phenyl ether (PPE), in which one of the methylenes of DPP has been replaced by oxygen.

The near-backscattering spectrometer, BASIS, at SNS was used to measure the quasielastic neutron scattering from samples of DPP and PPE tethered to the interior pore surface of MCM-41. The research was conducted by a team consisting of A. T. Ruffin of Fisk; M. K. Kidder, A. C. Buchanan, Phil Britt, and Ken Herwig of ORNL; and M. Zamponi of Institut für Festkörperforschung in Germany. Quasielastic neutron scattering is uniquely capable of simultaneously probing both the length and time scales of molecular motion. BASIS provides an unprecedented dynamic range of time scales that can be investigated from $<10^{-12}$ s to approximately 10^{-9} s. The samples were prepared and characterized in the Chemical Sciences Division at ORNL. Both samples were prepared on MCM-41 having pore diameters of 2.8 nm and surface areas of 913 m^2/g. The grafting density of the DPP sample was 0.84 molecules/nm^2, and that of the PPE sample was 1.17 molecules/nm^2. PPE-3 indicates that the location of the O-atom is farthest from the tether point. The samples were measured over a range of temperatures from 50 to 370 K.

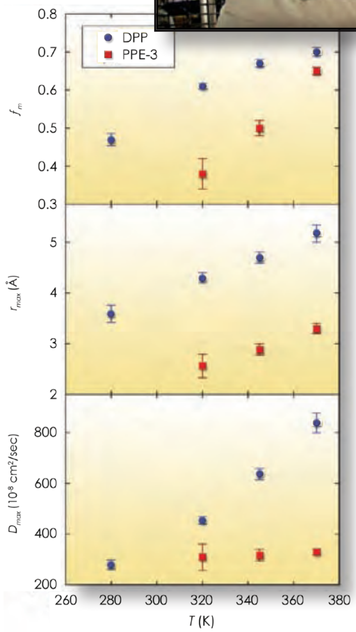
The figure at right shows the spectra collected on BASIS for the DPP sample at a temperature of 370 K. The red solid lines are fits to the data for a model of a single Lorentzian line shape, along with an elastic response, both convoluted with the resolution function of the instrument. As is typical, the resolution function was determined from a low-T (~50 K) measurement where all diffusive motions were frozen out. A sloping background was also included in the fits. The half-width at half-maximum of the Lorentzian component, Γ, clearly tends toward a finite value at momentum transfer, Q = 0, indicating the confined nature of the motion. As the molecules remain attached to the surface at all temperatures investigated in this study, they can explore only a restricted spatial volume.

In order to provide a physical context for a more quantitative description, a model previously employed to describe the motion of phospholipid tails and the alkyl chains of a liquid crystalline phase of dicopper tetrapalmitate was adapted for use here. In this model, each of the hydrogen atoms along the molecule backbone or alkyl chain is assumed to diffuse randomly, exploring the volume of a sphere of radius *r*. An analytic form for the dynamic structure factor, *S(Q,ω)* where ω is the energy transfer, is well known. In this adaptation, the radius of the sphere was taken to vary linearly with distance of the hydrogen atom from the tether point; and the diffusion constant, *D*, was taken to vary with the cube of the relevant sphere radius. This allows atoms farther from the tether point to explore a larger spatial volume, while it is assumed that each hydrogen atom explores its sphere volume with the same time constant.



Spectra (colored circles) and fits (red solid lines) for the DPP sample at 370 K.


Ariel Ruffin, first user of BASIS, July 19, 2007.

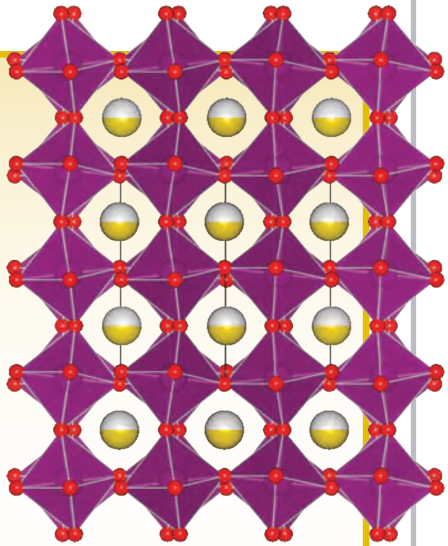


Parameters fit to the diffusion-in-a-sphere model described at right.

The extracted parameters are then the maximum sphere radius, rmax, and diffusion constant, Dmax, associated with the hydrogen atom furthest from the tether point. Additional elastic intensity associated with hydrogen atoms immobile on the maximum time scale of this measurement and the substrate (MCM-41) was included. After the contribution from the MCM-41 was removed, the fraction of mobile molecules, fm, could be determined from the ratio of the intensity associated with the sphere diffusion model to the total scattering from either the DPP or PPE-3.

The DPP molecules clearly exhibit faster dynamics and explore larger spatial volumes than their PPE-3 counterparts, as seen in the lower two panels of the figure at left. At the lower temperatures of these measurements, a larger fraction of the DPP molecules are mobile as well. It is interesting that there seems to be an asymptotic approach to unity for the DPP with a faster slope exhibited by the PPE-3 molecules. The difference in grafting density for the two samples may be responsible for some of the differing behavior illustrated in the figure; however, both of these samples are rather far from a typical saturation grafting density of ~1.7 molecules/nm², and the effects from packing density should not be dominant. The most likely explanation is that the additional hydrogen bonding interaction of the PPE-3 with either the surface or neighboring molecules results in the slower and more confined motion observed in this series of measurements.

Exploring Lattice Dynamics in CMR Manganites



Structural drawing of perovskite-type oxide, one of the crystal phases for which researchers conducted inelastic neutron scattering.

During the 1990s, some materials were discovered to have a property called "colossal magnetoresistance" (CMR) that causes them to dramatically change their level of electrical resistance under the influence of a magnetic field. Scientists were already familiar with materials capable of giant magnetoresistance, a change in resistance of 20% or so. But CMR materials can change by orders of magnitude, decreasing or increasing their resistance to electrical current by 1000 times or more as conditions change.

CMR has been observed mostly in crystalline manganese oxides called manganites. In these materials, there is a strong interplay between the magnetism, due to the electronic spins, and the electron transport. If the spins in the atoms in these materials are aligned in the same direction (as in a paramagnetic material), the resistance to electrical current is low and electrons can flow easily from atom to atom. If the spins are pointing in random directions, resistance is high (as in an antiferromagnetic material). In manganite crystals, the presence of a magnetic field at a threshold temperature can cause random spins to align and switch regions of higher resistance to low resistance—the CMR effect. The research discussed in this highlight describes how the lattice vibrations in CMR-related manganites change near the charge/orbital ordered state.

A curious set of manganese-based crystalline materials called "colossal magnetoresistance" (CMR) manganites has attracted a lot of attention from materials researchers during the past decade because of their potential for use in electronics and computing applications (e.g., magnetic memory and electronic switches). These materials exhibit an enormous decrease in electrical resistance when an external high magnetic field is applied.

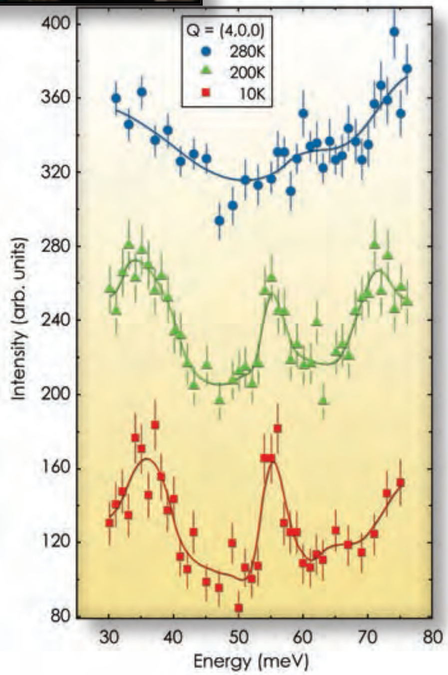
Researchers also are intrigued by the richness of the materials' physical properties, which arises from the competition of a multitude of electronic ground states that can lead to large responses to subtle changes in chemical doping (i.e., the intentional introduction of impurities), structural manipulation, or small changes in external stimuli such as magnetic fields. The fundamental physics behind these phenomena is related to the complexity arising from the interplay of electronic charge, spin, and orbital and crystal lattice degrees of freedom.

One of the ground states observed in CMR manganites is that in which the electric charges and associated electronic orbitals form an ordered three-dimensional pattern. The charge order/orbital order (CO/OO) in these materials is one of the most interesting collective phenomena in transition metal oxides. Although neutron scattering is not sensitive to the ordering of the charges or electronic orbitals in a material, it can easily detect the crystal lattice distortions associated with this ordering. In many cases, the CO/OO transition is followed by a change to an antiferromagnetic state, in which the electron spins of neighboring atoms point in alternate directions in an ordered pattern.

Because of the strong interplay between different degrees of freedom in CMR manganites, researchers want to study how the lattice dynamics is affected by the CO/OO transition in these materials. To understand the effect on the lattice dynamics, Hao Sha and Jiandi Zhang of Florida International University have used the HB-3 Triple-Axis Spectrometer at HFIR to perform inelastic neutron scattering measurements on a single crystal of $Pr_{0.65}Sr_{0.35}MnO_3$. This material exhibits a CO/OO transition at a charge and orbital ordering temperature (T_{CO}) of 230 K and an antiferromagnetic transition at TN = 140 K. (TN is Néel temperature, the temperature above which antiferromagnetic materials become disordered and cease to be antiferromagnetic.) The Mn^{3+} and Mn^{4+} ions and the *E*g orbital of Mn^{3+} form the so-called CE-type order state below T_{CO}, which serves as the precursor state for the antiferromagnetic transition.

Sha and Zhang have observed a strong temperature (T) dependence of the Jahn-Teller (JT) active phonon modes across CO/OO transition temperature T_{CO}. The figure at right presents the T-dependent phonon spectra at the Brillouin zone center (G point) measured at the HB-3 spectrometer. Three bond-bending and bond-stretching modes of the MnO_6 octahedra in the studied compound appear in the measured energy range of the spectra. These preliminary measurements reveal well-defined phonon excitations at E= 36, 58, and 74 meV in the CO/OO phase below T_{CO} = 230 K, whereas these modes are severely broadened and damped above T_{CO}.

These dramatic changes suggest that the system undergoes an order-disorder transition from dynamic JT to a static, cooperative JT effect. The JT distortion of MnO_6 octahedra above T_{CO} is averaged out by the fluctuation between Mn^{3+} and Mn^{4+} states as a result of a finite exchange hopping rate of the *E*g electrons. Below T_{CO}, the formation of CO/OO-ordered domains leads to a static or quasi-static orthorhombic distortion where the electron hopping rate is strongly suppressed. Similar behavior of Raman-active modes has been observed with Raman spectroscopy. Further experiments are under way to elucidate the nature of this coupling. A complete phonon band mapping and phonon band structure calculation are necessary to understand these observed phonons.



Top: User Hao Sha, Florida International University, conducts research at the HFIR HB-3 Triple-Axis Spectrometer. Bottom: T-dependent phonon spectra at the Brillouin zone center (Γ point) measured at the HB-3 spectrometer.

Contact:
Jiandi Zhang
(zhangj@fiu.edu)

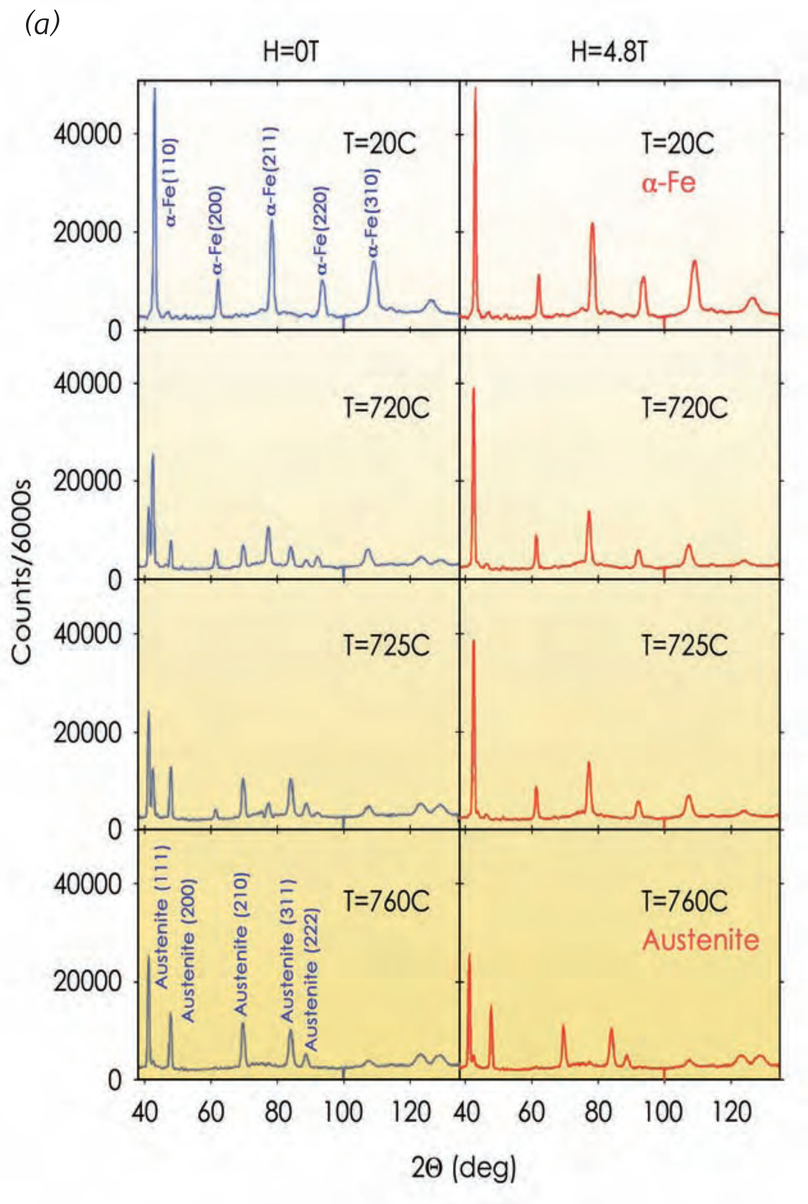
Processing Alloys Under High Magnetic Fields

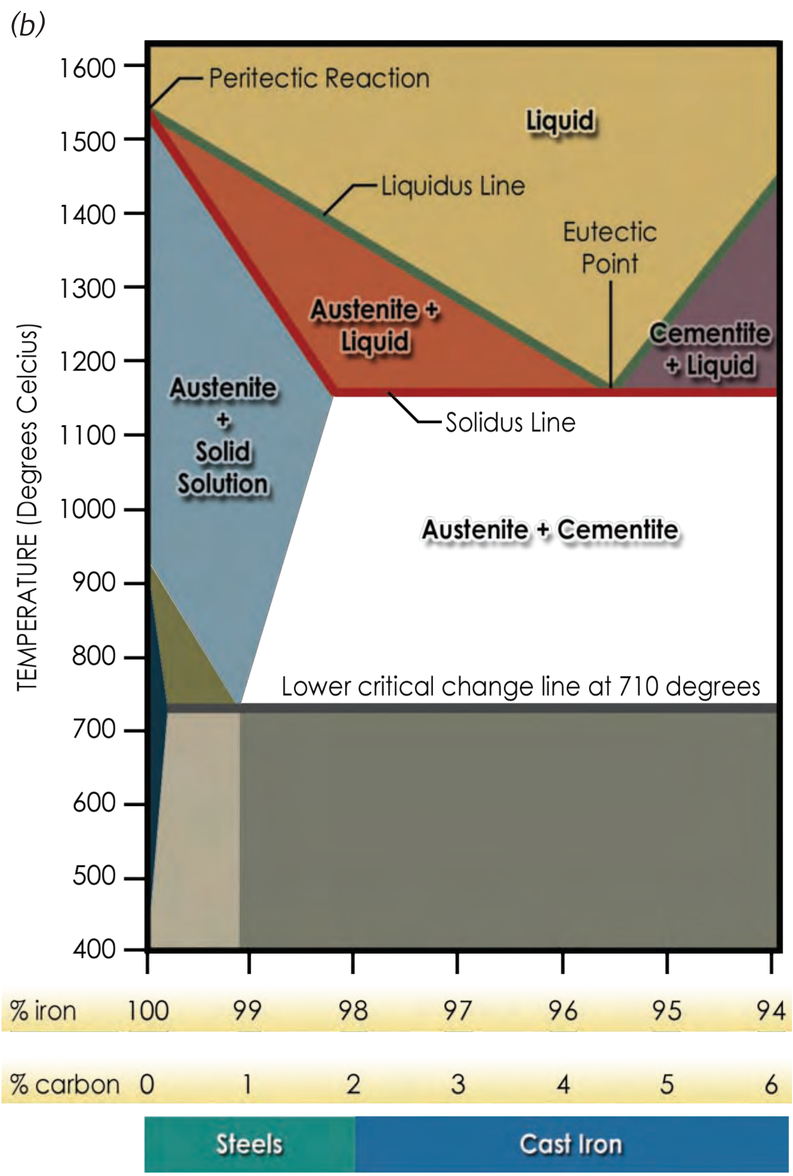
Materials scientists need to be able to see how alloys perform under the influence of high magnetic fields and high temperatures. However, previously, experiments have not been able to trace how materials react during actual simultaneous exposure to a magnetic field and high temperatures; instead, samples had to be examined after the conditions were no longer in force. In a breakthrough accomplishment for materials processing studies, researchers working at the Wide-Angle Neutron Diffractometer at HFIR designed and built a heater that can be inserted into a powerful magnet to expose samples to magnetic fields of 5 Tesla while temperatures are quickly ramped up to as high as 1200°C. The research team used in situ neutron scattering to analyze how the microstructure of an iron-carbon alloy reacted to the influence of the magnetic field and elevated temperatures, validating previous theoretical studies.

X-ray radiograph of the induction coil insert for the cryomagnet. The dark rectangle (0.5 cm wide) is the sample with thermocouple leads attached. The induction coil wraps around the sample volume.

The use of thermal-magnetic processing to manipulate alloy phase diagrams has great potential as a tool for developing the next generation of structural and functional materials. Applying a high magnetic field to an alloy alters the free energy in the material (i.e., the amount of energy that can be harnessed to do work). It also causes increases in the temperatures at which materials undergo phase transformation, or change from one state to another (i.e., solid to liquid, liquid to gas, etc.), and in the amount of a material that can be dissolved in a solvent.

A team of ORNL researchers is developing the capability to conduct neutron scattering at high magnetic fields and elevated temperatures to clarify the transformations that occur in materials when they are processed under those conditions. An interdisciplinary research team (Gerry Ludtka, Gail Mackiewicz-Ludtka, Cam Hubbard, John Wilgen, Roger Kisner, and Jaime Fernandez-Baca) is using the Wide-Angle Neutron Diffractometer (WAND) at HFIR to explore how processing alloy materials under high magnetic fields affects their behavior.





(c)

Tempera-ture (°C)	Phase(s) present for H=0	Phase(s) present for H=4.8 T
25	α	α
720	$\alpha+\gamma$	α
725	$\alpha+\gamma$	α
760	γ	γ

Demonstration of in situ WAND neutron diffraction measurements on an ultrahigh purity Fe-0.75 wt % C binary alloy using the thermal magnetic insert. (a) Neutron powder diffraction patterns recorded for different in situ conditions. (b) Equilibrium phase diagram without applied magnetic field. (c) Table of observed phases.

As a first step, the researchers designed and constructed an induction heater high-temperature insert for a 5-Tesla cryomagnet at HFIR. The insert provides a protective inert gas environment around the sample being studied and allows rapid temperature changes up to 1200°C at high magnetic fields. The insert system includes a programmable feedback temperature control system designed to meet the requirements for performing neutron scattering experiments.

Using this thermal magnetic system, the researchers used in situ, time-resolved neutron diffraction to measure the shift in equilibrium phase transformation temperatures that occur in an Fe-C binary alloy when a high magnetic field is applied at elevated temperatures. The measurements were made using WAND, which enabled several diffraction peaks to be monitored simultaneously as the microstructure evolved under the influence of the external magnetic field.

Thermal magnetic system installed at WAND.

These measurements (see page 25) showed that a 4.8-Tesla magnetic field (H) stabilizes the room-temperature α-Fe phase of Fe-C to higher temperatures (see the 720°C and 725°C plots) than does the no-magnetic-field condition. Austenite (γ-Fe) is normally the high-temperature stable phase for this Fe-C binary alloy, as shown in the 760°C plots. α-Fe and γ-Fe are two different phases in which the Fe atoms are arranged in a body-centered cubic or face-centered cubic structure, respectively.

Before this unique capability was established at HFIR, the influence of high magnetic fields on phase equilibria had to be inferred from samples that were no longer under the applied field. Such measurements do not capture the microstructural evolution of the samples during the high magnetic field exposure. The breakthrough results from the HFIR experiments validate the predictions of theoretical calculations and substantiate prior research and development efforts at ORNL in this emerging research area of extreme sample environment science and technology.

WAND is operated jointly by ORNL and the Japan Atomic Energy Agency, Tokai, Japan, as part of the US/Japan Cooperative Program on Neutron Scattering.

Contact: Jaime Fernandez-Baca (fernandezbja@ornl.gov)

Three-Dimensional Magnetic Correlations in a Multiferroic Compound

Ferromagnetism is the type of magnetism most people are familiar with—the type that makes refrigerator magnets stick. Ferromagnetism allows a material to be magnetized by exposure to a magnetic field and remain magnetized after it is removed from the field. Ferromagnetic materials are characterized by a particular type of order at the atomic level that causes the magnetic moments to line up in parallel, contributing to the magnetism. Ferroelectricity is the electrical analog to ferromagnetism in which, instead of a magnetic moment, an electric dipole moment is formed. The orientation of the dipoles of ferroelectric materials will switch direction in the presence of an electric field. Ferroelectric materials are important in applications such as energy storage devices, memory devices, telecommunication, and medical imaging systems.

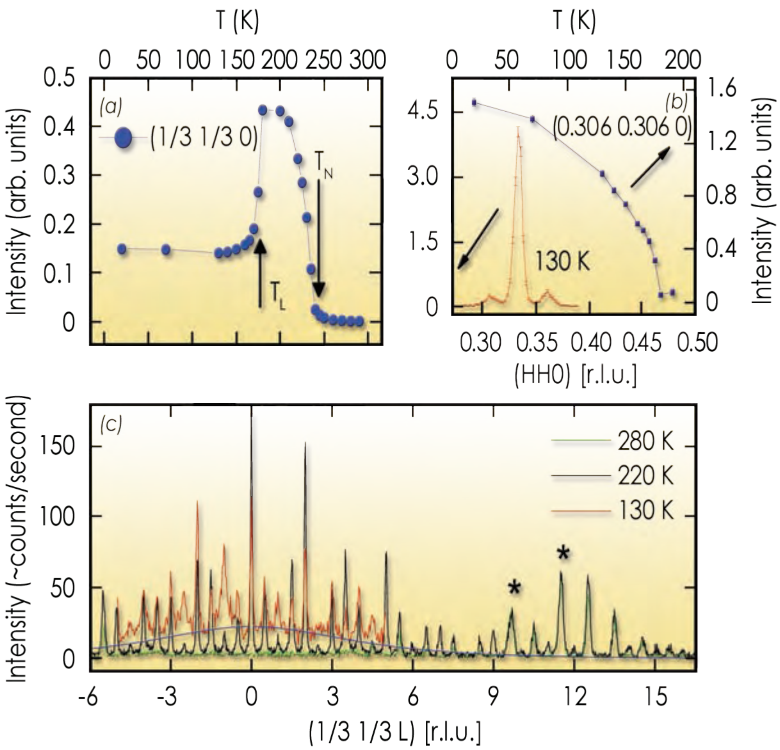
Multiferroic materials combine ferromagnetic and ferroelectric properties. Such materials are rare and not well understood. Research indicates that the magnetic properties of multiferroics can be manipulated by applying an electric field and the electrical properties changed by applying a magnetic field. Scientists are intrigued by the potential for using multiferroics to create new types of multifunctional materials and devices.

Ferromagnetism and ferroelectricity are central issues for scientists investigating collective behavior in condensed matter systems, both because of the interesting physics they present and because of the technological innovations possible from exploiting the ferromagnetic or ferroelectric properties of materials. A combination of ferromagnetism and ferroelectricity in a single device is an intriguing avenue for new hi-tech applications. Indeed, there is a surge of interest in multiferroic materials, in which ferroelectric and magnetic order coexist.

To provide insight into multiferroic behavior, scientists at ORNL and the National Research Council of Canada[1] have conducted neutron diffraction measurements of high-quality single crystals of the multiferroic material $LuFe_2O_4$ using the HB-1 Triple-Axis Spectrometer at HFIR and the N5 Triple-Axis Spectrometer at Chalk River Laboratories in Canada.

$LuFe_2O_4$ is an example of a new class of materials in which the origin of the observed ferroelectricity is subtle and complex. One of the contributing factors is the existence of so-called “charge order,” where ions of possibly different charge valences are arranged in an ordered pattern in a crystal. In $LuFe_2O_4$, for example, Fe^{2+} and Fe^{3+} ions are found in equal numbers at high temperatures but are randomly distributed. At temperatures below 320 K, the Fe^{2+} and Fe^{3+} ions settle into a charge-ordered state leading to the formation of a ferroelectric polarization. In addition, dielectric constant measurements in $LuFe_2O_4$ under applied magnetic fields show a giant magnetocapacitance at room temperature. At 240 K, magnetic order appears, along with a simultaneous anomaly in the electric polarization that indicates a coupling between the magnetic and ferroelectric degrees of freedom. To better understand the origin of the multiferroic behavior, it is essential to know the microscopic magnetic structure as a function of temperature and applied magnetic field. Neutron diffraction is the ideal technique for elucidating this structure.

In the figure at right, *(a)* shows the integrated intensity versus temperature for the (1/3 1/3 0) magnetic peak as measured by neutron diffraction. These data clearly indicate two phase transitions, one at 240 K (T_N) and another at 175 K (T_L). The changes that occur at each of these transitions can be examined by comparing scans along the (1/3 1/3 *L*) direction, (*c* above), at various temperatures (*L* is the orientation of the crystal lattice plane). The scan at 280 K shows peaks at large values of *L* with ½ integer indices. These peaks are not magnetic and in accord with previous work are attributed to the onset of 3-dimensional (3D) charge order at 320 K. Comparing the data at 220 K with those at 280 K (where there is no long-range magnetic order) shows new intensity appearing on peaks at integer and half-integer values of *L*, with the strongest enhancement at small *L* values. Such enhanced scattering at small *L* values is expected for scattering from the ordered magnetic moments of Fe^{2+} and Fe^{3+}. Thus the neutron scattering data demonstrate 3D magnetic correlations below 240 K in $LuFe_2O_4$.

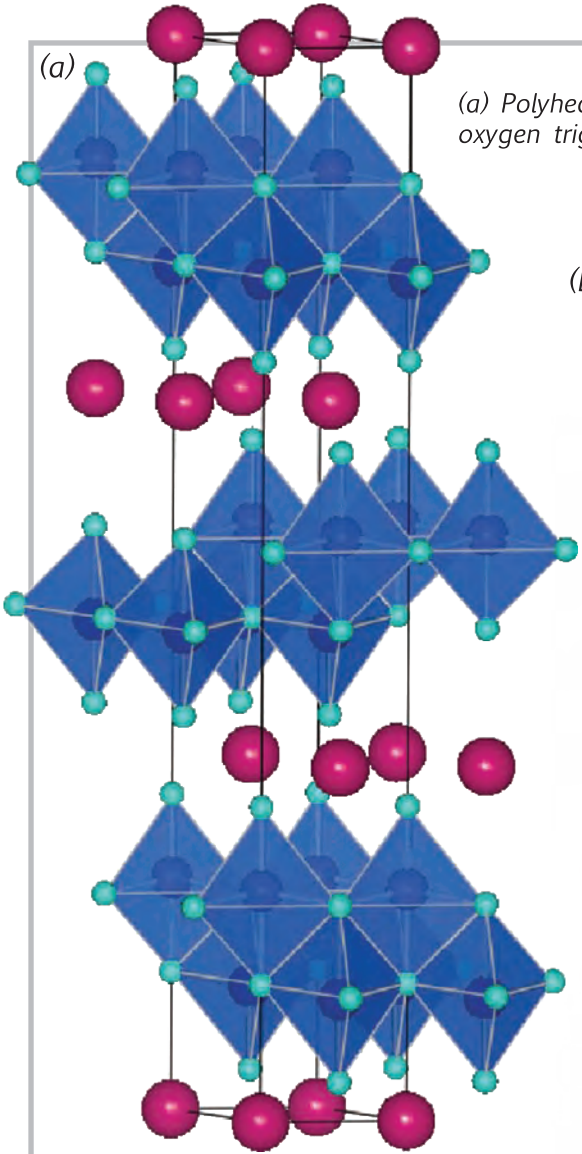


*(a) Temperature dependence of the (1/3 1/3 0) magnetic peak intensity. Two transitions are indicated at T_N (240 K) and T_L (175 K). (b) Appearance of a new set of satellite reflections below 175 K. (c) Scans along (1/3 1/3 L) at several temperatures. The blue line is proportional to the magnetic form factor. The * symbols indicate peaks contaminated by aluminum background scattering.*

A large number of reflections were measured at 220 K by scanning along the (1/3 1/3 *L*), (2/3 2/3 *L*), and (4/3 4/3 *L*) directions to constrain models for the symmetry allowed spin configurations in $LuFe_2O_4$. Based on analysis of the data, the research team concluded that the spin configuration is described by a ferrimagnetic structure with an ordering wave vector (1/3 1/3 0), with ½-integer reflections occurring as a result of the charge ordering that decorates the lattice with differing magnetic moments on Fe^{2+} and Fe^{3+} sites with a periodicity of (1/3 1/3 1/2). A model was fit to 58 observed reflections using two domain population factors, an overall scale factor, and a Debye-Waller factor yielding an overall reduced χ^2 of 1.39. The proposed magnetic structure shown on the following page has 2/3 of the spins pointing in one direction and 1/3 in the opposite direction.

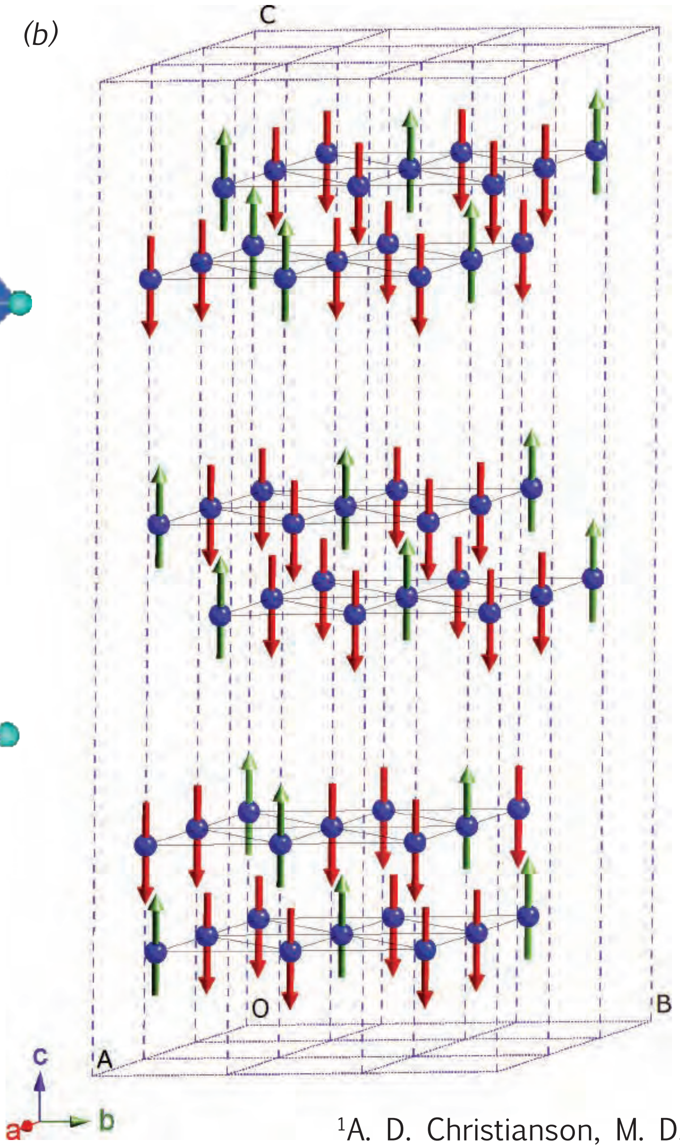
Below T_L, profound changes occur in the magnetic scattering, as shown above. In particular, a component to the scattering builds up that is extremely

(a)



(a) Polyhedral crystal structure drawing showing the slabs of edge-sharing iron oxygen trigonal bipyramids. (b) Ferrimagnetic structure determined below 240 K.

(b)



broad along (1/3 1/3 L) but sharp along (HH0). Section (*c*) of the graph also shows that below T_L, significant changes occur in the magnetic peaks along (1/3 1/3 L). The intensity along (1/3 1/3 L) for magnetic reflections changes rather dramatically, with some peaks becoming more intense (e.g., [1/3 1/3 1]) and some becoming less intense (e.g., [1/3 1/3 0]). Thus 3D magnetic correlations persist below T_L, albeit with a shorter correlation length than found for T_N. Scans along (110) have revealed the existence of a new set of satellite peaks indexed as (1/3±δ 1/3±δ 3L/2) where δ~0.027 (part *b* of graph) below T_L.

These experiments have demonstrated that $LuFe_2O_4$ has two transitions below 300 K that involve a 3D magnetically correlated structure with a finite correlation length along the c-axis. Below T_N a ferrimagnetic spin configuration is found with a magnetic propagation vector of (1/3 1/3 0) with magnetic intensity occurring at (1/3 1/3 *L*), where *L* is a half integer arising as a result of the charge ordering at 320 K.

Theoretical models that account for the 3D nature of the magnetic interactions and the sequence of magnetic phase transitions described should provide additional insight into the multiferroic behavior of $LuFe_2O_4$.

[1]A. D. Christianson, M. D. Lumsden, M. Angst, Z. Yamani, W. Tian, R. Jin, E. A. Payzant, S. E. Nagler, B. C. Sales, and D. Mandrus, "Three-dimensional magnetic correlations in multiferroic LeFe2O4," *Physical Review Letters* **100**, 107601 (2008).

Contact: Andrew Christianson
(christiansonad@ornl.gov)

Probing Crack Growth Retardation During Cyclic Loading

The aircraft industry leads the effort to understand and predict the growth of cracks caused by cyclic fatigue (on-and-off stress) in materials. Aircraft makers have developed a fail-safe design approach, by which a component is designed so that if a crack forms, it will not grow to a critical size between specified inspection intervals. If the crack growth rate characteristics of materials are known and all components are inspected regularly, a cracked component may be kept in service for an extended useful life.

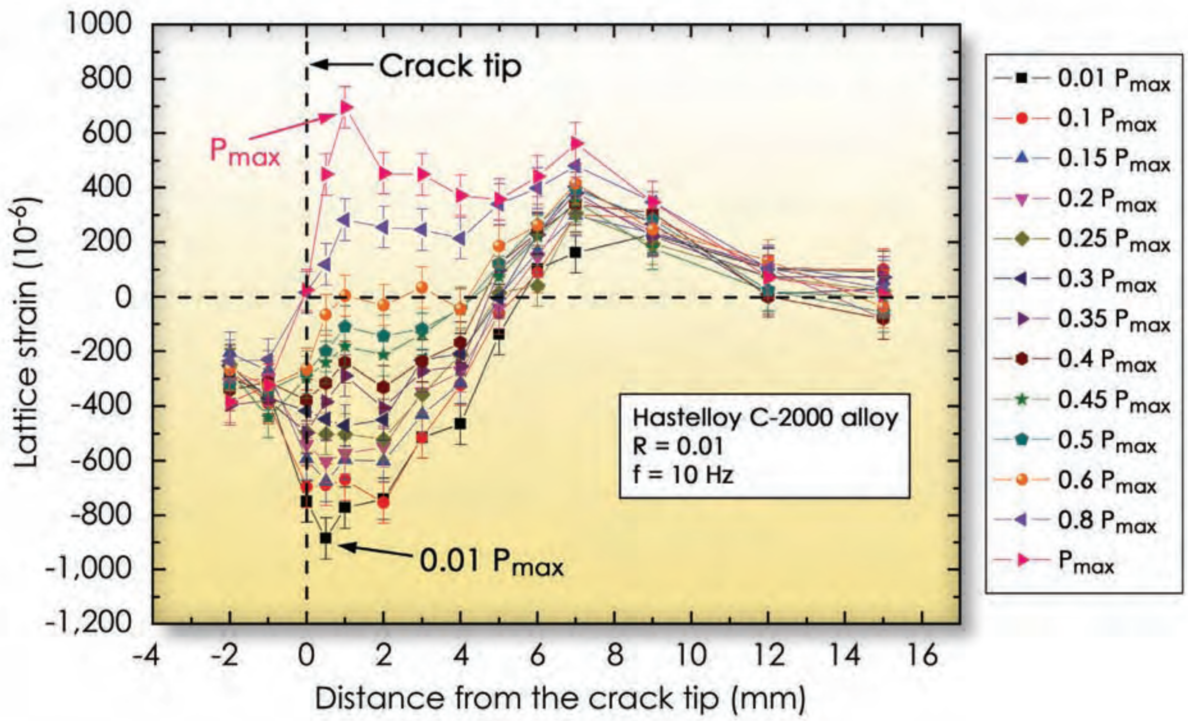
New materials with improved crack resistance can be designed once an understanding of the damage mechanisms is established. Two poorly understood issues are the *overload effect* and *crack closure behavior* in structural materials subjected to cyclic fatigue loading. Advances in fundamental understanding of the overload effect (a sudden increase in the load in the cyclic mechanical loading pattern) and the crack closure mechanism (responsible for changes in the fatigue crack growth rate) are valuable in enhancing capabilities to predict material lifetimes and improving safety models, and they help improve designs for critical applications subjected to random loading.

Ph.D. student Sooyeol Lee (University of Tennessee), a first-time user of neutron diffraction, performing the in situ loading measurements using the NRSF2 at HFIR.

A variety of crack closure measurements have been used to investigate mechanisms for retarding crack growth in structural materials. However, because of a lack of experimental capabilities for measuring strain/stress fields inside materials under applied loads, the relationship between overload

Cyclic fatigue is one of the most frequent causes of failure in structures and machinery. In cyclic fatigue, damage to a material accumulates not necessarily because of a heavy load but because of a dynamic load, one that stresses and then releases or waxes and wanes constantly over a prolonged period of time. Any type of machine, vehicle, or structure that stops and starts repeatedly or flexes constantly is subject to cyclic fatigue; aircraft are a prime example. Fatigued constituent materials become more damaged with each load cycle and eventually may wear out and fail if not repaired or replaced. A cyclic load may cause failure in a material that could withstand a heavier static load. In a material under cyclic fatigue, the damage typically begins as a crack on the surface, often at a point where the stress is high. The crack grows slightly every time the load is applied until the material finally fractures.

and crack retardation has not been quantitatively established. Using the NRSF2 Engineering Neutron Diffractometer at HFIR, a team of scientists recently used neutron diffraction to probe the crack closure phenomena after an overload during fatigue crack growth. Because neutrons penetrate deeply into the interior of a component, they enable the study of bulk crack closure behavior rather than only the surface crack closure phenomena that can be observed using strain gauges. Moreover, the NRSF2 measured the changes in internal strains in situ under the applied load using a load frame as a function of the distance from the fatigue crack tip.



Evolution of internal lattice strains when the applied load is increased right after overload during fatigue crack growth.

The internal strain evolutions were investigated while the applied load was increased near a crack tip after overload (see graph above). After a single tensile overload was imposed following a period of cyclic loading, large compressive strains were observed within ±5 mm near the crack tip. At 0.5 mm in front of the crack tip, the largest compressive strain of –880 $\mu\varepsilon$ (microstrain) was examined. As the distance from the crack tip increased, the strain changed from compressive to tensile. The maximum tensile strain was observed about 9 mm ahead of the crack tip. As the applied load increased, strains behind the crack tip did not change much, whereas strains in front of the tip evolved as the applied load increased. When $0.6P_{max}$ (60% of maximum load) was applied, the compressive strains ahead of a crack tip disappeared and became zero. This load value corresponds to the crack opening load. As the load increased from $0.6P_{max}$ to P_{max}, strain gradually increased, especially at the region in front of the crack tip. At P_{max}, the maximum tensile strain of 700 $\mu\varepsilon$ was observed 1 mm ahead of the crack tip.

From this combined in situ loading and spatially resolved strain scanning measurement, bulk internal strains were successfully measured as a function of the applied load, which allowed the researchers to determine the crack opening level at different stages of fatigue crack growth. The results will help establish the relationship between effective crack-tip driving force and crack growth rate.

Contact: Cam Hubbard (hubbardcr@ornl.gov)

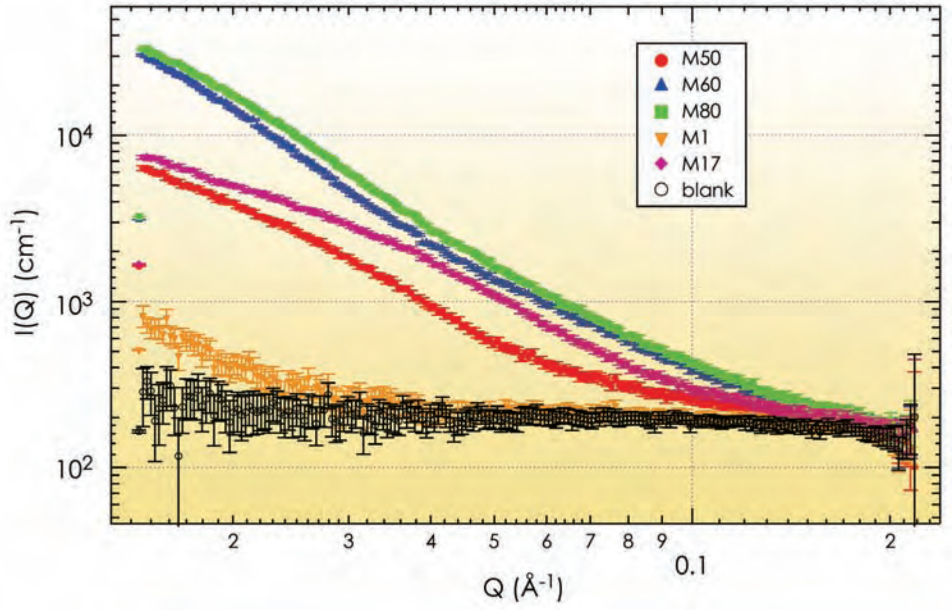
Correlating Defects with Thermal Conductivity in Crystalline Ceramics

In nonmetallic materials such as ceramics, heat is transmitted via lattice vibrations; that is, the energy from a heat source causes nearby atoms to vibrate, in turn causing other surrounding atoms to vibrate. The vibrations propagate through the lattice of atoms in quantized waves called "phonons." The thermal conductivity in a ceramic material is degraded as the phonons scatter off tiny defects or irregularities in the structure of the material. Just as rocks or other obstructions in a stream slow the flow of the water, so defects in a ceramic material slow the progress of the phonons by deflecting the waves. This process, called "phonon defect scattering," causes the thermal conductivity of ceramic materials to become highly degraded under neutron irradiation. Such degradation can have a great negative impact on the performance of some ceramics, such as those used in reactors where they are frequently bombarded with neutrons. However, a better understanding of the scattering process could help scientists tailor the thermal conductivity of thermoelectric materials to improve their performance.

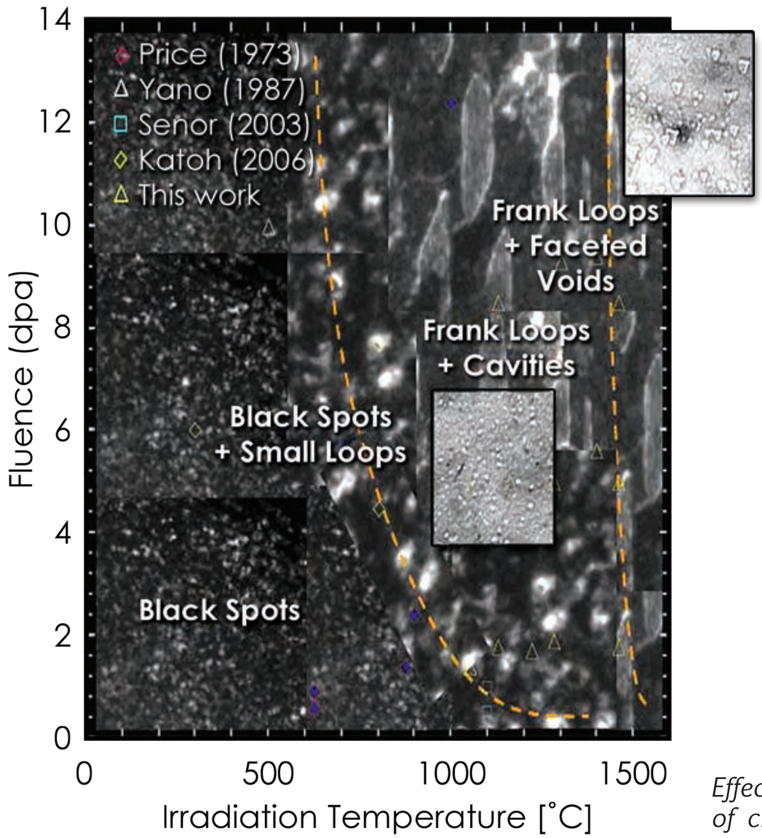
The way quantized waves of thermal energy, or phonons, bounce off defects (or scatter) in ceramic materials is important because it affects how quickly and evenly heat is transferred through the material. A theoretical understanding of the scattering process could enable materials scientists to manipulate defects in ceramics to tailor their thermal conductivity for specific applications. To date, though, researchers have not been able to experimentally validate a description of the phenomenon of phonon defect scattering in ceramics.

Recently, however, a theoretical approach was developed to quantify the strength of phonon scattering associated with each individual defect in a ceramic sample, such as vacancies, vacancy clusters, anti-site defects, and extended defects (e.g., loops and voids). Lance Snead and Ken Littrell of ORNL are leading an effort to validate this theoretical treatment through irradiation and characterization of highly pure, crystalline silicon carbide (SiC) samples. These model materials have been irradiated in the flux trap position of HFIR, and the resulting microstructure has been analyzed by high-resolution transmission electron microscopy (TEM) and HFIR's new general-purpose small-angle neutron scattering (SANS) instrument (SANS1).

The experiments show that after neutron irradiation, significant swelling of the sample material occurs, which is attributed to the temperature-dependent formation of interstitials and interstitial clusters. The result is a dramatic reduction in the thermal conductivity of the material. Because the theoretical treatment of phonon transport requires an accurate definition of the types of defects present in the material, their sizes, and their number density, these characteristics were quantified for irradiated SiC samples. The figure below gives a compilation image of the temperature and dose dependence of the microstructure of the sample as determined using high-resolution TEM. This image clearly indicates that defects larger than 3 nm include vacancy clusters, Frank loops, and dislocation networks. Although these defects are abundant, they do not come close to accounting for the amount of swelling or degradation in thermal conductivity measured; this indicates that the primary defects responsible for these property changes are less than 3 nm in size. The most likely candidates are vacancies, small vacancy clusters, or anti-site defects (e.g., a carbon atom on a silicon sub-lattice site).



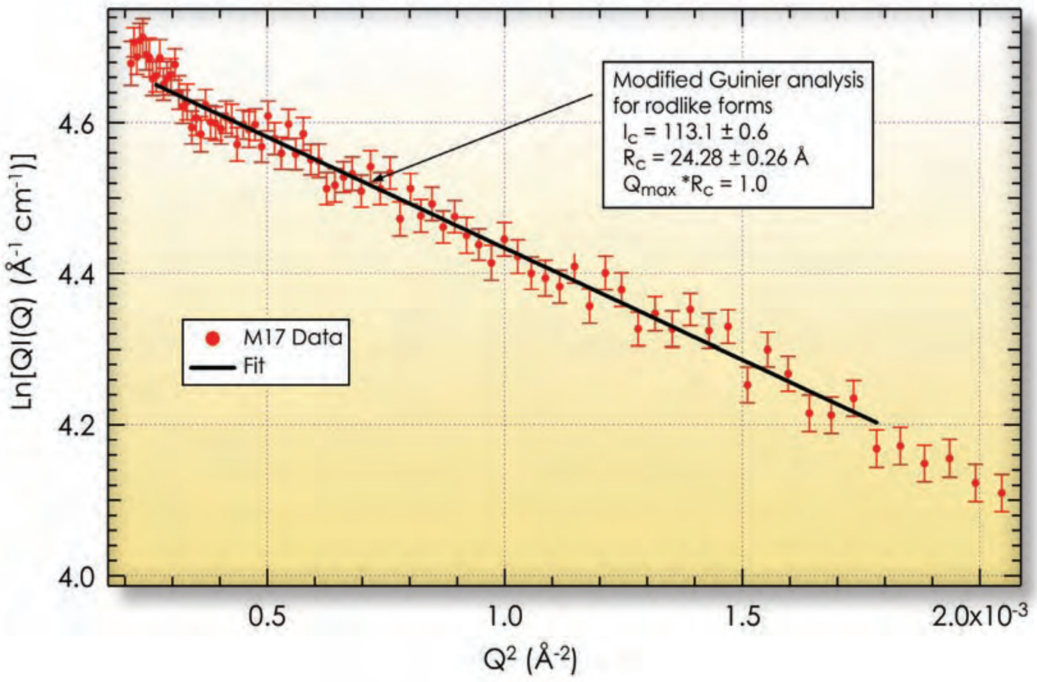
Small-angle scattering data from irradiated SiC samples. These data show structural defects increasing in size as the irradiation dose increases.

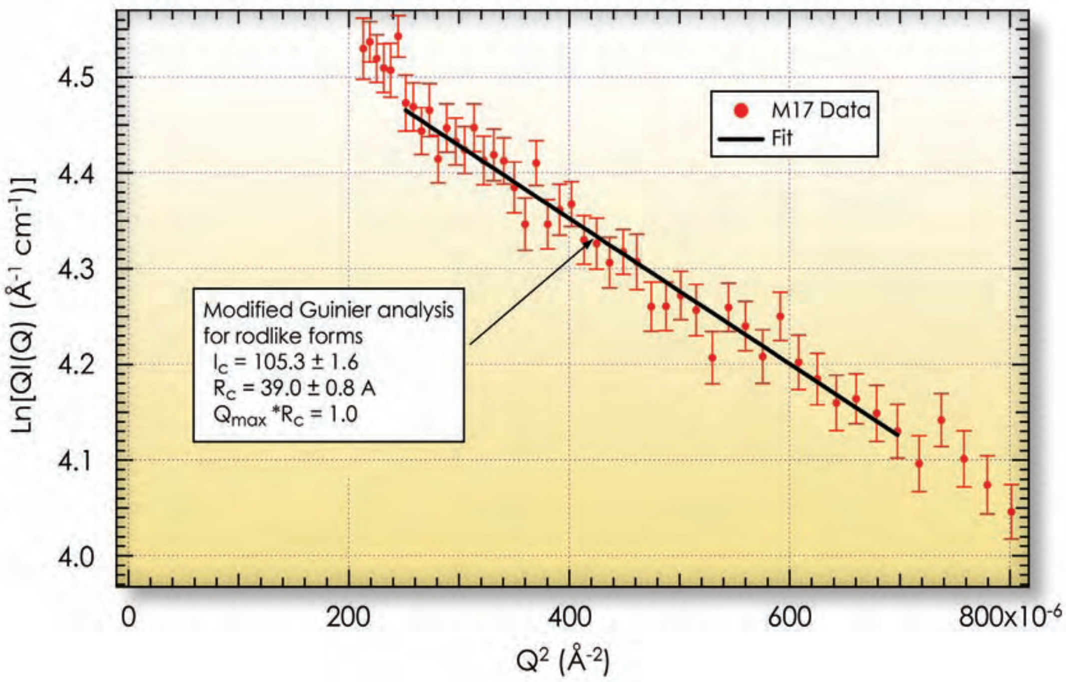


Effect of neutron irradiation on the microstructure of chemical-vapor-deposited SiC.

Characterization of the defect structure at the lower limit of TEM resolution is being carried out with SANS1. In this first step, SANS1 is being used to confirm what can be directly observed by TEM; the final objective is characterizing defects currently invisible to TEM. The measured scattering curves are shown above. The sample irradiated to the highest dose at the lowest irradiation temperature (M1, 8 displacements per atom or dpa, 1064°C,) was essentially indistinguishable from an empty holder at the length scales measured.

However, for a higher irradiation temperature at the same dose (M17, 8 dpa, 1267°C), there are hints of something large at low Q. This becomes even clearer in the sample irradiated near the highest irradiation temperature of this study (M50, 2 dpa, 1500°C). A modified Guinier analysis indicates the presence of rodlike structures (see page 34). This result sup-



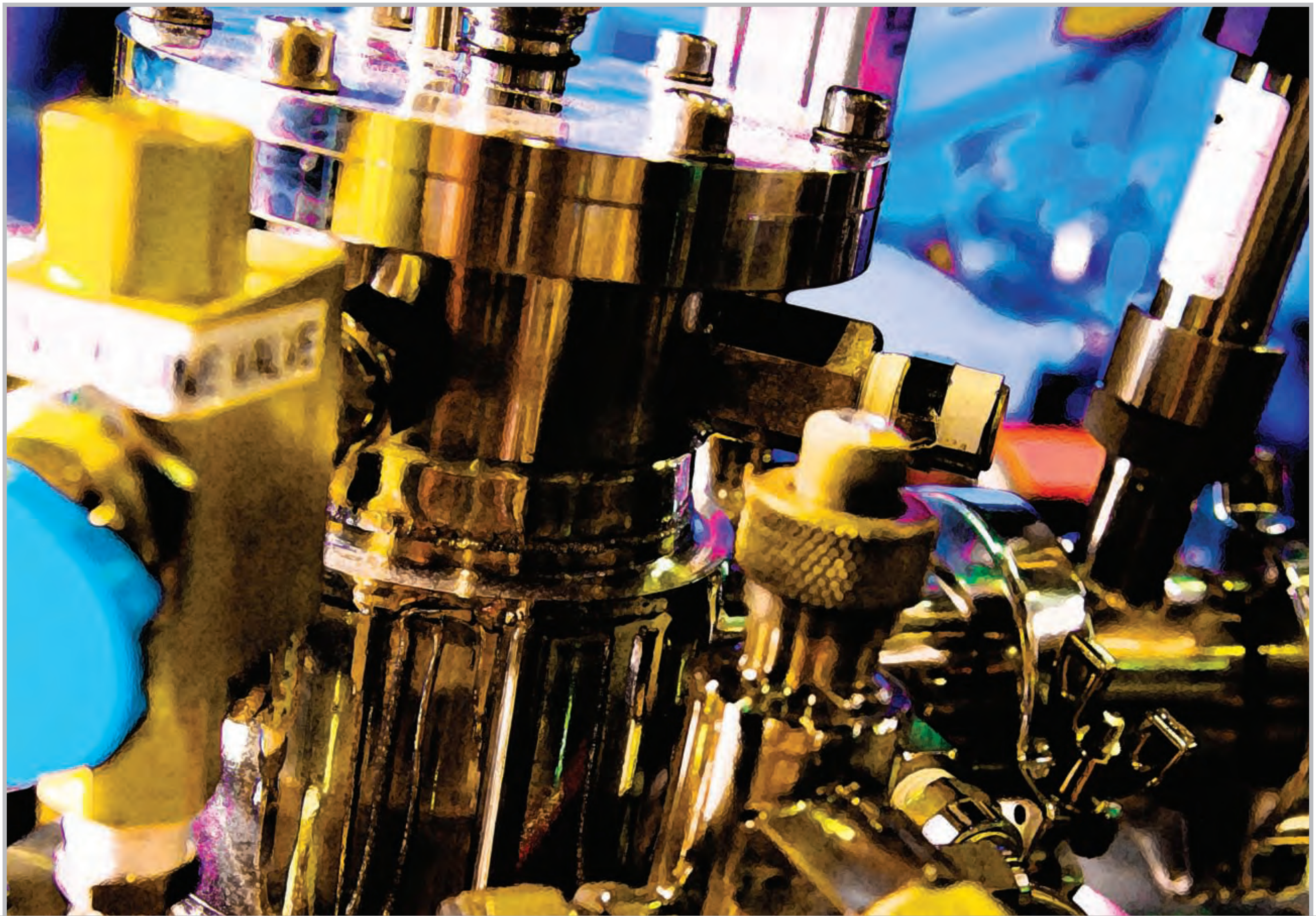


Modified Guinier analysis for rodlike forms showing the clear presence of extended, rodlike structures in the M17 and M50 samples.

ports the TEM findings for this microstructure. The M60 and M80 samples (both irradiated at 1500°C to 5 and 8 dpa, respectively) scatter strongly with a signal characteristic of very large objects, supporting the evidence for decreased density and the growth of tetragonal voids in the observed microstructure.

In this initial work, we have gained confidence that SANS1 can be used to quantify the defects responsible for phonon scattering in ceramic materials, at least at the lower end of resolution for TEM observation. The next hurdle is to apply this technique to those defects we cannot currently image, which is also the scale at which most of the phonon scattering defects exist. With the final description of these small vacancy complexes in irradiated SiC, the phonon scattering from all defects can be accounted for and the general theory for phonon transport in defected ceramics validated.

Contact: Ken Littrell
(littrellkc@ornl.gov)

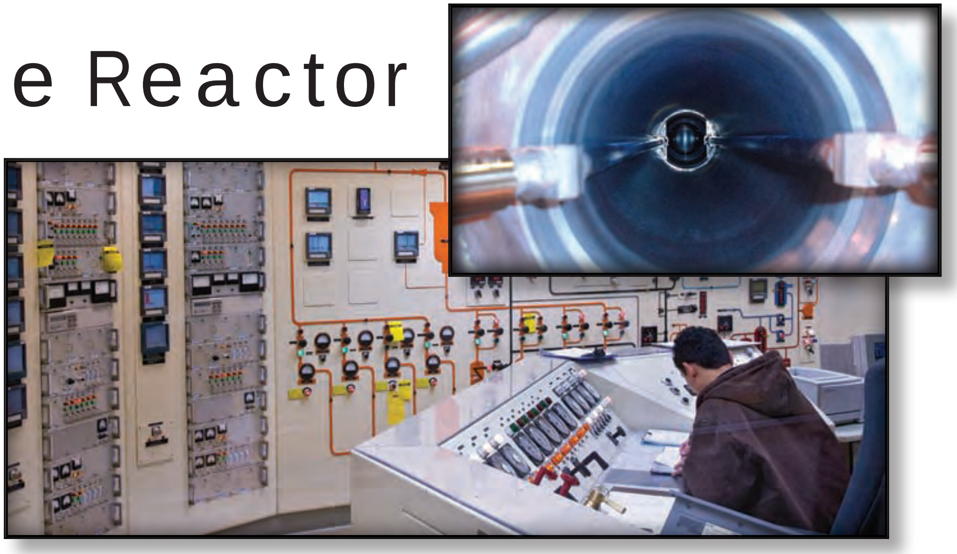


Operations

For neutron sciences at ORNL, "operations" was the buzz word for 2007. Although a great deal of design, installation, and testing was and is still taking place, successful operation of HFIR and SNS was the focus. This banner year included reactor, accelerator, and instrument performance that exceeded expectations in many cases. Another step forward was the beginning of integration with other ORNL facilities, expanding the resources readily available to users. Most important, 2007 was a safe year thanks to dedicated staff and effective programs that keep safety at the forefront of all neutron science work.

High Flux Isotope Reactor

In 2007, HFIR completed the most dramatic transformation in its 40-year history. During a shutdown of more than a year, the facility was refurbished and a number of new instruments were installed, as well as a cold neutron source. The reactor was restarted in mid-May; it attained its full power of 85 MW within a couple of days, and experiments resumed within a week.



Top: View of the cold source moderator vessel looking up into the beam tube during fabrication. Bottom: HFIR control room.

Improvements and upgrades to HFIR include an overhaul of the reactor structure for reliable, sustained operation; significant upgrading of the eight thermal-neutron spectrometers in the beam room; new computer system controls; installation of the liquid hydrogen cold source; and a new cold neutron guide hall. The upgraded HFIR will eventually house 15 instruments, including 7 for research using cold neutrons.

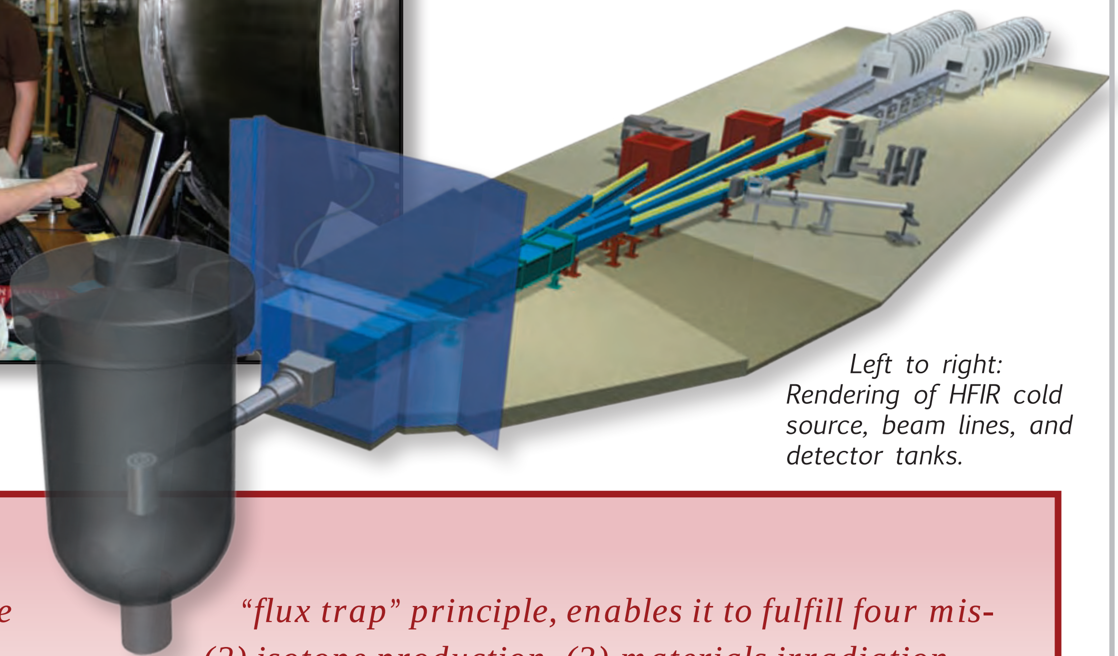
The cold source was tested successfully during the first few months of 2007. Testing verified the design assumptions and demonstrated that the cold source would support safe, reliable operation of the reactor. Since the initial startup with the cold source installed, both the reactor and cold source have operated safely and reliably for five fuel cycles.

Completion of all the testing was followed by a highly productive period of reactor operation. From May through December, HFIR operated for 9169.6 MW-d at its 85-MW full-power rating with the exception of a few hours at lower power to perform the HB-4 brightness measurements. This provided valuable neutron scattering instrument commissioning time and 1178 facility operating hours for users. During this time, 72 users performed 35 neutron scattering experiments. In addition to neutron scattering work, HFIR staff performed isotope production, neutron activation analysis, and materials irradiation experiments for a variety of customers.

An aggressive operating schedule is planned for 2008, with a tentative schedule of 140 operating days. This schedule assumes six operating cycles during the calendar year. Steady-state operation of HFIR will eventually provide neutron beams 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)

Greg Smith, acting deputy director for the Neutron Scattering Science Division, explains HFIR cold source operations to HFIR Family Day visitors.



Left to right: Rendering of HFIR cold source, beam lines, and detector tanks.

HFIR Design and Operation

The HFIR design, based on the "flux trap" principle, enables it to fulfill four missions: (1) neutron scattering, (2) isotope production, (3) materials irradiation, and (4) neutron activation. The reactor has a fuel region surrounding an unfueled moderating region or "island." High-energy neutrons are released from the fuel and then cooled and slowed in the island. The design produces a region with a very high (2.0×10^{15} neutrons/cm^2•s) flux of thermal (room-temperature) neutrons at the center of the island.

The neutrons "trapped" in the island are used to produce isotopes for medical, research, and industrial uses. Other neutrons are guided through beam lines into research instruments outside the reactor shielding, where neutron scattering studies are conducted. Holes in the reflector outside the fuel region allow researchers to irradiate samples of materials that are then retrieved and analyzed to determine the effects of the radiation. The beryllium reflector contains numerous experimental facilities with thermal-neutron fluxes of up to 1.0×10^{15} neutrons/cm^2•s.

Spallation Neutron Source

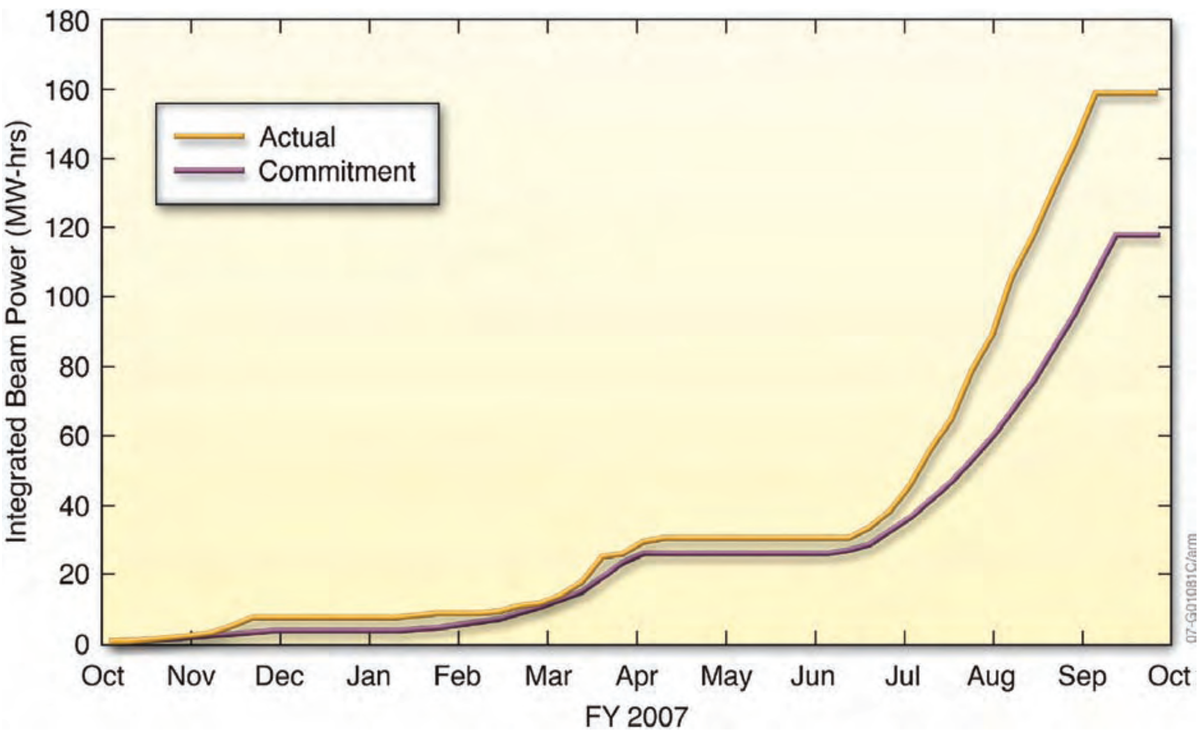
This was the first full year of operation for SNS. A positive accelerator readiness review in April permitted an increase in the administrative beam power limit from 100 kW to 2 MW. Since then, power levels, intensity, neutron production, and reliability have all steadily increased. By the end of 2007, SNS had achieved

- Continuous operation at 183 kW
- A record number of protons per pulse: 1.1×10^{14}
- A 60-Hz beam to target at ~70 kW
- 160 MWh of beam to target
- Accelerator availability of 79%
- 1500 neutron production hours

In regard to instrumentation, the Wide Angular-Range Chopper Spectrometer came online in 2007, joining the already operating Magnetism and Liquids Reflectometers and the Backscattering Spectrometer. The first user experiments were completed in August and September. Eventually SNS will make available to researchers a suite of up to 25 best-in-class instruments, which will allow measurements of greater sensitivity, higher speed, higher resolution, and in more complex sample environments than ever before.

A vibrant and engaged neutron scattering user community is vital to the success and scientific productivity of both HFIR and SNS. The user community was engaged from the beginning of the SNS project in the prioritization and selection of the neutron scattering instrument suite and is now beginning to use the instruments. As SNS completes more of

This graph shows the increase in integrated beam power delivered during FY 2007 versus the commitment from SNS. For the next year, plans are to operate for 4000 hours, reach an operating power of 750 kW, and produce neutrons for 2700 hours. In addition, machine availability is expected to increase to about 83%.



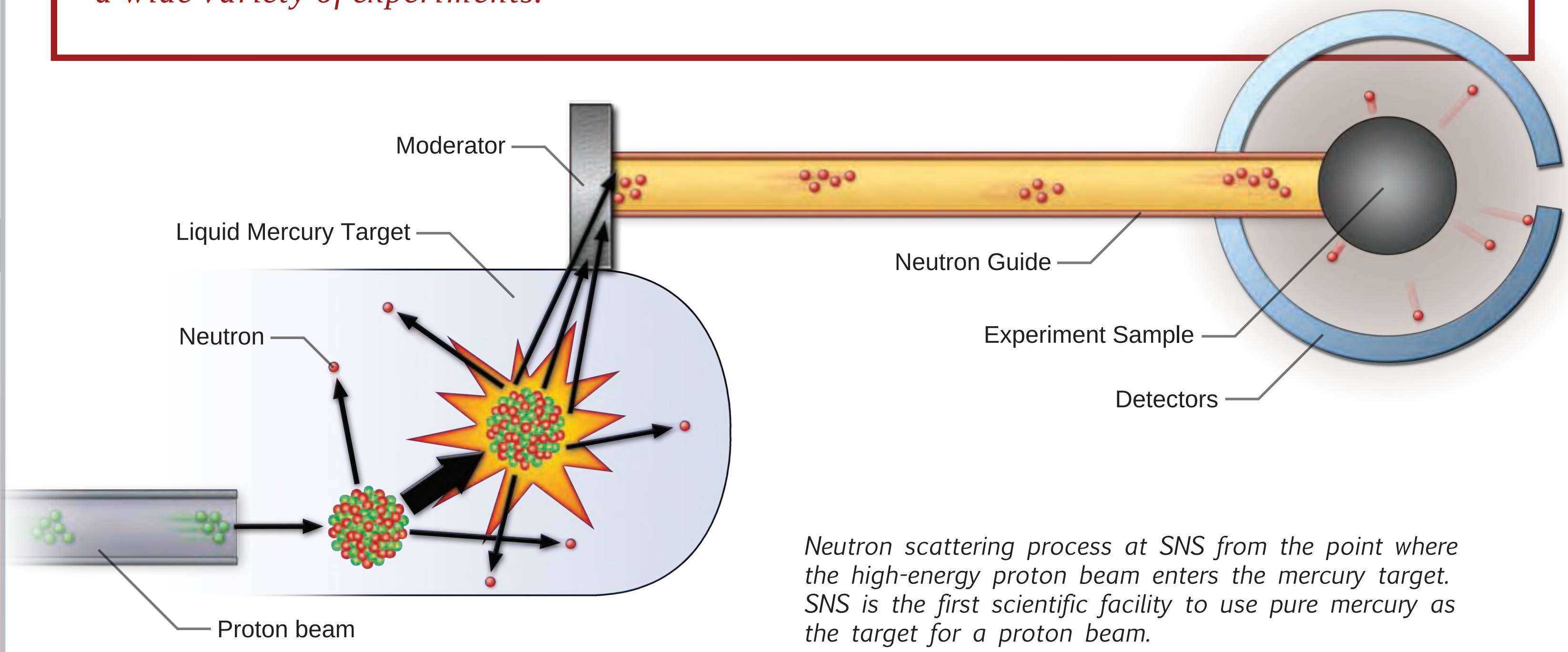
Actual versus committed integrated beam power performance at SNS during FY 2007.

these instruments and adds more operating hours over the next several years, it is anticipated that 1000 to 2000 researchers per year from all areas of science and industry will use these facilities.

SNS Design and Operation

The SNS process begins with injecting negatively charged hydrogen ions into a linear accelerator (linac), which accelerates them to very high energies (a billion electron volts, or 1 GeV). The ions pass through a foil that strips off their electrons and converts the electrons to protons. The protons accumulate in a ring, from which brief (a millionth of a second), powerful pulses of protons are released 60 times a second to strike a target containing liquid mercury. As the protons strike the target, pulses of neutrons are ejected or "spalled" from the mercury nuclei.

The neutrons shooting from the target are too high in energy to be usable as is. They are slowed down, or moderated, by passing them through vessels of water (to produce room-temperature or "thermal" neutrons) or liquid hydrogen at 20 K (for cold neutrons). The neutrons are then guided through a set of beam lines to specialized instruments that use the neutrons in a wide variety of experiments.



Neutron scattering process at SNS from the point where the high-energy proton beam enters the mercury target. SNS is the first scientific facility to use pure mercury as the target for a proton beam.

Facility Integration

Research capabilities at HFIR and SNS are enhanced by the proximity of other ORNL user facilities, most with the same access and training requirements. An important goal for Neutron Sciences is improving integration between the facilities, making it easier for users to access the support they need. Major user facilities at ORNL include

- Center for Structural Molecular Biology (CSMB)
- 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, which supports and develops user programs in the neutron bio-sciences. Small-angle neutron scattering (SANS) provides information on the global shape, form, and internal structure of complex biological systems in solution and makes it possible to study their response to environmental changes, chemical cofactors, and ligands important to their physiological function. CSMB develops technologies and methodologies for the structural molecular biology research community and develops computational tools to reduce, analyze, model, and interpret SANS data.

CSMB postdoc Kevin Weiss uses a laboratory scale fermentor to culture organisms in isotopically labeled growth media to produce biomolecules for neutron scattering studies.

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

CSMB has established a Bio-Deuteration Laboratory for in vivo production of hydrogen/deuterium–labeled bio-macromolecules for research at HFIR and SNS. The laboratory provides facilities and expertise for cloning, protein expression, purification, and characterization of deuterium-labeled biological macromolecules. Users can design and produce proteins, complexes, and macromolecular assemblies optimized for neutron scattering; and the data can be used to construct biologically meaningful models of protein complexes, assemblies, and hierarchical structures.

Current research efforts at CSMB include modeling the structure of the Putidaredoxin Reductase (Pdr) and Putidaredoxin (Pdx) complex, visualizing morphology changes in biomass during pretreatment for conversion to biofuel, investigating peptides that have the protein context of huntington exon 1, associated with Huntington's disease, and elucidating the impact of the water-miscible ionic liquid [bmim]Cl on the protein fold in aqueous solutions.

Contact: Dean Myles (mylesda@ornl.gov)

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

CNMS is a research facility for nanoscale science and technology. Housed in an 80,000-ft^2 building adjacent to SNS, CNMS allows users access to a complete suite of unique capabilities for studying nanoscale materials and assemblies. CNMS integrates nanoscale science with three other research areas: neutron science at SNS and HFIR; synthesis science facilitated by a new Nanofabrication Research

Deanna Pickel, a polymer chemist at CNMS, prepares a glass reactor for an anionic polymerization experiment that requires high purity and high-vacuum conditions to create well-defined materials. Many of these materials are already being incorporated into experiments at ORNL neutron facilities.

Laboratory and other labs; and theory, modeling, and simulation using the Nanomaterials Theory Institute and access to high-performance computers at ORNL's NCCS and the National Energy Research Supercomputing Center at Lawrence Berkeley National Laboratory.

Contact: Linda Horton (hortonll@ornl.gov)

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

NCCS hosts the Cray XT4 "Jaguar" supercomputer, which was capable of more than 119 trillion calculations per second (119 teraflops) at the end of 2007 and was being upgraded to 250+ teraflops. A petaflops supercomputer, capable of a quadrillion calculations per second, is to be installed in 2008. NCCS is also home to several smaller supercomputers. Allocations for large supercomputing projects (i.e., millions of processor-hours) are awarded through a proposal process that issues a yearly call for proposals. Smaller allocations are occasionally awarded to "director's discretion" projects.

Contact: Jim Hack (jhack@ornl.gov)

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

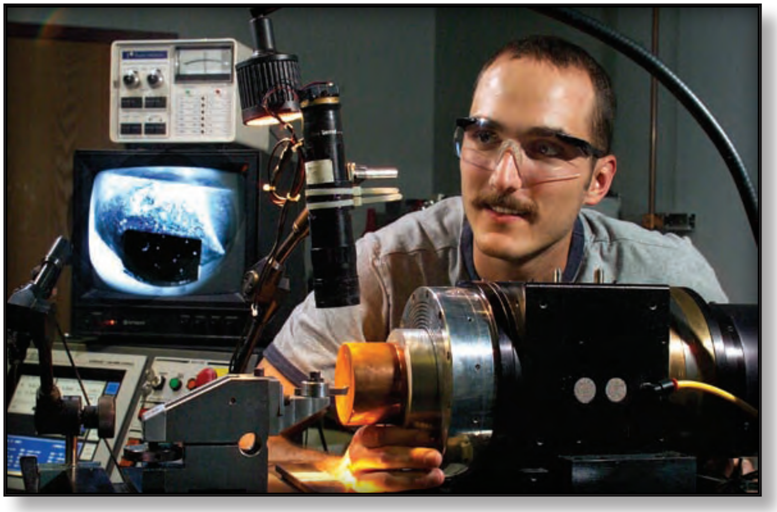
SHaRE provides access to a suite of advanced instruments and expert staff scientists for the micrometer-to-nanometer-scale characterization of materials in several focused research areas: transmission and scanning electron microscopy, atom probe tomography, X-ray photoelectron spectrometry, and dual-beam focused ion beam and ultramicrotomy specimen preparation and support. Researchers submit research proposals for review and approval to gain access to SHaRE's characterization facilities. Proposals are accepted at any time.

Contact: Carolyn Wells (wellscb@ornl.gov)

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

HTML helps solve materials problems that limit the efficiency and reliability of automotive systems. Six user centers are available to researchers. The centers are staffed by experts in the materials sciences and are equipped with instruments that can characterize the structural, chemical, physical, and mechanical properties of materials at the nanoscale and microscale over a wide range of temperatures and pressures. Research capabilities include microstructural analysis; X-ray and neutron diffraction; residual stress analysis; thermophysical properties studies; mechanical characterization; and analysis, thermography, and tribology.

Contact: Edgar Lara-Curzio (laracurzioe@ornl.gov)



Jason Braden demonstrates use of a diamond tool to turn a concave mirror onto a piece of copper.

Safety

Safety is critical to the success of the Neutron Sciences work at ORNL. Efficient operation and safety are inextricably linked and are an integral part of every individual's performance plan. This total safety awareness led to the formation of the Integrated Safety Management Program, the cornerstone of our operations. Our primary goal is to operate the best neutron facilities in the world. Achieving this goal means involving staff in all levels of work, from planning through post-task analyses, and incorporating the best ideas from those with the most knowledge of the hazards.

Saad Elorfi, Sample Environment Group, checks one of the main vacuum valves on the pumping station for the Backscattering Spectrometer to ensure that the systems are functioning properly.

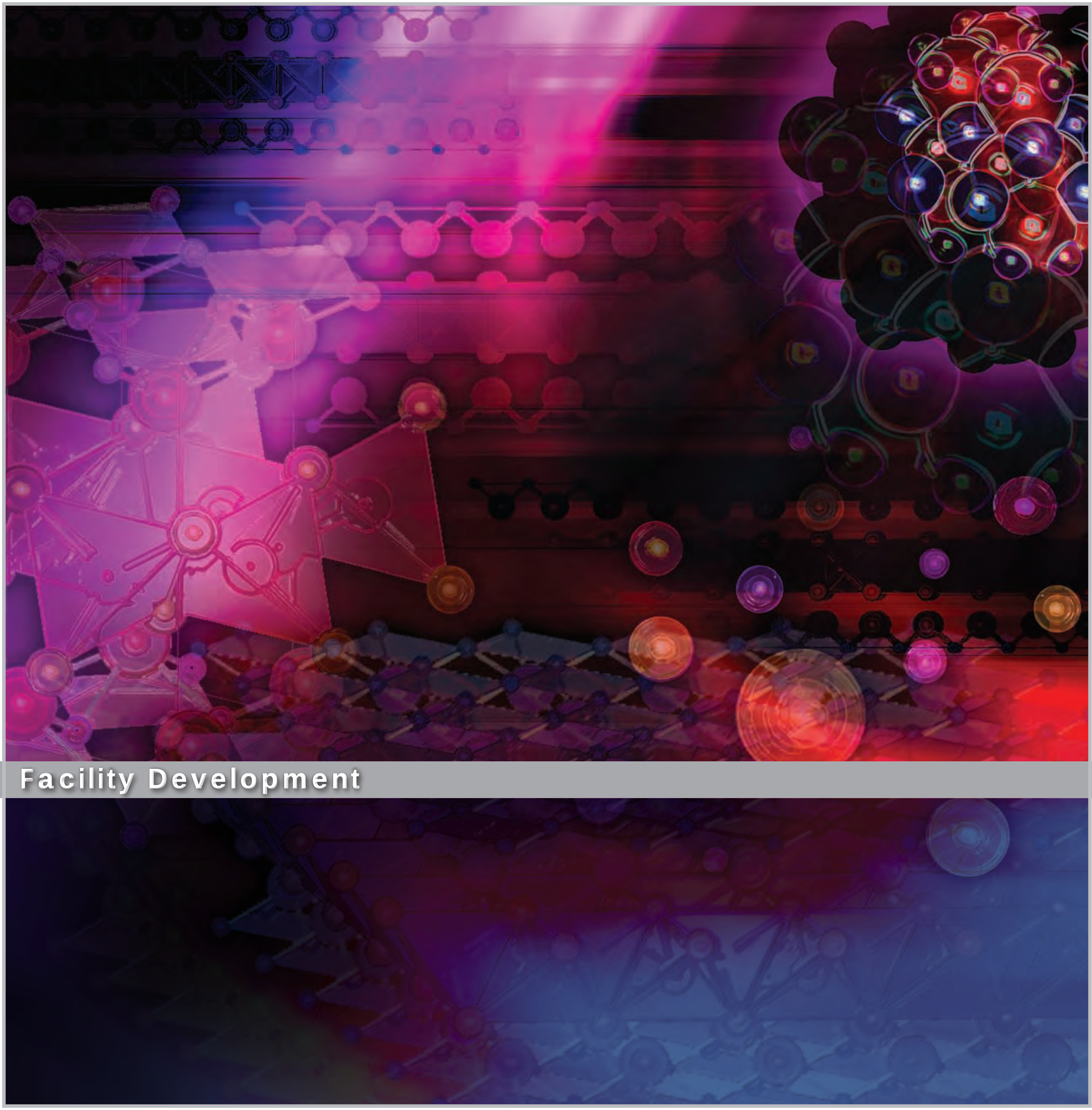
The focus on safety at all levels resulted in impressive safety statistics for FY 2007. SNS employees and contractors had zero lost work-day injuries in FY 2007, and the rate of injuries resulting in restrictions was only 0.2 per 200,000 hours worked. This rate is below the DOE Office of Science goal of 0.25 injuries per 200,000 hours worked. Neutron Sciences personnel working at HFIR have worked 303,699 hours without a lost workday case (the last case occurred in June 2006).

Our facilities are regulated by DOE requirements for both 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. Staff members strive to reduce or eliminate pollution and waste materials, as well as to conserve energy and other resources.

Even though all of ORNL's neutron facilities operate safely and efficiently, a number of programs are being implemented to move to more in-depth levels of safe operation. Incorporating human factors information into work planning helps identify potential pitfalls before workers begin a task. Managers are trained to identify conditions and requirements that "trap" workers through unclear expectations or conflicting requirements. Through human factors training, managers have the tools they need to clarify directions given to workers and to deal with potential conflicts associated with work activities.

Enhancing interactions with staff in the workplace through the Management Observation Program also increased worker involvement and ownership of the safety programs and increased the efficiency of operations. For example, involving workers in planning activities during the major maintenance periods at SNS reduced the radioactive dose by about 90% from the levels initially estimated for the work. This task-level planning led to using as-low-as-reasonably-achievable (ALARA) goals even more effectively than for previous jobs and resulted in the use of real-time dose feedback that provided immediate dose information to the workers. This instant-feedback method is now used for maintenance and other tasks and is implemented throughout the entire work control process.

Contact: Frank Kornegay (kornegayfc@ornl.gov)

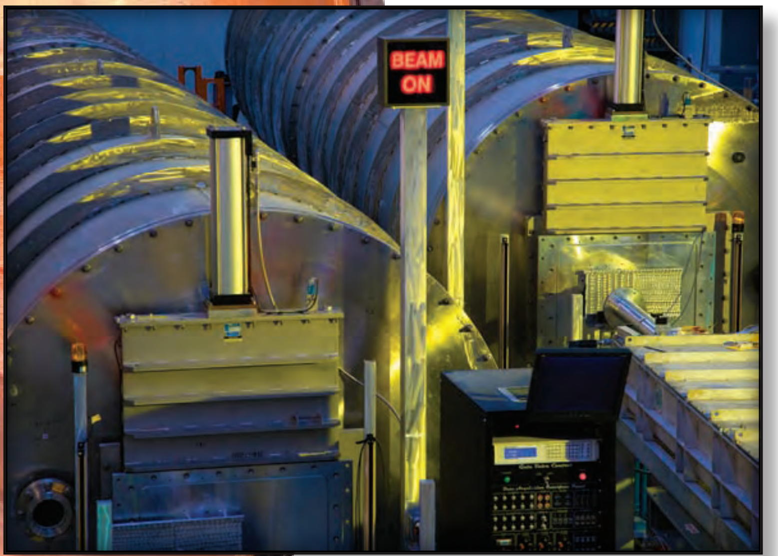


Facility Development

Instruments

High Flux Isotope Reactor

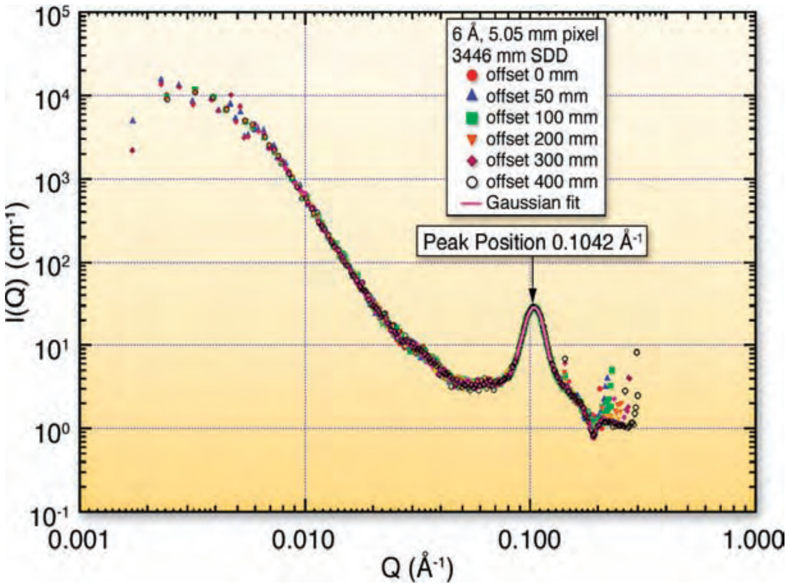
HFIR has six operating instruments available to users (see table below). During 2007, 9 external users performed 16 experiments on the triple-axis spectrometers and 2 experiments on the Wide-Angle Neutron Diffractometer in support of ORNL Laboratory Directed Research and Development projects. Commissioning of the Neutron Residual Stress Mapping Facility 2 was completed, and the facility was able to support six user projects (conducted by both industry- and university-based researchers). In total, 35 scattering experiments were conducted (out of more than 70 proposals).



Detector tanks for the new SANS instruments at HFIR. On the left is the tank for the general-purpose, high-resolution instrument; the tank on the right is for the Bio-SANS instrument, which is constructed specifically for biological research.

Small-Angle Neutron Scattering Instruments

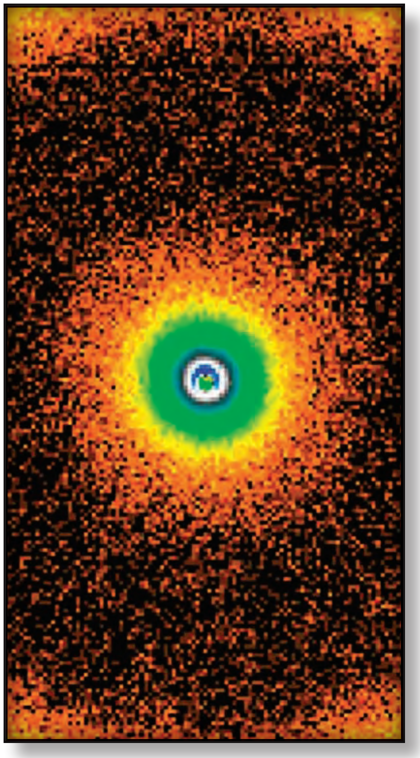
HFIR's new cold neutron source provides beams to two new small-angle neutron scattering (SANS) instruments, the SANS1 for general SANS analysis and a Bio-SANS for biological research. Even though the SANS instruments were still being commissioned during 2007, proposals were accepted and experiments run on both instruments.



Reduced scattering curve from a standard calibration sample of a polymer blend with diffraction peaks taken from data generated at the Bio-SANS instrument.

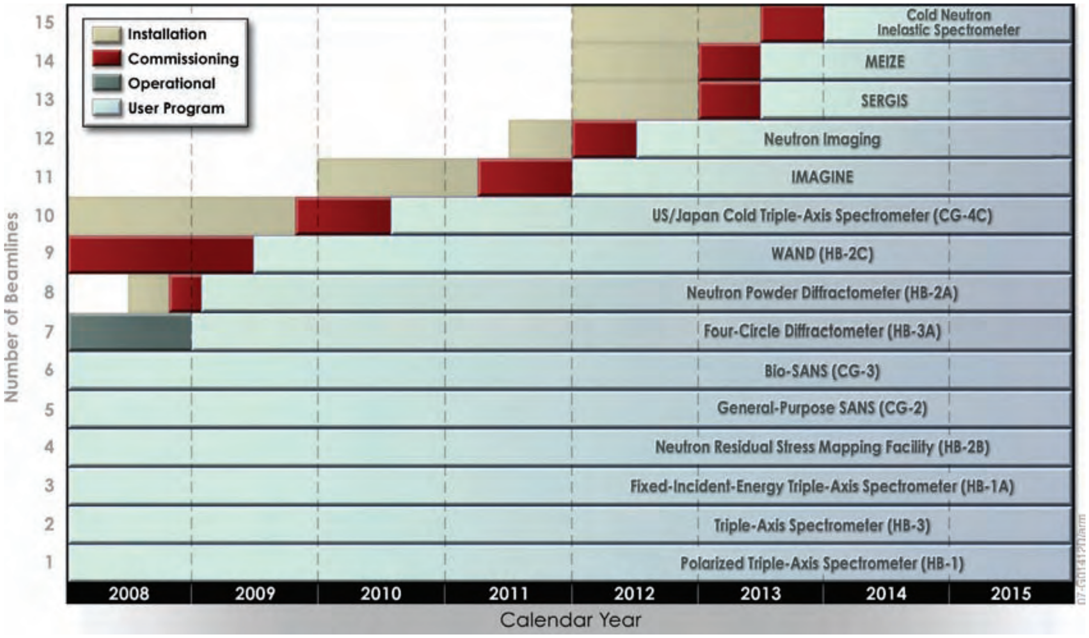
HFIR instruments currently in the user program

Beam line	Instrument
HB-1	Polarized Triple-Axis Spectrometer
HB-1A	Fixed-Incident-Energy Triple-Axis Spectrometer
HB-2B	NRSF2—Neutron Residual Stress Mapping Facility
HB-3	Triple-Axis Spectrometer
CG-2	SANS1—Small-Angle Neutron Scattering Diffractometer
CG-3	Bio-SANS—Biological SANS instrument



Two-dimensional scattering pattern of a polymer from data taken at the Bio-SANS instrument.

Major milestones for instrumentation at HFIR.



SANS1

SANS1 is optimized to provide information about structure and interactions in materials on the scale of 5 to 2000 Å. It has cold neutron flux on sample and capabilities comparable to those of the best SANS instruments worldwide. Its capabilities include a wide range of neutron wavelengths (λ = 5-30 Å), resolution $\delta\lambda/\lambda$ = 9.45%, and a 1-m^2 area detector with 5 x 5 mm pixel resolution with a maximum counting capability of up to 200 kHz. The sample-to-detector distance can be varied from 1 to 20 m, and the detector can be offset horizontally by up to 45 cm, allowing a total accessible Q range from <0.001 to 1 Å^{-1}. The 2-m sample environment area will accommodate large, special-purpose sample environments such as cryomagnets, furnaces, mechanical load frames, and shear cells. SANS1 is ideal for studies of soft condensed materials (e.g., complex fluids, glassy systems, polymers); hard condensed materials (e.g., metallurgical alloys, nanocomposites, ceramics, catalysts); and magnetic systems (e.g., flux lattices in superconductors, ferrofluids).

Bio-SANS

Bio-SANS is operated by the Center for Structural Molecular Biology (see "Facility Integration" in the Operations Section) and provides the most advanced capabilities in the world for analysis of biological systems. The instrument provides detailed structural data for bio-materials from 10 to 1000 Å in length, enabling scientists to build a detailed understanding of the internal structures of complex biological systems and study their responses to changing conditions.

Bio-SANS is designed to have a low background to enable studies of weakly scattering systems. The instrument's sample area has a 2-m footprint, making it suitable for sample environments ranging from traditional liquid cells to large, high-field magnets. Its enclosed sample chamber can handle most samples, and it has a temperature-controlled, multiposition sample changer.

More information about the two SANS instruments is available in the Facts and Figures section.

Four other HFIR instruments are being commissioned or will be commissioned in 2008 and 2009:

- US/Japan Wide-Angle Neutron Diffractometer (WAND), beam line HB-2C
- Four-Circle Diffractometer, beam line HB-3A
- Neutron Powder Diffractometer, beam line HB-2A
- US/Japan Cold Triple-Axis Spectrometer, beam line CG-4

Efforts are also under way to establish instrument projects for each of the five open positions on the HFIR beam lines (one thermal and four cold neutron positions). The plan is to initiate two projects in 2008 and the remaining three in 2009. All open instrument positions are expected to be occupied by 2012. Instrument development teams (IDTs) have been formed for three possible instruments: a quasi-laue diffractometer (IMAGINE) for beam line CG-4, a cold triple-axis spectrometer for beam line CG-1, and a neutron imaging instrument. The IDTs have submitted letters of intent for IMAGINE and the cold triple-axis spectrometer to the Neutron Scattering Science Advisory Committee, and both were approved for the submittal of full proposals.

Spallation Neutron Source

The Backscattering Spectrometer, Liquids Reflectometer, and Magnetism Reflectometer were commissioned in spring 2006 and have been available to a limited number of users since then. (Please see the Science Highlights section for some of the experiments that have been conducted.) All three instruments are performing well and are expected to continue to expand in reliability and capability.

SNS instruments currently in the user program	
Beam line	Instrument
2	Backscattering Spectrometer
4A	Magnetism Reflectometer
4B	Liquids Relectometer

SNS instrument development and construction continues at a fast pace. In September, the Wide Angular-Range Chopper Spectrometer (ARCS) at beam line 18 was completed and measured its first neutrons. Commissioning then began, and the first user experiments are expected in 2008. The Spallation Neutrons and Pressure Diffractometer (SNAP) began receiving neutrons in January 2008, and progress is on schedule for six other instruments scheduled for completion and commissioning during 2008:

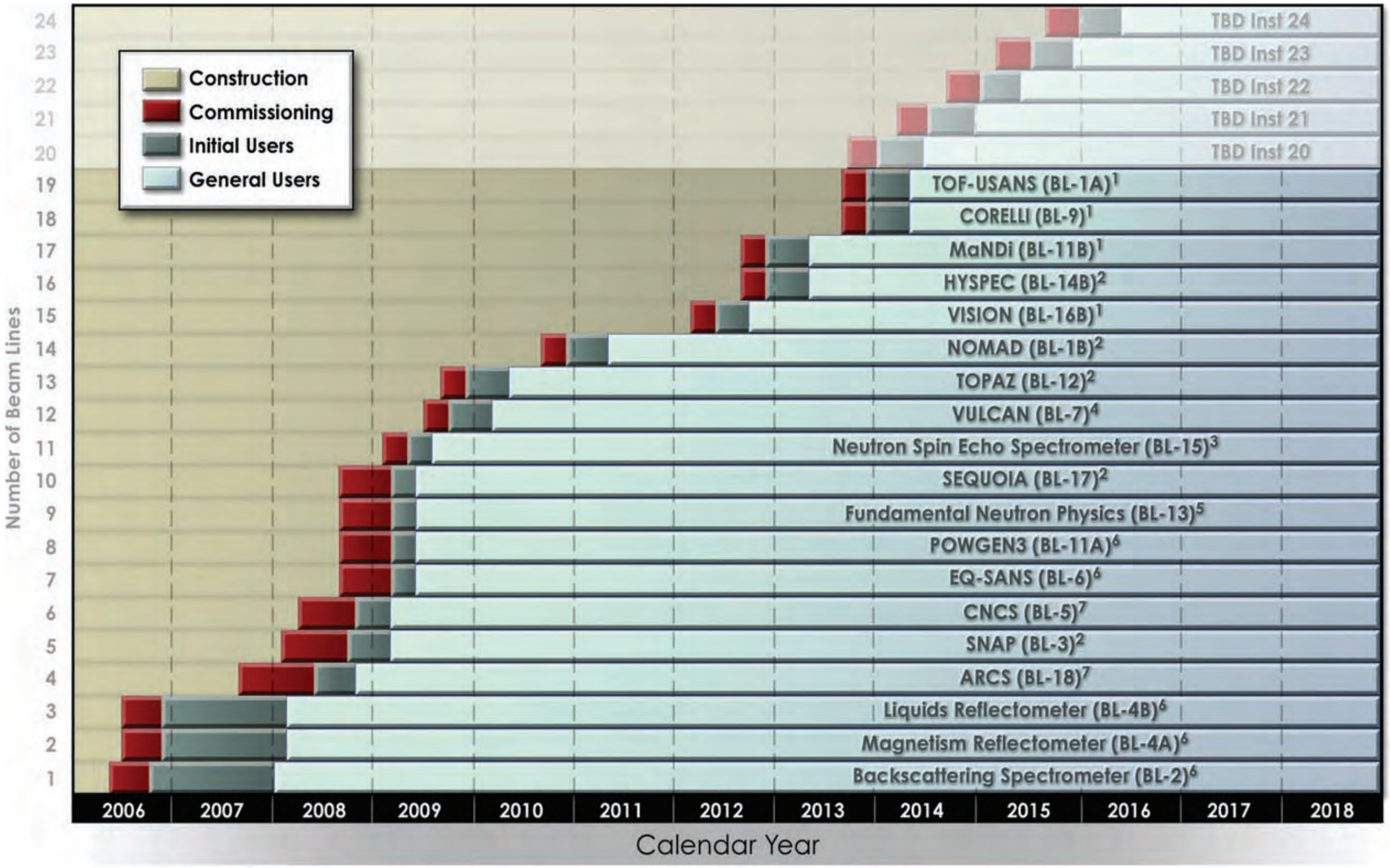
- EQ-SANS (Extended Q-Range Small-Angle Neutron Scattering Diffractometer), BL-6
- CNCS (Cold Neutron Chopper Spectrometer), BL-5
- POWGEN (Powder Diffractometer), BL-11A
- FNPB (Fundamental Neutron Physics Beam Line), BL-13
- SEQUOIA (Fine-Resolution Fermi Chopper Spectrometer), BL-17
- VULCAN (Engineering Materials Diffractometer), BL-7

The Neutron Spin Echo Spectrometer is scheduled for commissioning in 2009.

Two "SNS Instruments—Next Generation" (SING) projects will add nine more instruments to the SNS lineup between 2008 and 2013. SING I—a suite of five best-in-class instruments—is more than 50% complete. The construction, commissioning, and schedule for the current SNS instrument suite availability is shown at right.

SING I	
Beam line	Instrument
1B	Nanoscale-Ordered Materials Diffractometer (NOMAD)
3	Spallation Neutrons and Pressure Diffractometer (SNAP)
12	Single-Crystal Diffractometer (TOPAZ)
14B	Hybrid Spectrometer (HYSPEC)
17	Fine-Resolution Fermi Chopper Spectrometer (SEQUOIA)

SING II	
Beam line	Instrument
1A	Time-of-Flight Ultra-Small-Angle Neutron Scattering Instrument (TOF-USANS)
9	Elastic Diffuse Scattering Spectrometer (CORELLI)
11B	Macromolecular Neutron Diffractometer (MaNDi)
16B	Chemical Spectrometer (VISION)



Funding: [1]SING-II; [2]SING-I; [3]Jülich; [4]Canada Fund for Innovation; [5]DOE-NP; [6]SNS; [7]DOE-BES.

Sample Environment

The Sample Environment teams at HFIR and SNS joined forces in 2007 to create a single group and a more unified program. The group purchased and commissioned a number of standard, workhorse sample environments to support the user community at the two facilities.

The most exciting Sample Environment projects involved research and development collaborations with scientists using the neutron scattering instruments. One such project opened up a new way to study the science behind materials processing under extreme conditions. ORNL scientists wanted to perform the first in situ study of phase transformation under simultaneous high magnetic field and high temperature. This proof-of-principle experiment required building a high-temperature sample insert to fit inside a magnet on the Wide-Angle Neutron Diffractometer (WAND) at HFIR (see Science Highlights). The new technique was successful, opening the door to greater understanding of the role of magnetic fields in structure changes and phase equilibria at high temperatures.

Instrument developer John Wenzel tests engineering changes to improve the efficiency and performance of a top-loading cryostat.

Collaborations with research teams also led to the development of controlled atmosphere furnaces, gas pressure cells, and a controlled humidity cell that was tested and commissioned on the SNS Liquids Reflectometer during the summer. A 1700°C controlled atmosphere reaction (CAR) furnace was tested offline in October. The CAR furnace will be commissioned on the HFIR WAND and will be available for use on other HFIR and SNS instruments. Additional furnace designs are under development. New gas pressure cells were also designed, including a sapphire cell optimized for inelastic measurements on the SNS Backscattering Spectrometer.

The completion of laboratory automation projects has been a significant boost to the Sample Environment program. The Fast Exchange Refrigerator for Neutron Science (FERNS) was developed to meet the demands of high-throughput powder diffractometers such as POWGEN at SNS. FERNS includes a benchtop encapsulation station for sealing powder samples into vanadium cans, a 24-sample automatic changer module, a sample can identification system, and a cryogenic module that cools the sample below 10 K within 10 minutes and regulates sample temperature throughout the range of 10 K to room temperature. FERNS, delivered to SNS in 2006, underwent rigorous testing and upgrades in 2007 to make it a user-ready system. It is now available as a commercial product.

The FERNS cryogenic sample changer for handling sample cans (right) was also delivered in 2006 and was tested and upgraded in 2007 to make it user ready. It is also now commercially available. At the other end of the spectrum, the SNS Single-Crystal Diffractometer will be cooling and remotely manipulating salt-grain-size samples using a special system that is under development.

Cryogenic sample changer (FERNS) for the SNS Powder Diffractometer (POWGEN).

For the SNS Liquids Reflectometer, a system was designed and fabricated to handle sample plates for horizontal scattering geometry. It features an articulating robotic arm and environmentally controlled storage racks.

A project to develop a 16-Tesla actively shielded split-coil vertical field magnet for neutron scattering is progressing on schedule. The analysis phase was completed in April 2007, and the design phase was completed in April 2008. The magnet will be delivered to SNS in 2009. Smaller systems have already arrived: a 5-Tesla actively shielded vertical magnet was commissioned in May 2008, and a 2-Tesla electromagnet and integrated Displex system is operating on the SNS Magnetism Reflectometer.

The Spallation Neutrons and Pressure Diffractometer (SNAP) is a single-crystal instrument that positions very small samples held in a complicated sample environment. To meet the needs of this instrument, the following equipment is being commissioned:

- 8 large-volume Paris-Edinburgh (P-E) presses
- 5 large-volume gas devices
- 15 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.

Landon Solomon (left) and Bruce Hill (right) prepare a liquid helium cryostat that will be used to hold a research sample in the neutron beam.

A list of Sample Environment equipment for each facility is available in the Facts and Figures section.

Contact: Lou Santodonato (santodonatol@ornl.gov)

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 HFIR and SNS beam lines. Detectors count the number of incoming neutrons, and, more important, they record the position and arrival time (i.e., energy) of every single neutron that is seen by the detectors. Ongoing efforts are being made to count neutrons more efficiently and at finer spatial and temporal resolution to increase the capacity and resolving power of all of the neutron scattering instruments.

Although the Detector Group is beginning to support needs for HFIR instruments, in 2007 most of the development work was for the three operating SNS instruments. The Detector Group focused its efforts on development of three neutron detector systems: linear position-sensitive detector (LPSD) "8-pack" modules, shifting scintillator detectors, and neutron Anger cameras with position-sensitive photomultiplier tubes. These three new designs, along with traditional multiwire proportional chambers, make up the four detector types used at SNS.

Pam Morrison and Will Reynolds of the SNS Detectors Group install a 2-meter-long LPSD into 8-packs for the Cold Neutron Chopper Spectrometer on beam line 5.

LPSD 8-Pack Modules

LPSD 8-pack modules, based on GE Reuter-Stokes ^3He proportional tubes, were initially developed for the Wide Angular-Range Chopper Spectrometer (ARCS) and have been chosen for several other instruments as well. A 112-tube array has been running on the Backscattering Spectrometer since its commissioning in 2006. The electronics, mounted on each module, include low-noise preamplifiers and a "ROC" board that digitizes the signal, determines position by charge division, and sends the position and time for each neutron to the data acquisition system. The detector bias supply is also mounted on each module. The low-power electronics are designed for normal operation within the instrument vacuum tank.

One of the highlights this year was development of Pharos, a highly efficient neutron detector array that can operate on solar power and can be located anywhere without support facilities (see the Honors and Awards section for more details).

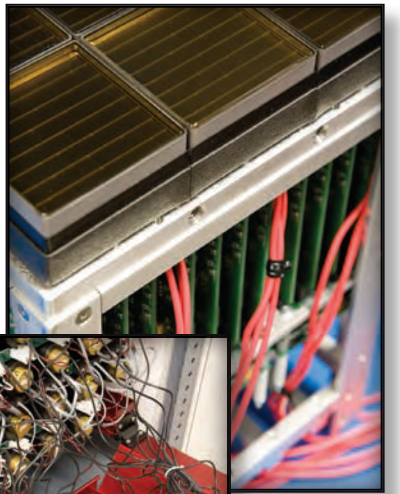
During 2007, all 115 ARCS modules (920 LPSD tubes, 2.5 cm in diameter × 100 cm in length) were completed and calibrated. In September, eight modules were used in the ARCS commissioning measurements. The full ARCS array was installed in early November.

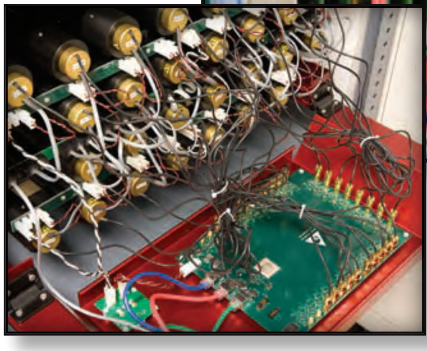
LPSD tubes have been acquired and assembly is in progress for three more SNS instruments scheduled for 2008 commissioning, including the Extended Q-Range Small-Angle Neutron Scattering Diffractometer (300 tubes, 0.8 × 100 cm), the Cold Neutron Chopper Spectrometer (660 tubes, 2.5 × 200 cm), and the Fine-Resolution Fermi Chopper Spectrometer (1440 tubes, 2.5 × 120 cm). In addition, the LPSD systems will be used on the

Hybrid Spectrometer, VISION Chemical Spectrometer, Nanoscale-Ordered Materials Diffractometer, and Corelli Diffractometer. All of these instruments are now undergoing design and prototyping. Other laboratories also have expressed interest in the LPSD system.

Shifting Scintillator Detectors

The shifting scintillator detectors, developed for the POWGEN Powder Diffractometer and the VULCAN Engineering Materials Diffractometer, are now in production for commissioning of these instruments in 2008. These detectors use ^{6}LiF/ZnS:Ag scintillators to convert neutrons to blue photons, which are then collected by a grid of wavelength-shifting fibers and transported to an array of photomultiplier tubes for position encoding. The fiber assembly technique has been transferred to a small business, PartTec, Ltd., which is now producing fiber assemblies for SNS. Eight POWGEN and three VULCAN modules have been assembled and will be ready for instrument installation in late 2008.





Top right: View inside an Anger camera showing the input windows of the position-sensitive photomultiplier tubes and their preamplifier boards.

Bottom left: Back of a shifting scintillator detector for the VULCAN instrument showing the photomultiplier tubes and the high-speed-comparator readout card, CROC.

Neutron Anger Cameras with Position-Sensitive Photomultiplier Tubes

An all-new neutron Anger camera system was developed for the Spallation Neutrons and Pressure Diffractometer (SNAP) and the Single-Crystal Diffractometer (TOPAZ). The two-dimensional resolution goals, 1.3 mm for SNAP and 1 mm for TOPAZ, had not been achieved previously with neutron Anger cameras (or by any large-area, time-of-flight-capable neutron detector).

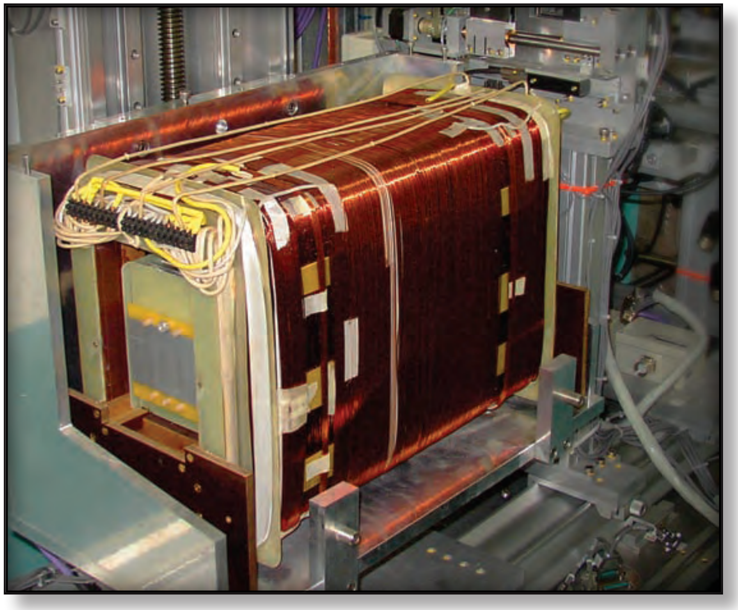
Each module uses 9 Hamamatsu 8500 position-sensitive photomultiplier tubes (PSPMT), each with 64 elements, in a 3 × 3 array behind a single 15 × 15 cm^2 GS20 ^{6}Li glass scintillator plate. A glass diffuser plate and an innovative paraheדral lens are located between the tube and the scintillator. The optics serve to spread the scintillation signal for position determination using Anger logic and to minimize the effects of gaps between PSPMTs. The preamplified and summed photon signals are analyzed using the "Anger ROC" board and readout software, which allows the module to operate as a single element. Modules assembled and tested for SNAP have achieved the 1.3-mm SNAP resolution requirement; further development is in progress to reach the 1-mm TOPAZ requirement. Additional Anger cameras are planned for the MaNDi Diffractometer. The Anger team achieved a major milestone by installing 18 assembled modules in SNAP in September.

In addition to developing detectors for installation, the Detector Group works to maintain detectors on operating instruments, including the Brookhaven area detectors on the SNS reflectometers. The group is also developing low-efficiency monitor assemblies for the SNS instruments. A new scintillator detector assembly laboratory went into service in 2007, and the group maintains two 35-μg ^{252}Cf neutron sources for test and calibration, a smaller check source, and the interim HB-2DS Detector Test Station at HFIR. The SNS group is also participating in external development projects on scintillators, scattering detectors, and imaging detectors.

Contact: Ron Cooper (cooperrg@ornl.gov)

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

Data Acquisition Systems



The resonance spin flipper at the SNS Magnetism Reflectometer. This system and other magnetic equipment are now operational and controllable via the data acquisition system.

Over the next few years, the data rates and intensities produced at HFIR and SNS are expected to be among the fastest and highest possible. To prepare for that onslaught of information, the Data Acquisition Systems (DAS) Group has been working to develop and test software and electronics to meet the unique data collection and handling requirements of the neutron scattering instruments. Chief among these efforts is development of software that allows real-time control and visualization of instrument operation and neutron scattering data; coordination of hardware interfaces of various subsystems, such as sample environment; and design and assembly of custom electronics for detector systems.

Software development was a major emphasis in 2007, and the power of the Neutron Sciences DAS was demonstrated throughout the year as instruments were restarted and commissioned at both facilities. Software such as C++ library modules and LabView VIs were tested extensively for ease of use and reliability under a variety of operational conditions with more than a dozen different users. New software features requested by the instrument scientists, such as region of interest and handling of polarization/analyzer state live views, were added during the commissioning and first user cycles, offering new methods of controlling long experimental sequences.

Additional software developments by the DAS group were key to successful data acquisition and real-time translation. During commissioning of the Wide Angular-Range Chopper Spectrometer at SNS, the DAS successfully provided real-time views of d-spacing while data was collected at a rate of two million events per second. These high data rates allow experiments to be completed in much shorter times, freeing up time for additional experiments. The popular SPICE software, which was developed to control and collect data on the HFIR triple-axis instruments, was expanded and upgraded to run the SANS instruments at HFIR. Automated notification of the data management server allowed real-time translation of non-Nexus files into NeXus format, which allows for easier sharing of data between collaborators. Python software was used as a scripting language to develop custom-control graphical user interfaces for spin flippers and polarizers for the SNS Magnetism Reflectometer. These customized scripts allow for greater flexibility in the control of instruments, while hiding many of the complexities of hardware control. In addition, version control for software development in the DAS Group was successfully migrated from CVS to Subversion, which is now the version control standard for both the data analysis and the data acquisition groups.

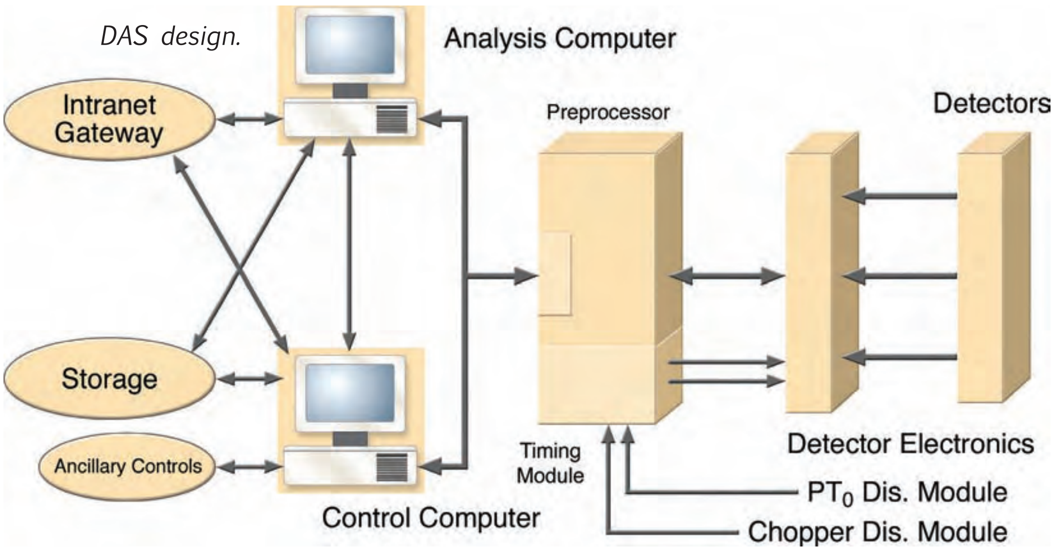
The adaptability of the software architecture was demonstrated at SNS, where custom user equipment was integrated with DAS control in less than a day. Field gate programmable array code was developed for the Anger readout card and comparator readout card boards using new techniques for position determination in the Anger camera detectors and cross-fiber detectors. These innovations allow greater resolution, higher rates, and lower backgrounds for the detector systems.

As part of the buildout of the SNS instrument suite, the DAS Group oversaw the manufacture of about 1,000 large electronic boards designed for a variety of uses, such as position determination and time stamping, cross-fiber detection, Anger camera detector systems, data concentration, supply of detector bias, optical transmission of detector data, communication to and from detector systems, and optical transmission of digital signals. All of the electronics were designed by the SNS DAS Group and represent a suite of state-of-the-art electronics for large-area, high-rate detector systems. Build kits were coordinated by Neutron Sciences staff and were manufactured by outside vendors.

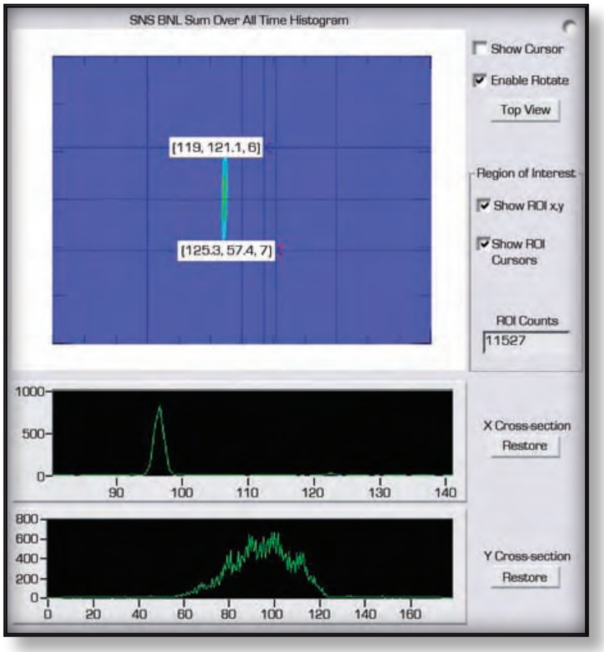
Data acquisition needs will continue to grow as more instruments and ancillary equipment come online. In response, the DAS Group continues to work hard developing the best possible new software and improved hardware for data acquisition.

Contact: Rick Riedel (riedelra@ornl.gov)

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



DAS design.



This screen shows region-of-interest (ROI) capability for live display of data. An ROI can be defined in the two-dimensional display area, which controls what data are used to update other graphical displays of reduced data such as d spacing or energy transfer.

Data Analysis

The Scientific Computing Group helps researchers transform their experimental data into scientific results. This year marked a transition from developing infrastructure to providing commissioning support for instrument teams and to supporting the first facility users. As a result of these efforts, a framework is in place that automatically flows experimental data from the HFIR and SNS data acquisition system (DAS) into the centralized data management system via a process called "live cataloging."

Experiment data are compiled into NeXus format. As mentioned in the previous DAS section, NeXus files allow for more flexible sharing of data among different systems. NeXus is based on the Hierarchical Data Format (HDF5) supported broadly via commercial data processing applications such as IDL and IgorPro and community packages such as ISAW. A Web-based data access system called the Neutron Sciences Portal (the portal) provides users with ubiquitous access to data. Cataloging the data enables users to search and discover data of interest via the portal, while keeping the data accessible only to the experiment team.

Integrated with the portal are data reduction applications for the SNS Backscattering Spectrometer (BASIS) and the Liquids and Magnetism Reflectometers (the SNS instruments available to users 2007). These same data reduction applications are available both on site and off site via the portal. By (manually) cataloging data sets from both the Lujan Neutron Powder Diffractometer at the Los Alamos Neutron Science Center and the LENS Small-Angle Neutron Scattering instrument at the Indiana University Cyclotron Facility, we've also demonstrated that the data portal concept can be extended. The plan is to support live cataloging for these and additional instruments outside ORNL in the future, providing a centralized location for users to access and process their experiment data.

The portal currently provides access to a number of existing applications developed by the Scientific Computing Group. Applications are developed in

Applications Available Via the Portal		
Developed by the Neutron Sciences Scientific Computing Group	Community Developed	Commercial and Open Source (availability might depend on license availability)
BASIS data reduction	DAVE	IDL
Liquids Reflectometer and Magnetics Reflectometer data reduction	EXPGUI	Matlab
Reflectometry data scaling utility	FullProf	SigmaPlot
NeXus file creation utility—converts event lists into NeXus files	ISAW	Origin
Geometry generator utility—used in conjunction with data reduction	McStas (still in beta test)	IgorPro
	PDFgui	Python
	WinPLOTR	Open Office

Instrument	NeXus files	Event file size (MB)	Histogram size (MB)	NeXus file size (MB)	Compression (%)
BASIS	280	73.0	703	5.80	99.2
Liquids Reflectometer	2191	2.4	233	6.80	97.0
Magnetism Reflectometer	1346	27.0	148	7.58	95.0

As instruments produce larger and larger histograms, the value of data reduction made available through the portal will continue to grow.

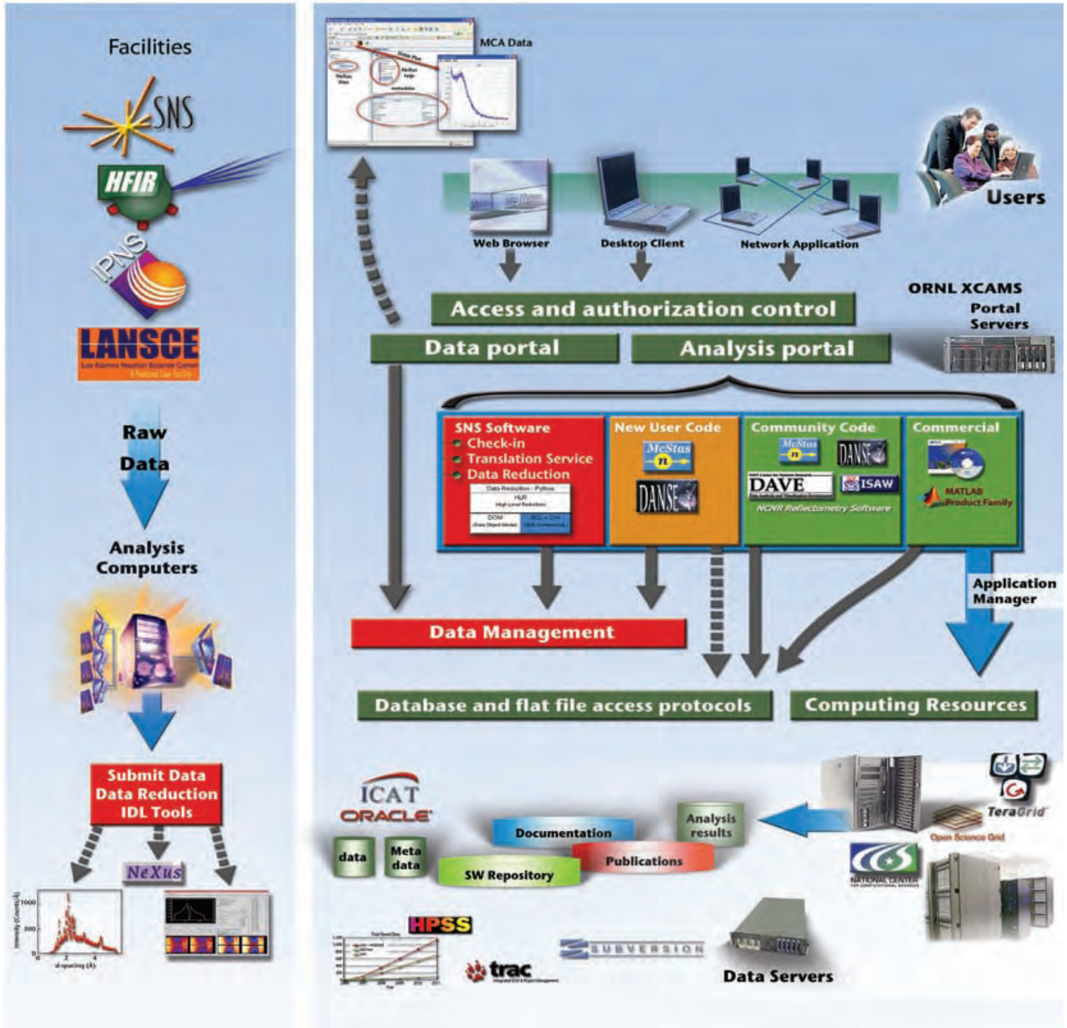
conjunction with instrument commissioning in close collaboration with the instrument teams. Initially, data reduction applications were the primary focus. These applications can be segmented into two primary components, the graphical user interface (GUI) and the reduction engine. In essence, the GUI provides a convenient means of interacting with data, setting parameters, and configuring options in order to create command-line execution calls identical to those that could be manually typed on the analysis computer command line. It allows for significant flexibility as to which computers the GUI and reduction engines can be placed on, including installation on separate computers. The GUIs used on the instrument analysis computers are also accessible via the portal. Separating the GUI from processing provides flexibility and insight into the requirements for portal-based computing and data management architectures.

Data analysis capability will also be significantly enhanced by the incorporation of software being developed in the neutron scattering community within the DANSE (Distributed Data Analysis of Neutron Scattering Experiments) project, which is funded by the National Science Foundation. A number of DANSE applications are beginning to make their way into the portal. Leading the way is software developed for diffraction applications; however, the final suite will include small-angle neutron scattering, reflectometry, and inelastic software applications. New and improved DANSE applications will be made accessible via the portal as they become available.

Users can request computer access via https://portal.sns.gov/accounts/.

Contact: Steve Miller (millersd@ornl.gov)

neutrons.ornl.gov/instrument_systems/computing/



Instruments at neutron facilities produce raw data that flow into the data management system via instrument-associated analysis computers to be prepped, cataloged, and archived. Users have access to data, applications such as data reduction, and computing resources through a portal interface. Via the portal, users can access both data and applications using a Web browser. Behind the scenes, a series of servers transact user requests, locating data and automatically selecting computer resources. Community-produced analysis applications such as PDFgui, ISAW, and DAVE are also made available to users. The portal provides a home area for storing data created by users.

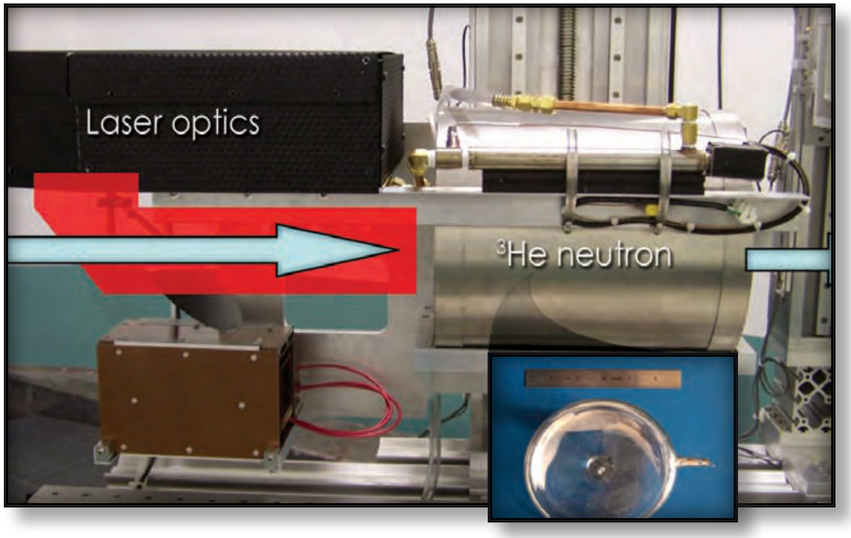
Polarized Neutron Development

Polarized neutrons are used in studying magnetic structure and magnetic excitation phenomena in materials. Recently, neutron polarizers and analyzers based on spin-dependent neutron absorption by ^{3}He have become viable for neutron scattering. This type of neutron spin filter can accommodate a neutron beam with a wide bandwidth, large beam cross section, and large angular divergence. There is little if any background caused by small-angle scattering from the spin filter.

SNS staff have been working with the polarized ^{3}He R&D community to develop polarized ^{3}He neutron spin filters for scattering. In a series of experiments carried out at the Single Crystal Diffractometer (SCD) at the Intense Pulsed Neutron Source (IPNS), they developed a compact neutron polarizer that can be installed at an instrument as needed. Improving upon the conventional use of such spin filters, in which the ^{3}He polarization decays over time, the new system maintained a stable non-decaying ^{3}He polarization online by continuously polarizing the ^{3}He for the duration of the experiment.

The SNS team also used the adiabatic fast passage (AFP) technique in nuclear magnetic resonance to flip the ^{3}He polarization with respect to the field, thereby creating a combined neutron polarizer and neutron spin flipper. A ^{3}He cell that reached 67% polarization at the SCD was used. The polarization of 3-Å neutrons was determined by measuring the spin positive and negative beam intensities downstream of the ^{3}He polarizer. Repeatedly flipping the ^{3}He polarization at an equivalence of one flip every 5 minutes showed no impact on the polarization. In the most recent polarized SCD experiment, the magnetic structure of a single crystal of $Yb_{14}MnSb_{11}$ was measured and a previously unknown ferromagnetic structure identified.

After completing these experiments, the SNS team developed a ^{3}He analyzer, constructed at the National Institute of Standards and Technology, for the SNS Magnetism Reflectometer (at left). As in the test system, the instrument incorporated continuous polarizing capability to keep the ^{3}He polarization at its maximum and AFP to flip the ^{3}He polarization for spin positive and spin negative measurements. Commissioning tests for the analyzer are under way.



Polarized ^{3}He-based neutron polarization analyzer on the SNS Magnetism Reflectometer. The ^{3}He cell (insert) is located inside the magnetostatic cavity.

To meet the future demand for polarized ^{3}He spin filters—especially wide-angle analyzers that cover up to a 120° span of scattering angles—SNS is developing a ^{3}He production system based on spin exchange optical pumping to polarize ^{3}He. A large-scale laboratory-based system (above) is being built that can produce a large volume of high-polarization ^{3}He gas and maintain the polarization until an experiment is conducted. It can also be used to fill sealed cells for online spin filter systems. A compact system is being designed for direct use at the SNS Hybrid Spectrometer and potentially at other instruments.

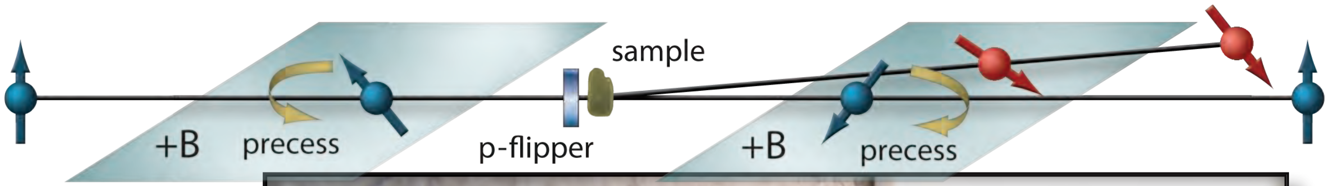
Polarized neutrons are also used in neutron spin echo (NSE), a technique based on the neutron spin precession in a magnetic field. NSE has conventionally been used to achieve high-energy resolution in neutron scattering, but spin echo scattering angle measurement (SESAME) techniques are being developed to extend the technique to achieving high-angular resolution that cannot otherwise be reached. As illustrated below, parallelogram-shaped magnetic field regions are imposed before and after a sample. Neutrons that are not scattered by the sample find the precession in the two field regions canceled, whereas scattered neutrons acquire a net precession angle. The scattering angle can therefore be determined with high precision by measuring the change of neutron polarization.

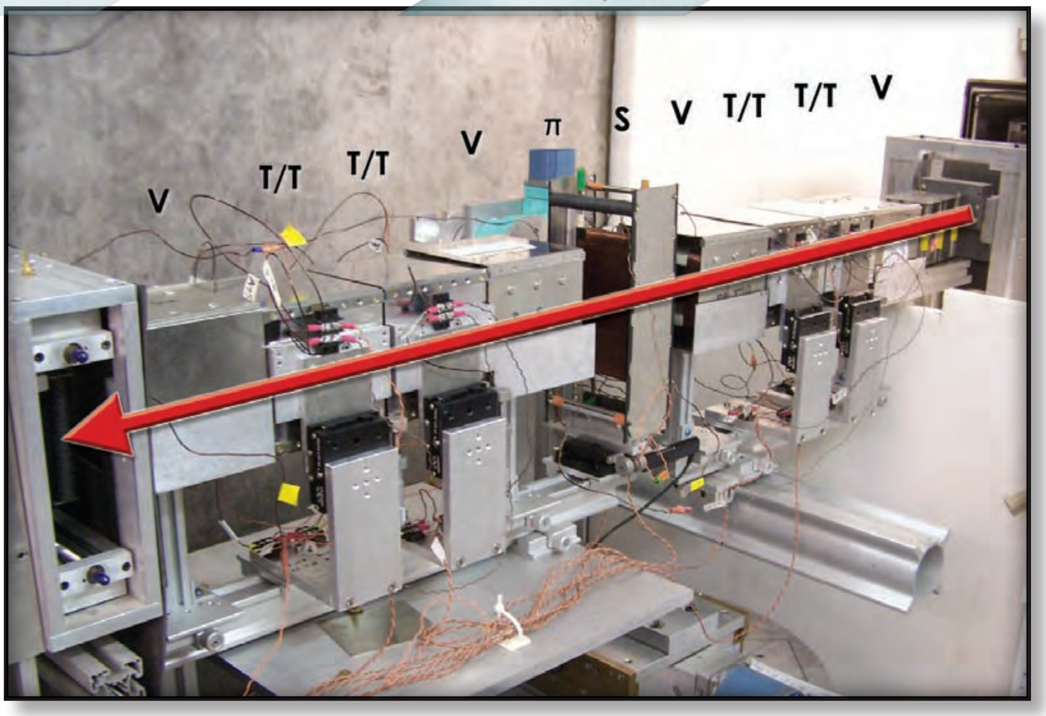
In collaboration with Roger Pynn (SNS and Indiana University Cyclotron Facility), we have been developing SESAME techniques for scattering. In 2007, an experiment was conducted at the Asterix polarized neutron reflectometer at the Los Alamos Neutron Scattering Center (LANSCE). The experiment aimed at testing an approach that uses a series of triangular-shape coils to produce parallelogram-shape magnetic fields while mitigating the complexity due to the inclined field boundaries. The setup, as shown at right, was tested for spin-echo small-angle neutron scattering measurements where 100-nm polystyrene spheres suspended in D_2O with volume concentrations of 8.2% and 10.7%, respectively, were used.

The ongoing collaboration on developing SESAME techniques focuses on reaching micron-scale spin-echo lengths and minimizing the amount of materials in the neutron beam. These developments will be applied either to expand the measurement capability of an instrument or on a dedicated state-of-the-art SESAME instrument.

Contact: Hal Lee (leewt@ornl.gov)

Principle of SESAME. For un-scattered neutrons, the spin precession in the parallelograms cancels, whereas for scattered neutrons, there is a net precession resulting in a change in the polarization.





SESAME experiment set up at Asterix, LANSCE. The red arrow shows the flight path of the polarized neutron beam. The symbols are: V= π/2 flipper using v-coil, T/T = triangular shaped precession coils, S = sample, π = π-flipper.

Future Initiatives

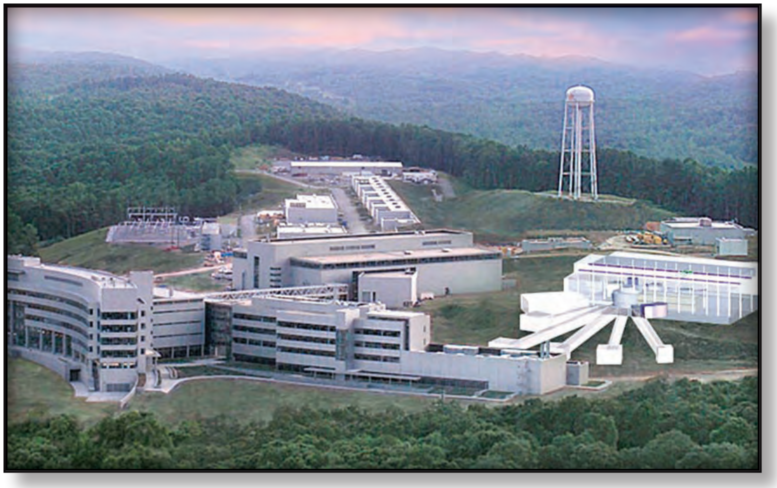
SNS Power Upgrade and Second Target Station

To improve the performance of the SNS neutron source, a power upgrade project is in the works that will double the proton beam power by the end of 2016, making twice as many neutrons available for the SNS neutron scattering science programs. This additional beam power will be achieved by increasing the energy of the protons by 30% from 1.0 to 1.3 GeV and from raising the beam current by 60%. The project will include an upgrade of the target systems to withstand the higher power. The project is waiting on approval to begin planning and preliminary engineering, and construction is expected to start in 2010.

To provide a second source of neutrons to more instruments, SNS is developing plans and conceptual designs for a second target station. Studies show that this station will improve performance by more than an order of magnitude for broad areas of forefront science and could open totally new areas to exploration. Construction could be finished in 2019.

Contact: Kent Crawford (crawfordrk@ornl.gov)

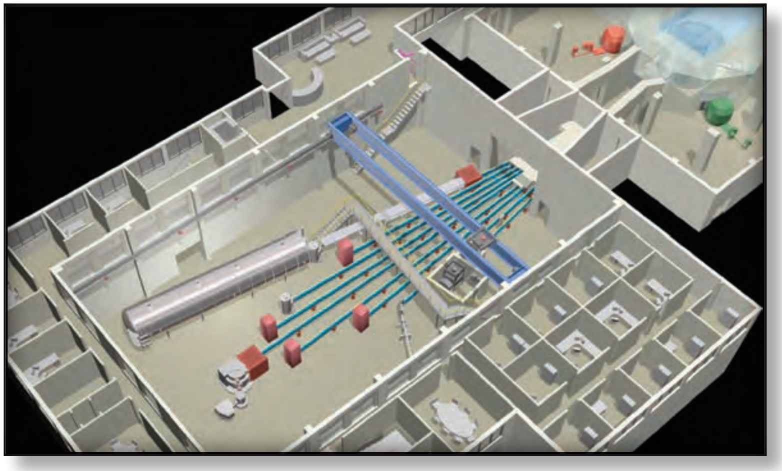
neutrons.ornl.gov/facilities/proposed_upgrades.shtml



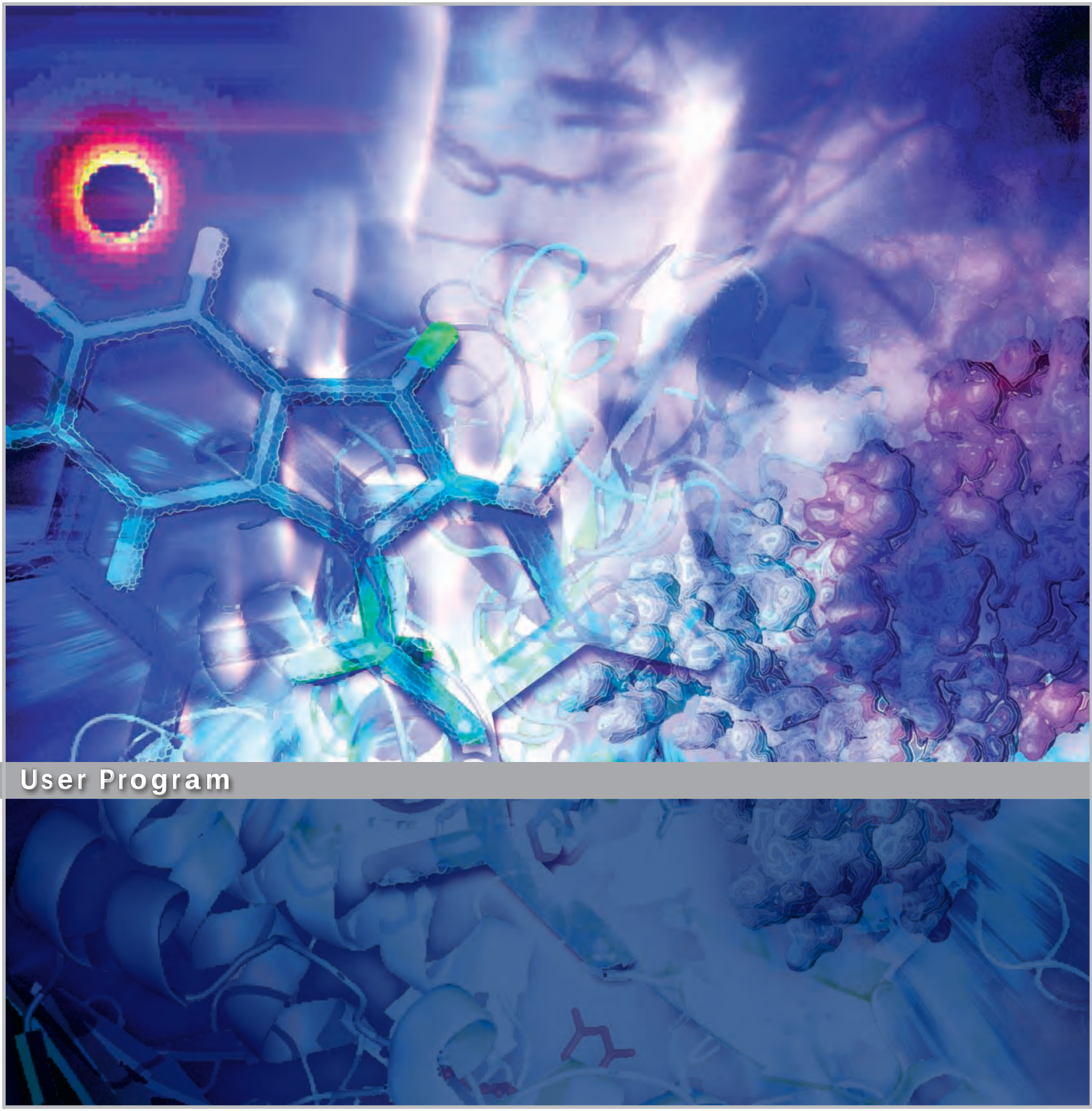
SNS site on Chestnut Ridge. On the right is the projected location of the second target station.

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.

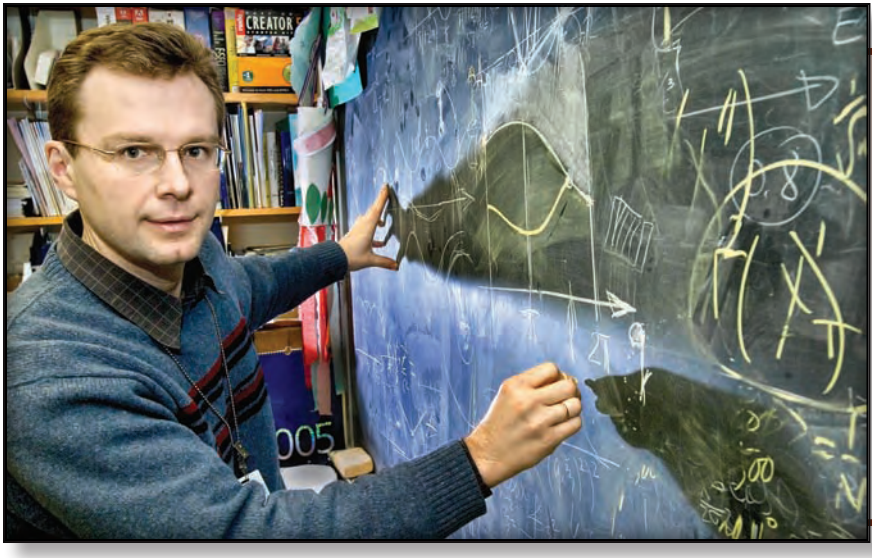


Top image: Rendering of the HFIR cold source and guide hall with nine beam lines. Bottom image: Artist's conception of the proposed HFIR Neutron Science Center.



User Program

SNS-HFIR User Group



Igor Zaliznyak, SHUG Executive Committee Chair

SHUG welcomes anyone interested in using the neutron scattering facilities at ORNL. It provides input to Neutrons Sciences management on user concerns, provides a forum for keeping the entire neutron science community informed of issues and progress at the ORNL facilities, and serves as an advocacy group for neutron scattering science at these facilities. For more information, see neutrons.ornl.gov/shug/

Fellow HFIR and SNS users,

It is my pleasure to serve as chair of the SNS–HFIR User Group (SHUG) at a time of good news and exciting events. Thanks to dedicated efforts by ORNL staff and many SHUG members, ORNL's neutron facilities are up and running. Users can now take part in the frontier science these facilities make possible.

Although not all instruments are yet online, the emphasis at SNS and HFIR is shifting toward reliable operation and development of the user program. A vibrant, vigorous user program is key to the success of these facilities—success that will ultimately be demonstrated by the quality of the research and the scientific advances that emerge.

Running an efficient user program requires close cooperation and coordination with the user community. The ORNL Neutron Sciences staff are eager to work with users, both by informing us of news and developments and by listening to our concerns and suggestions. The SNS–HFIR user meeting at ORNL on October 8–11 provided a forum for such communication. The scientific agenda presented an overview of scientific issues the neutron community will address using SNS and HFIR, as well as technical challenges the facilities face. On behalf of the meeting organizers and the SHUG Executive Committee, I thank all those who participated.

Development of software tools was mentioned as a top challenge for the facilities, particularly for the new instruments. Another important challenge is developing funding models for user support and education, including travel support for new users. Several such programs have already been established at ORNL, among them an undergraduate summer research program, the Clifford Shull and Instrument Development fellowships, and the Joint Institute for Neutron Sciences.

An important goal for the user program is increasing the size of the user community. Steps toward this goal will include finding new ways to attract students and researchers from universities and industry, as well as working to obtain new funding sources. As a core user group, SHUG must play a central role in community building and educational and outreach activities, expanding the ranks of researchers using neutron tools.

I wish you success with your upcoming experiments at SNS and HFIR.

Igor Zaliznyak, SHUG Executive Committee Chair

HFIR and SNS: Open to Users

Within a few years, HFIR and SNS are expected to host more than 1000 users annually. One user program serves both facilities and was developed from experience at HFIR and other national and international user facilities, with the best practices adapted to the environment at ORNL. The goal of the program is to provide world-class user services at these facilities. Current user program activities are focused on three areas: the proposal system, user administration, and outreach and education.

Proposal System

The user program's most important effort in 2007 was development of the Integrated Proposal Tracking System (IPTS). This Web-based system became available to the user community during the July call for proposals, which resulted in more than 200 submissions. The second call for proposals ended in January 2008. We anticipate at least two annual calls for proposals, each to be announced about two months before the proposal window opens.

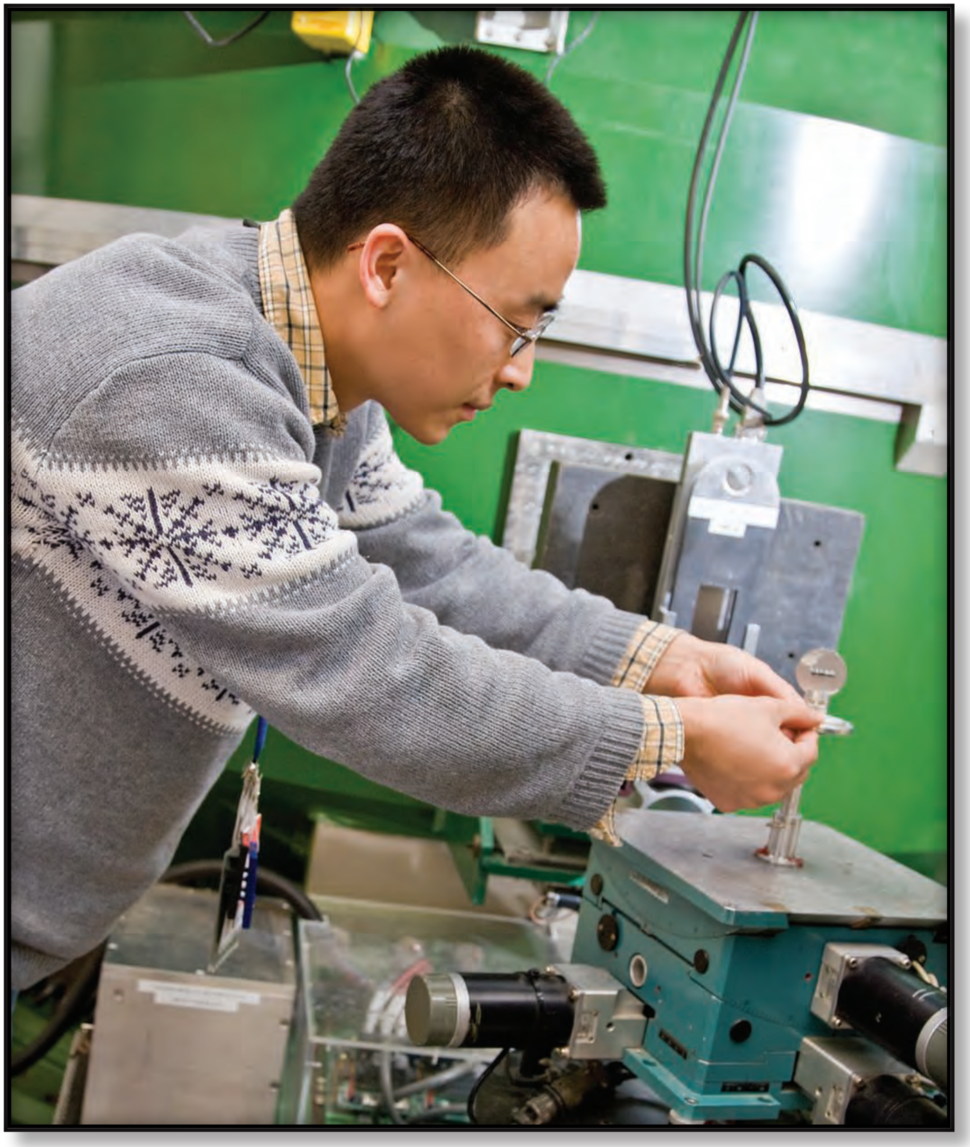
The Center for Nanophase Materials Sciences (CNMS), located adjacent to SNS, has a strong interest in materials characterization using neutrons. Because of these close ties and the adaptability of the IPTS to other user facilities, CNMS will also use IPTS for its proposals in the future.

The 2007 effort was just the first stage of IPTS development. Future IPTS enhancements will include expanding the flexibility of processing reviews; initiating scheduling and sample management systems; and linking to other ORNL systems, including those related to site and facility access, training, and publications.

Users Joon Ho Roh (University of Maryland) and Sheila Khodadadi (University of Akron) talk with Eugene Mamontov (right), instrument scientist for the SNS Backscattering Spectrometer. Along with two other users from the University of Akron, the team conducted an experiment on the relaxation dynamics of hydrated RNA.

User Administration

After proposals are reviewed and beam time is awarded, users prepare to visit ORNL. Protocols are in place for all users to take three Web-based courses, each requiring about an hour, before arriving at ORNL. Completing the courses before coming to ORNL expedites facility access and the completion of required training for which the courses are prerequisites. All users must successfully complete a radiological worker training practicum for neutron scattering users and about 2 to 4 hours of hands-on training specific to the instruments and labs they will be using. Users also receive dosimeters and reference cards with key telephone numbers and safety reference information. Our goal is to have new users ready to begin their experimental work in about a half day. Training is valid for two years, and returning users can receive their badges and dosimeters and begin work immediately if their training is current.



Feng Ye of ORNL works with the HB-3 Triple-Axis Spectrometer at HFIR.

At the end of an experiment, a user completes an online survey; returns the ORNL badge, dosimeter, proximity card, and reference cards; and notifies the user office of any publications resulting from the research.

The Neutron Sciences Web site (neutrons.ornl.gov) provides more information about policies, practices, and expectations for users. Information about the Oak Ridge and East Tennessee area and links to other on-site resources are also available.

Outreach and Education

Outreach and education are necessary not only to develop a user community but also to identify the resources needed to perform cutting-edge science. In response to requests from the user community for additional information, several means of communication have been established. Monthly progress reports are distributed electronically to the 1400 individuals on the Neutron Scattering Science Division mailing list and are

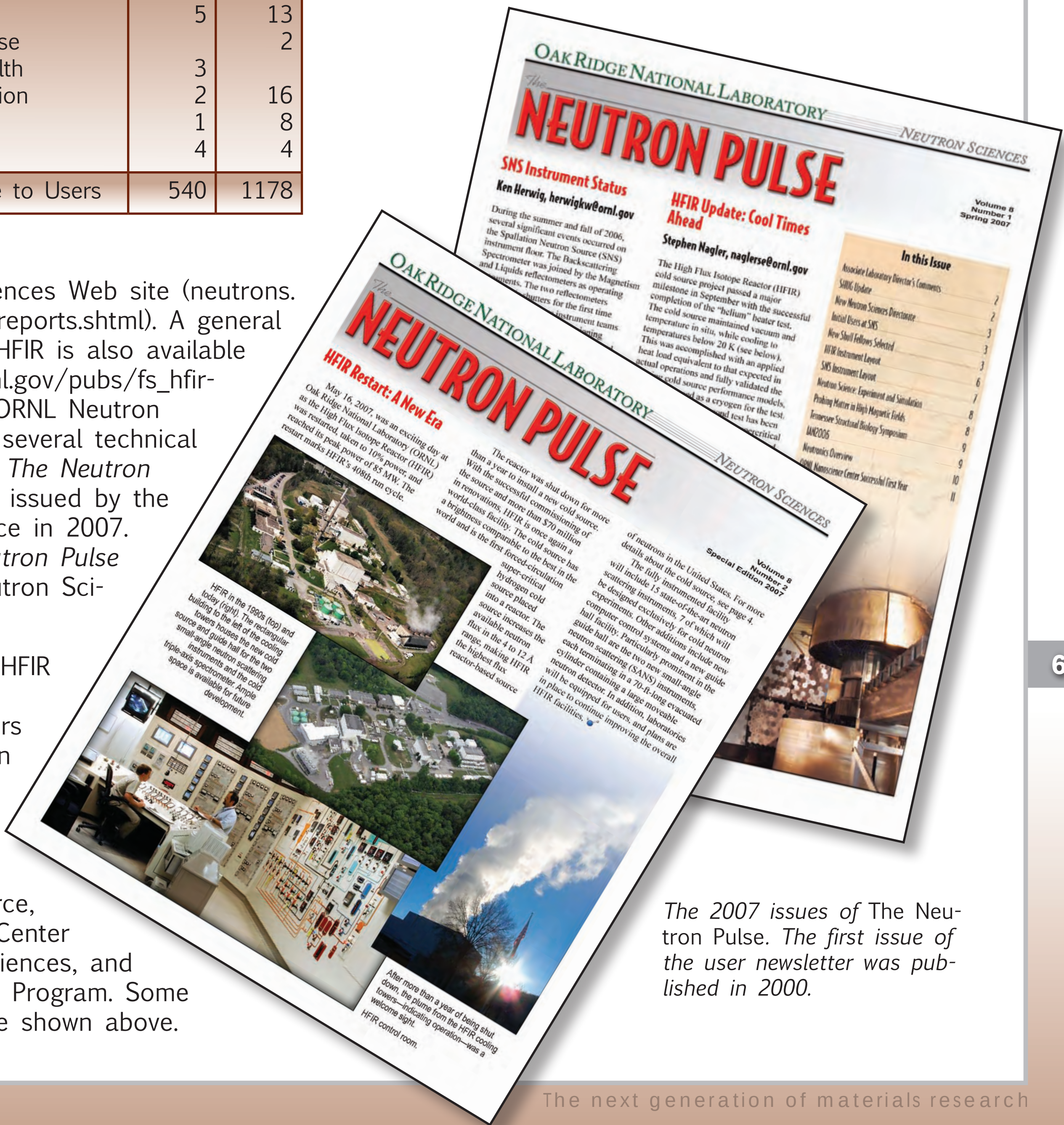
User Statistics for 2007	SNS	HFIR
Badged Users (total)	24	72
• First-time users	24	43
• Students	10	14
• Postdocs	4	18
Support Sources		
• U.S. Department of Energy (DOE) Office of Basic Energy Sciences	10	30
• DOE other	5	13
• U.S. Department of Defense		2
• National Institutes of Health	3	
• National Science Foundation	2	16
• Industry	1	8
• Other	4	4
• Operating Hours Available to Users	540	1178

posted on the Neutron Sciences Web site (neutrons.ornl.gov/snsnews/progress_reports.shtml). A general fact sheet about SNS and HFIR is also available on the Web at neutrons.ornl.gov/pubs/fs_hfir-sns.pdf. Articles about the ORNL Neutron Sciences have appeared in several technical journals, and two issues of *The Neutron Pulse* users newsletter were issued by the Neutron Sciences User Office in 2007. Beginning in 2008, *The Neutron Pulse* will be replaced by the Neutron Sciences annual report.

On October 8–11, the SNS-HFIR User Group helped stage a highly successful ORNL Users Week. The event focused on the scientific resources of four ORNL user facilities funded by the DOE Office of Basic Energy Sciences: the Spallation Neutron Source, High Flux Isotope Reactor, Center for Nanophase Materials Sciences, and Shared Research Equipment Program. Some statistics from the event are shown above.

Current and prospective users became acquainted with the research capabilities of the user facilities through presentations, tours, and workshops. Attendees were also introduced to the user proposal process.

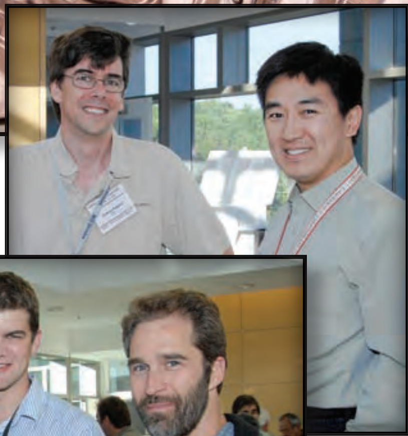
Contact: Judy Trimble (trimblejl@ornl.gov)
neutrons.ornl.gov/users/



The 2007 issues of The Neutron Pulse. *The first issue of the user newsletter was published in 2000.*

SNS Liquids Reflectometer users Joe Strzalka (left) and Venkata Nagarajan (right) participated in the first measurement of a free liquid surface on the instrument. Both users are from the University of Pennsylvania.

ORNL Users Week Statistics	
Number of registrants	367
Institutions represented: • Colleges and universities	78 55
Regions represented: • U.S. states and District of Columbia • Foreign countries	 32 7
Sessions registered for: • Nanoscience • Neutrons • Combined sessions	 36% 28% 36%
Registrants for nine tutorial sessions	200



Attendees at the 2007 ORNL Users Week Workshop.

Accessing Beam Time at HFIR and SNS

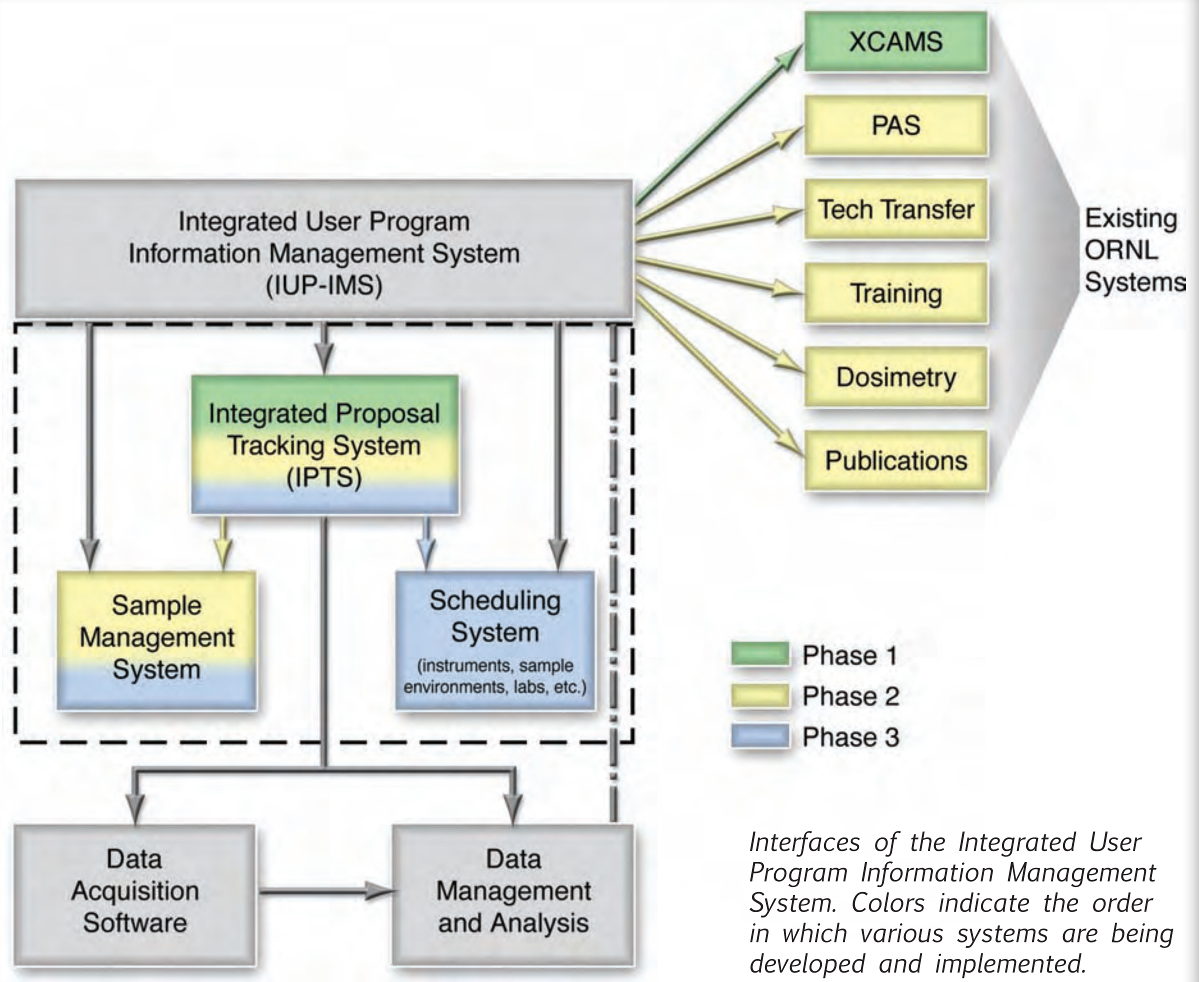
Access to Oak Ridge user facilities such as HFIR or SNS is a two-step process:

1. Review and approval of the user's proposal.
2. Signed agreement between the user institution and UT-Battelle, LLC, the managing contractor of ORNL.

ORNL's Neutron Science User Program supports research at HFIR and SNS. General users receive at least 75% of the beam time allocation for the instruments included in the general user program. Proposals for time on the instruments are submitted electronically through the Integrated Proposal Tracking System (IPTS), which will also be used for the Center for Nanophase Materials Sciences, located adjacent to SNS. This system provides easy, convenient access to all three facilities. Details about IPTS, including policies and guidelines, are available at neutrons.ornl.gov/users.

When a proposal has been accepted, ORNL's Technology Transfer and Economic Development Office executes a user agreement with the user institution. This agreement, which can be either proprietary or nonproprietary, stipulates the terms and conditions for the interaction (including disposition of intellectual property). Most user research will be in the public domain and must be disseminated by publication in the open literature; policies for access for proprietary research are listed at the Web site just mentioned.

Each external user must have an ORNL contact who works closely with the principal investigator and



Interfaces of the Integrated User Program Information Management System. Colors indicate the order in which various systems are being developed and implemented.

the experiment team to prepare and perform the experiment. Prospective users should examine the appropriate instrument pages (neutrons.ornl.gov/instrument_systems) and contact instrument scientists when developing proposals. Each instrument has a Web site that describes the capabilities and functions of the instrument and identifies the instrument scientist. The instrument scientist can help to confirm the feasibility of a proposed experiment and the effectiveness of the research technique and answer questions about the capabilities of the instrument.

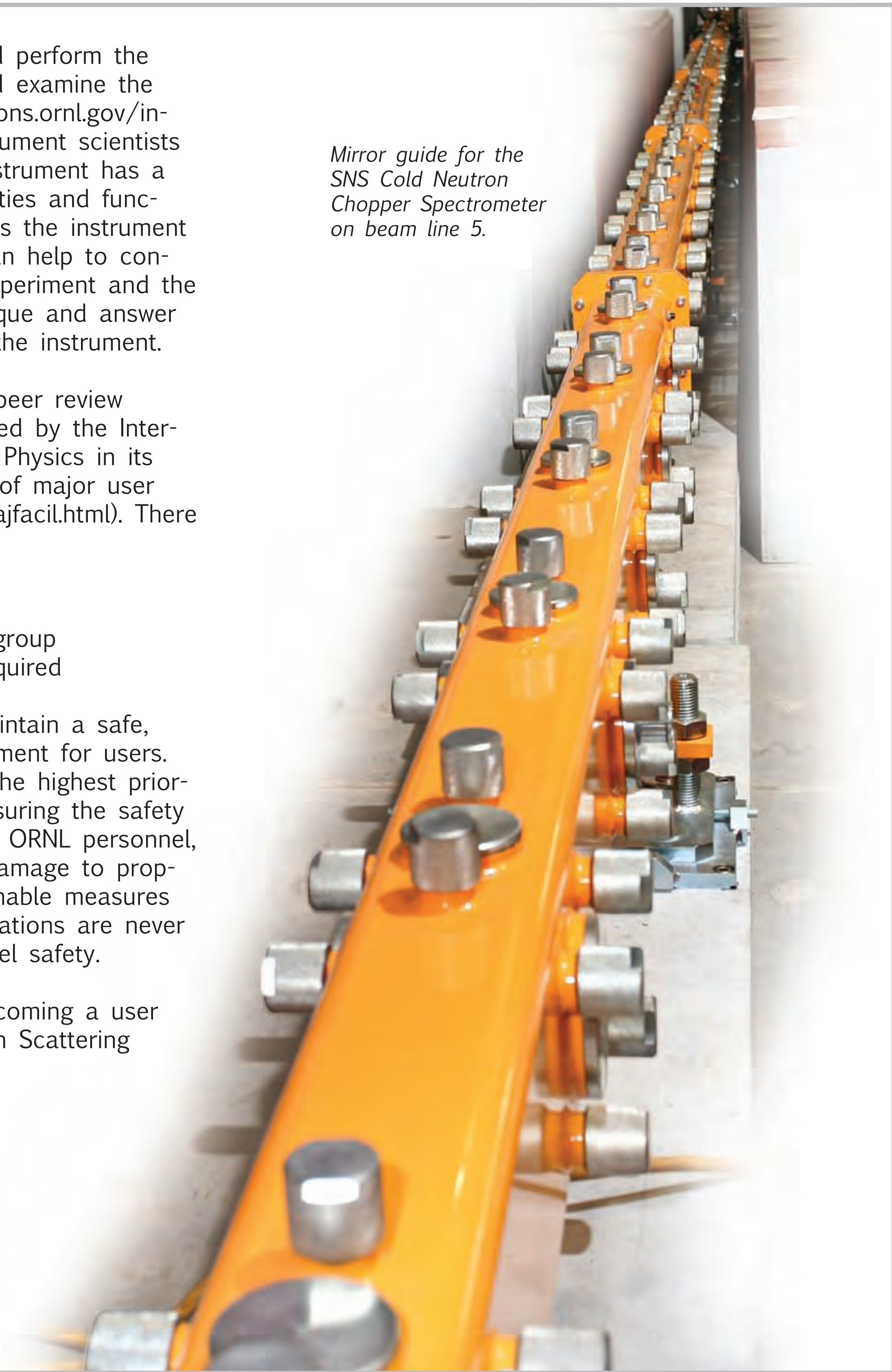
The evaluation criteria used in the peer review procedures for all users are proposed by the International Union of Pure and Applied Physics in its recommendations on the operation of major user facilities (www.iupap.org/ga/ga22/majfacil.html). There are four criteria:

- scientific merit
- technical feasibility
- capability of the experimental group
- availability of the resources required

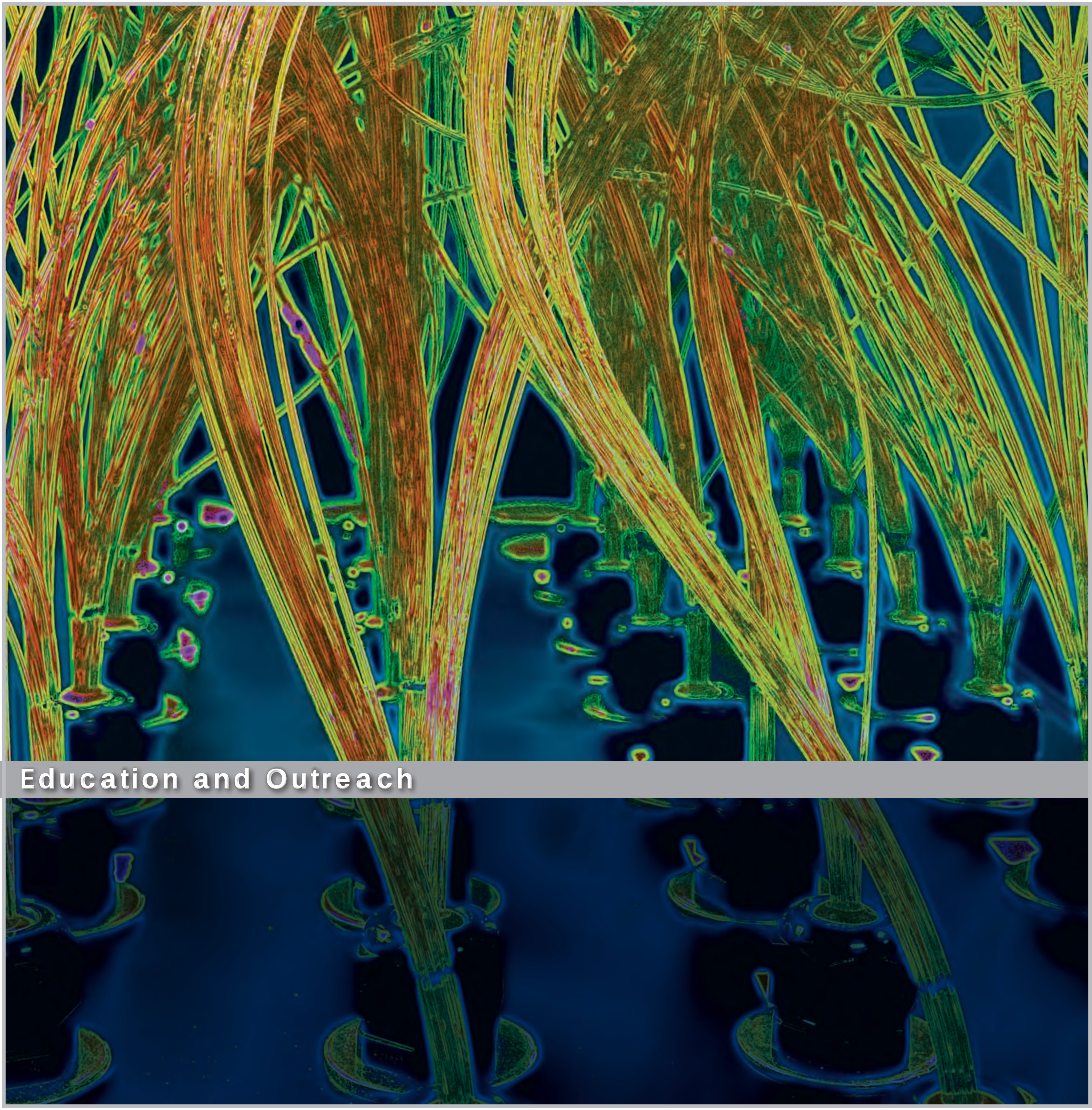
The goal of HFIR and SNS is to maintain a safe, ecologically sound research environment for users. Facility staff and users shall place the highest priority on protecting the health and ensuring the safety of HFIR and SNS users and visitors, ORNL personnel, and the public and on preventing damage to property and the environment. All reasonable measures will be taken to do so. Facility operations are never given a higher priority than personnel safety.

For additional information about becoming a user at HFIR or SNS, contact the Neutron Scattering Science Division User Office:

neutronuser@ornl.gov
865.241.3675
neutrons.ornl.gov/users.



Mirror guide for the SNS Cold Neutron Chopper Spectrometer on beam line 5.



Education and Outreach

On-Site Research and Educational Opportunities

One of the priorities of the Neutron Sciences is to educate scientists, students, and the public about the benefits and possibilities of neutron scattering research. Some of the ways we accomplish this include

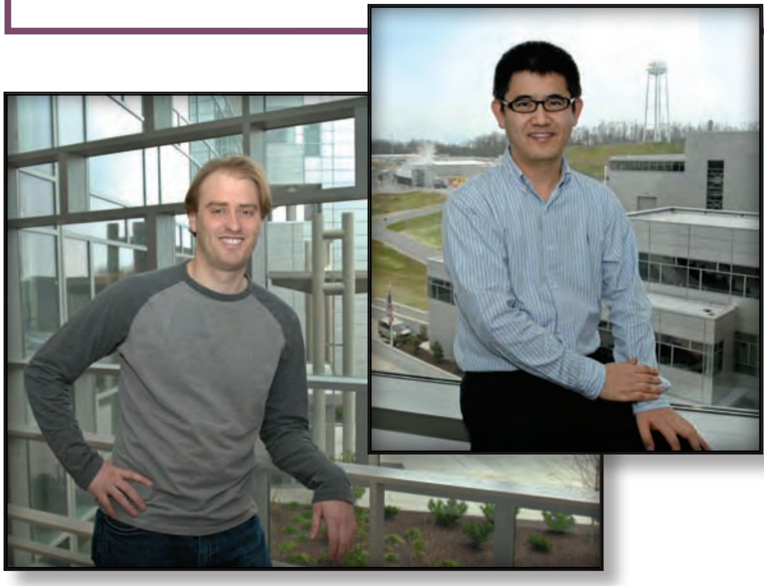
- *Fellowships and sabbatical opportunities for researchers*
- *Internships for high school and college students*
- *Meetings and workshops for the scientific community*
- *The Joint Institute for Neutron Sciences*
- *Presentations at local universities and public schools*
- *Presentations at meetings of local community organizations*
- *Facility tours for the public and special visitors*
- *Community days at HFIR and SNS that are open to the public*
- *Outreach materials such as publications, displays, and multimedia*
- *Neutron Sciences public Web site*

Fellowships

Two types of fellowships are funded by the Neutron Scattering Science Division: the Clifford G. Shull Fellowship and the Instrument Development Fellowship.

Clifford G. Shull Fellowship

The Clifford G. 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 has been 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 the 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



Shull fellows for 2006: Andrew Christianson (left) and Wei-Ren Chen (right).

Shull fellows for 2007: Christopher Stanley (left) and Sylvia McLain (right).

leadership. Appointments are for two years, with the possibility of being renewed for a third.

To date, four Shull fellows have been appointed, two each in 2006 and 2007:

- Andrew Christianson, Colorado State University
- Wei-Ren Chen, Massachusetts Institute of Technology
- Sylvia McLain, University of Oxford and ISIS
- Christopher Stanley, National Institute of Standards and Technology and the National Research Council

Instrument Development Fellowship

The Instrument Development Fellowship focuses on the development of novel neutron instrumentation and instrument components to be used for neutron science at ORNL or other U.S. neutron centers. The call is directed to scientists within 10 years of their Ph.D. who are located at academic, industrial, or government institutions. This fellowship was established in 2006, and the first appointment was made in 2007 to Thorwald Van Vuure, Institute for Transuranium Elements, Karlsruhe, Germany. Appointments will range from one to three years.

Candidates are evaluated through their proposal submissions. Proposals should contain ideas for novel concepts for neutron instrumentation that will enable unexplored areas of science to be addressed or that will significantly improve current methods in the field. Proposals may describe an entire instrument concept or a major component of an instrument including, but not limited to, detectors, polarization techniques, optical components, analysis software, or source components.

Internships and Postdoctoral Appointments

Every year the Neutron Sciences Directorate sponsors internships for high school and college students. In 2007, we hosted a record 42 summer students. Some of these students were invited to extend their appointments for longer periods. Applications from each student are reviewed, an interview is conducted, and selected students are assigned to a 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 ensuring that the student is given opportunities to learn and grow from the experience.

Postdoctoral appointments are also made throughout the year. During the past year, 16 postdoc assignments were made.

Contact: Bob Martin (martinrg@ornl.gov)

neutrons.ornl.gov/jobs/fellowships.shtml

Summer interns sponsored by Neutrons Sciences participate in a poster session during their tenure at ORNL. Each student is assigned a mentor in his or her field, who helps the student develop a poster summarizing the summer's main project. Right: DOE-Oak Ridge Federal Project Director David Arakawa talks with students at the poster session.

Joint Institute for Neutron Sciences

The Joint Institute for Neutron Sciences (JINS) promotes and supports research using the HFIR and SNS neutron scattering facilities. JINS was founded by ORNL and the University of Tennessee to serve as an intellectual center for the neutron sciences and as a gateway for users of ORNL's neutron facilities. It is one of four ORNL joint institutes funded by the state of Tennessee.

JINS sponsors fellowships and sabbatical opportunities to draw neutron scientists from all over the world, joint faculty appointments between ORNL and its university partners, and scholarships for graduate students and young faculty members to workshops related to HFIR and SNS programs.

The first researcher selected to visit ORNL on a JINS sabbatical is Julia Chan of the Chemistry Department of Louisiana State University (LSU). Chan will work at SNS in 2008. She will investigate the structures of new materials discovered in her LSU laboratory, including several highly correlated electron systems and cerium and ytterbium intermetallics (powder and single crystals). Neutron diffraction and scattering measurements will be invaluable to Chan's research to determine the atomic positions of lighter elements and elements with similar atomic numbers.

During 2007, JINS provided support to visiting scholars to attend these neutron science workshops:

- Educational Symposium on Neutrons for Materials Science and Engineering, April 2007
- Neutron Stress, Texture, and Phase Transformation for Industry, April 2007
- ORNL Users Week, October 2007

Construction of a JINS building near SNS is scheduled for 2008. This image below shows the layout of the JINS building on the Chestnut Ridge site. The facility is expected to be completed in late 2009.

Contact: Al Ekkebus (ekkebusae@ornl.gov)

neutrons.ornl.gov/jins/

Julia Chan (left) explaining single-crystal structure analysis with students at Louisiana State University.

Meetings and Workshops

To fulfill its goal of excellence in science, the Neutron Sciences Directorate aims to attract members of the science and engineering community and develop expertise to effectively use ORNL's neutron facilities. Two ways of accomplishing those goals are outreach efforts and leadership and active participation in the scientific community. The outreach effort includes active participation by Neutron Sciences staff in educational programs for the user community. These include special sessions at conferences or specialized workshops in which the benefits and capabilities of neutron scattering are described for at least one scientific discipline. Community leadership and participation involves staff taking a role in discussing, identifying, and planning a path forward for future research and enabling technologies.

Outreach Participation

Workshop	Date	Location
Educational Symposium on Neutrons for Materials Science and Engineering Oak Ridge Chapter of ASM	April 18, 2007	Oak Ridge, Tennessee
Neutron Stress, Texture, and Phase Transformation for Industry	April 19, 2007	Oak Ridge, Tennessee
American Crystallographic Association, 2007 Annual Conference	July 21–26, 2007	Salt Lake City, Utah
Renewable Energies for a Global Economy, Experimental Program to Stimulate Competitive Research Program Review Workshop	July 23–25, 2007	Golden, Colorado
2007 Denver X-Ray Conference	July 30–August 3, 2007	Colorado Springs, Colorado
SKIN 2007—Studying Kinetics with Neutrons	September 27–28, 2007	University of Göttingen, Germany
ORNL Users Week	October 8–12, 2007	Oak Ridge, Tennessee
MRS 2007 Annual Meeting	November 25–30, 2007	Boston, Massachusetts

These educational efforts will be complemented by the Workshop on Neutron Scattering Education to be held in 2008. The goal of the workshop is to develop a roadmap for neutron scattering education in the United States. The roadmap will serve as a plan for expanding current capabilities and opportunities within the neutron sciences community through collaboration between participating academic institutions and neutron scattering facilities.

Contact: Al Ekkebus (ekkebusae@ornl.gov)

neutrons.ornl.gov/calendar/past_events.shtml

Attendees at a 2007 Users Week Workshop at SNS.

Distinguished Visitors

HFIR and SNS welcome visitors for tours of their facilities. Distinguished visitors in 2007 included legislators and their staff members, officials of DOE and other federal agencies, Tennessee and local government officials, delegations from other countries, and representatives of other research institutions.

One of the big events for 2007 came in August when U.S. Senator Lamar Alexander and U.S. Congressmen Bart Gordon and Zach Wamp of Tennessee participated in a panel discussion at SNS about the America COMPETES Act. Other panel participants were DOE–Oak Ridge Office Manager Gerald Boyd, Oak Ridge Associated Universities President Ron Townsend, University of Tennessee Executive Vice-President David Milhorn, and Oak Ridge High School teacher Benita Albert. During the event, ORNL Director Thom Mason announced that SNS had officially become the world's most powerful pulsed spallation neutron source when the protons-on-target power passed the 180-kW mark earlier in August.

Contact: Al Ekkebus (ekkebusae@ornl.gov)

neutrons.ornl.gov/visitors/

DOE-Oak Ridge Office Manager Gerald Boyd, Congressman Zach Wamp, ORNL Director Thom Mason, and Senator Lamar Alexander during the August 2007 America COMPETES Act and SNS record announcement media event at SNS.

Neutron Sciences Visitors in 2007	
February 21	Staff from the office of U.S. Senator Bob Corker
March 8	Jeff Kupfer, Chief of staff for Energy Secretary Bodman
March 23	Ambassador Howard Baker, Jr.
April 5	Staff from the offices of U.S. Senators from New Mexico Pete Dominici and Jeff Bingaman
April 5	Japan Atomic Energy Agency
May 8–9	Tokyo Institute of Technology
May 17	General Kaname Ikeda, director of the International Thermonuclear Experimental Reactor project
June 20	National Council of State Legislatures Advisory Council on Energy
June 20	University of Tennessee Board of Trustees
August 29	British Consulate
August 30	U.S. Senator Lamar Alexander and Congressmen Zach Wamp and Bart Gordon
September 14	Oak Ridge Mayor Tom Beehan
September 26	Nuclear Regulatory Commission Commissioner Pete Lyons
September 28	University of Tennessee Chancellor Loren Crabtree

People

Neutron Sciences Staff

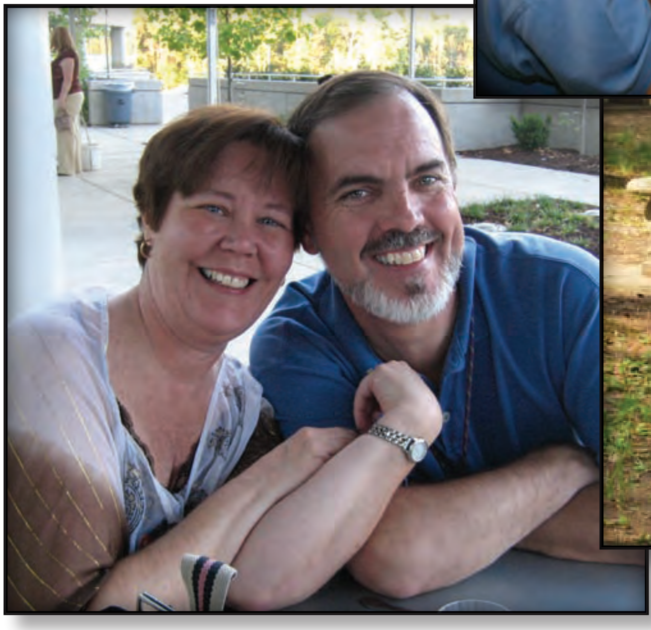
The ORNL Neutron Sciences Directorate is composed of four divisions, each focused on a specific mission:

- Neutron Scattering Science
- Neutron Facilities Development
- Research Accelerator
- Research Reactors

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 the Center for Nanophase Materials Sciences, other ORNL research divisions, 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.

The directorate hired 85 new staff members in 2007 and hosted 42 students throughout the year. The visiting 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 the 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. Employees also participate in Lab-sponsored activities such as community day and family day, when staff can invite their families to come visit the HFIR and SNS sites.



Clockwise left to right: Cathy and Bob Cummins at the SNS completion celebration. David Glasgow with his children, Brady (left) and Bailey (right), at the July 21 HFIR Family Day. Melissa Ward and her granddaughter, Aaliyah, at the directorate picnic.

Awards and Honors

Neutron Sciences staff received a number of prestigious honors and awards during 2007 from ORNL, the U.S. Department of Energy (DOE), and academic and professional organizations. Several other ORNL staff received awards based on research conducted at Neutron Sciences facilities.

Referred to by *The Chicago Tribune* as "The Oscars of Invention," the prestigious R&D 100 Awards were established in 1963 by what is now *R&D Magazine*. Each year awards are presented to recognize the 100 most technologically significant, innovative new products and processes in industry, academia, and government. The more than 50 outside judges who participate each year are chosen from among professional consultants, university faculty, and industrial researchers with expertise in the areas they are judging.

Pictured left to right are Cooper, Clonts, and Riedel.

Researchers Richard Riedel and Ronald Cooper (Neutron Scattering Science Division), and Lloyd Clonts (Energy and Engineering Sciences Division) received a 2007 R&D 100 Award for Pharos—a neutron detector system that can be used to identify nuclear materials at airports or other locations. Pharos can determine the direction and distance from which neutrons are coming, enabling it to track targets once they've been identified.

Stephen E. Nagler was named a UT-Battelle Corporate Fellow. Nagler is chief scientist for the Neutron Scattering Science Division, overseeing the development and implementation of strategies for leadership in neutron sciences. Designation as a Corporate Fellow recognizes exceptionally accomplished ORNL staff members for achievements in science or engineering. Corporate Fellows are characterized by innovation, dedication, and significant contributions to research and development that are acknowledged nationally and internationally.

Herbert A. Mook, Jr., was elected as a fellow of the American Association for the Advancement of Sciences (AAAS) and to the Neutron Scattering Society of America's (NSSA's) inaugural group of fellows. Mook, the first scientific director of SNS and former director of ORNL's Center for Neutron Scattering, is a UT-Battelle Senior Corporate Fellow.

The AAAS Council recognized Mook's "pioneering experiments using neutron scattering in materials that test theories leading to understanding of novel physics and new directions of research." Two of Mook's inventions—the neutron transmission polarizer and the ultrasonically pulsed neutron spectrometer—received R&D 100 awards. The NSSA honored Mook for his neutron scattering experiments on novel phenomena in condensed matter, including investigations of the magnetic interaction and its role in the properties of superconducting materials. The society also cited Mook's work advancing the art of neutron scattering research.

Ronald A. Crone, director of the Research Reactors Division, was honored at ORNL's Awards Night for "Administrative and Operational Leadership at the Director Level" for outstanding leadership in successfully establishing HFIR once again as a world-class research tool. Crone (right) is pictured with ORNL Director Thom Mason.

Frank Kornegay, SNS operations manager, was honored by Purdue University's Department of Earth and Atmospheric Sciences as an outstanding alumnus. Kornegay received his B.S. and M.S. degrees in atmospheric science from Purdue.

Awards for Research at Neutron Sciences Facilities

Saed Mirzadeh of the Nuclear Science and Technology Division received the American Nuclear Society's 2007 Seaborg Medal Award. Mirzadeh is internationally known for contributions to the development of radioisotopes. Mirzedeh works with the Nuclear Medicine Program, through which ORNL supplies many of the radioisotopes used for medical procedures. The award was based in part on research conducted at HFIR.

Steven Zinkle, director of the ORNL Materials Science and Technology Division, won DOE's Ernest Orlando Lawrence Award, which honors mid-career scientists and engineers for exceptional contributions in research and development. Zinkle's work has focused on physical metallurgy of structural materials and investigating radiation effects on ceramic materials and metallic alloys for fusion and fission reactors and space reactor systems. The award was based in part on research conducted at HFIR.

Lawrence Award presented to Steve Zinkle by Energy Secretary Samuel Bodman, left, and Undersecretary for Science Raymond Orbach, right.

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 Neutron Scattering Science Division (NSSD) director and the Neutron Facilities Development Division (NFDD) director 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.

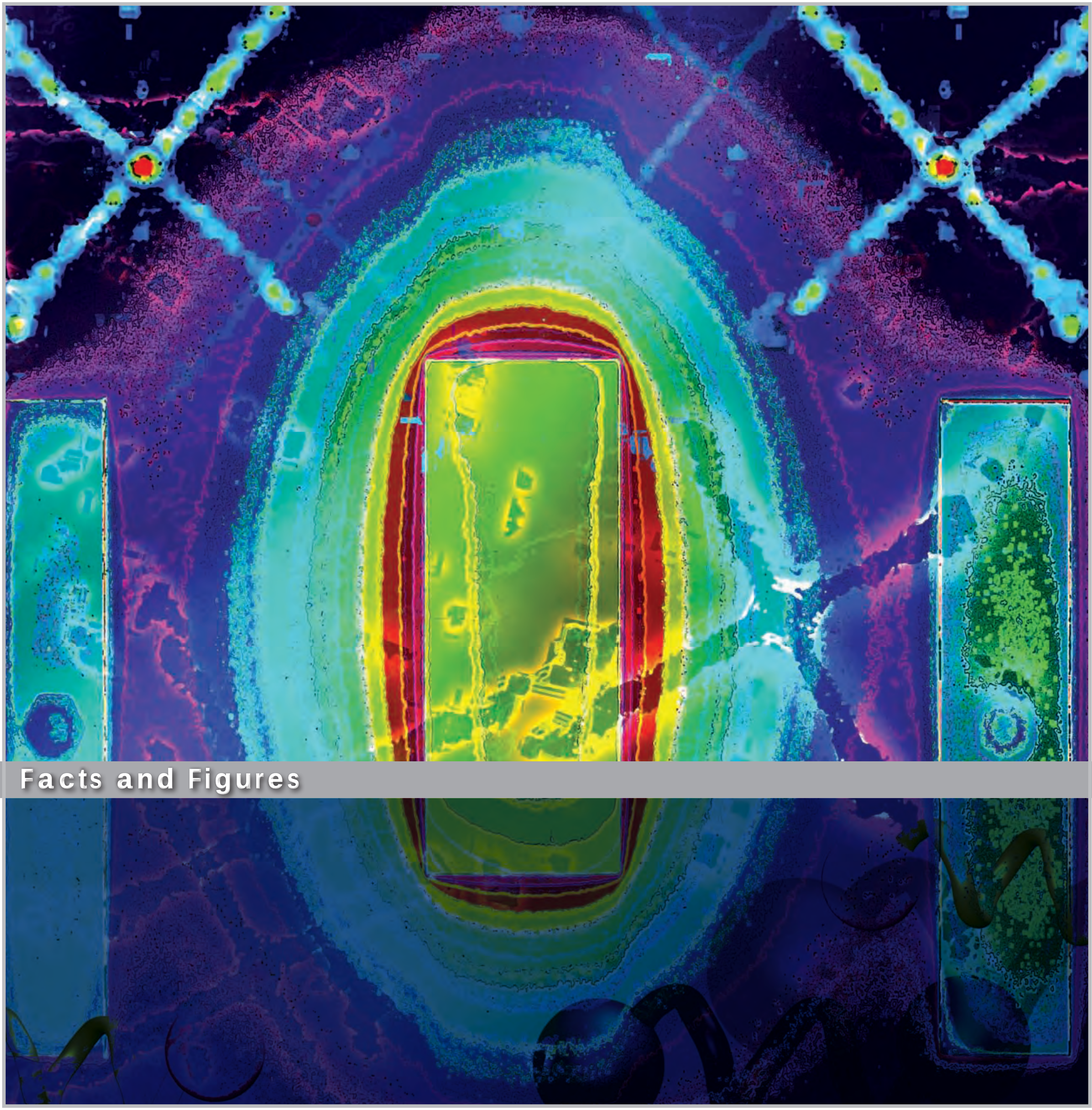
SNS Accelerator Advisory Committee

Chair, Gerry Dugan, Cornell University

This committee reports to the associate Laboratory director for Neutron Sciences and advises the Research Accelerator Division (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—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 • HB-1A	Triple-Axis Spectrometer Fixed-Incident-Energy Triple-Axis Spectrometer
Horizontal Beam Tube HB-2: Thermal Neutron Beam–Radial to Core	
• HB-2A • HB-1A • HB-2C • HB-2D	Neutron Powder Diffractometer (under development) Neutron Residual Stress Mapping Facility US/Japan Wide-Angle Neutron Diffractometer (WAND) Future development
Horizontal Beam Tube HB-3: Thermal Neutron Beam–Tangential to Core	
• HB-3 • HB-3A	Triple-Axis Spectrometer Four-Circle Diffractometer
Horizontal Beam Tube HB-4: Thermal Neutron Beam–Tangential to Core	
• CG-1 • CG-2 • CG-3 • CG-4A • CG-4B • CG-4C • CG-4D	Future development Small-Angle Neutron Scattering Diffractometer (SANS1) Small-Angle Neutron Scattering Instrument (Bio-SANS) Future development Future development US/Japan Cold Neutron Triple-Axis Spectrometer (under development) Future development

HFIR SAMPLE ENVIRONMENT

SE Description	Temperature Range (K)	Bore Size	Interface Connec-tions	Distance from Interface to Beam Center	Stick Distance to Beam Center	Special Features/ Comments	SE Team Comments	Helium Fill and Hold Time Estimates
High-temp displex-1AF	5-800	N/A	0.25-in. hole	2 in.	N/A			
Displex-1A	11-300	N/A	1/4-28 Female	2.325 in.	N/A	For use with standard sample can		
Displex-A	4-300	N/A	1/4-28 Female	2.325 in.	N/A			
Displex-B	6.5-300	N/A	1/4-28 Female	2.325 in.	N/A			
Displex-H	8-00	N/A	1/4-28 Female	2.325 in.	N/A	Optional saphirre window for SANS		
Displex-I	8-300	N/A	1/4-28 Female	2.325 in.	N/A	Turbo- 1 hour RT to base temp		
Displex-M	14-300	N/A	1/4-28 Female	2.325 in.	N/A	High capacity for use with high-pressure cells		
Omniplex-O	5.5-300	50 mm	1/4-28 Female	1.5 in. w/ +/-2 in. adj.	19-7/8 in.	Top-loading displex		
Omniplex-O2	4.8-300	50 mm	1/4-28 Female	1.5 in. w/ +/-2 in. adj.	19-7/8 in.	Top-loading displex		
4.5-Tesla horizontal field magnet	1.8-300	40 mm	M6 Male	2.325 in./59 mm	44.325 in./1125 mm	Access for SANS use only		Fill = 225 L/ 6 days at field
5-Tesla vertical field magnet	2-300	50 mm	Custom	1.97 in./50 mm	33.75 in./857 mm +/-15 mm	WAND[a] mount capable	Sample well depth = 35-7/16/40 mm be-low beam center	Fill = 60 L/ 1 day at field
7-Tesla vertical field magnet	2-300	25 mm	M6 Male	Nominal 1.5 in.	46 in.	Field limited to 5.5 T at HB-1A		Fill = 125 L/ 6 days at field
Helium cryostat-Variox 1	1.5-300	50 mm	M8 Female	Nominal 1.5 in.	46 in.			
Helium cryostat-old blue	Variable	N/A	Custom	N/A	N/A	For use with high-pressure cells		

[a] US/Japan Wide-Angle Neutron Diffractometer.

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 length[c]	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	68%
Ring extraction beam gap	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	Time-of-Flight Ultra-Small-Angle Neutron Scattering Instrument (TOF-USANS)
1B	TU	Hydrogen decoupled	Nanoscale-Ordered Materials Diffractometer (NOMAD)
S2	TU	Hydrogen decoupled	Backscattering Spectrometer (BASIS)
3	TU	Hydrogen decoupled	Spallation Neutrons and Pressure Diffractometer (SNAP)
4A	TD	Hydrogen coupled	Magnetism Reflectometer
4B	TD	Hydrogen coupled	Liquids Reflectometer
5	TD	Hydrogen coupled	Cold Neutron Chopper Spectrometer (CNCS)
6	TD	Hydrogen coupled	Extended Q-Range Small-Angle Neutron Scattering Diffractometer (EQ-SANS)
7	BU	Water	Engineering Materials Diffractometer (VULCAN)
8A	BU	Water	
8B	BU	Water	
9	BU	Water	Elastic Diffuse Scattering Spectrometer (CORELLI)
10	TU	Hydrogen decoupled	
11A	TU	Hydrogen decoupled	Powder Diffractometer (POWGEN)
11B	TU	Hydrogen decoupled	Macromolecular Diffractometer (MaNDi)
12	TU	Hydrogen decoupled	Single-Crystal Diffractometer (TOPAZ)
13	BD	Hydrogen coupled	Fundamental Neutron Physics Beam Line
14A	BD	Hydrogen coupled	
14B	BD	Hydrogen coupled	Hybrid Spectrometer (HYSPEC)
15	BD	Hydrogen coupled	Neutron Spin Echo Spectrometer (NSE)
16A	BU	Water	Chemical Spectrometer (VISION)
16B	BU	Water	
17	BU	Water	Fine-Resolution Fermi Chopper Spectrometer (SEQUOIA)
18	BU	Water	Wide Angular-Range Chopper Spectrometer (ARCS)

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

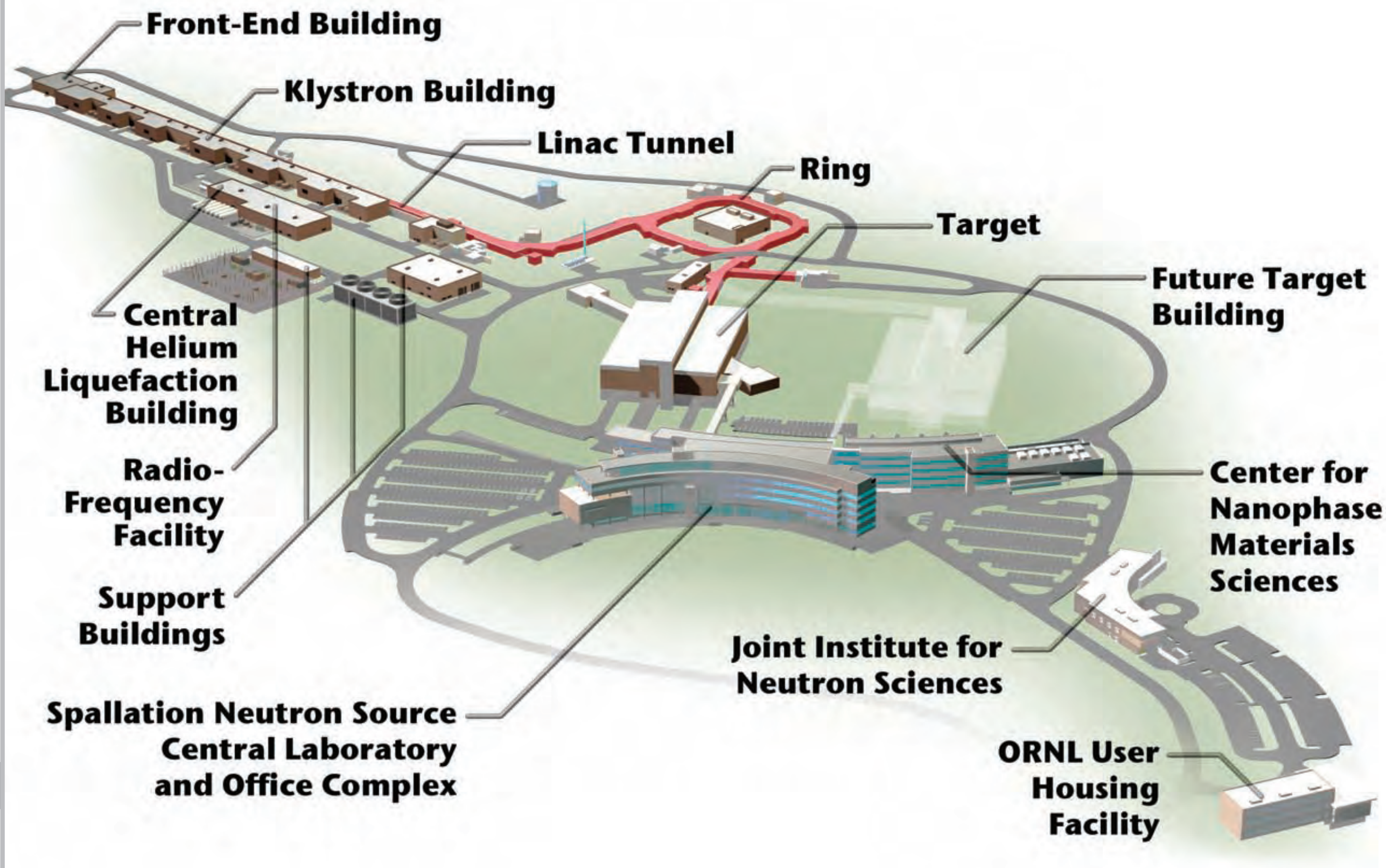
SNS SAMPLE ENVIRONMENT INVENTORY

Equipment ID	Description	Temperature Range (K)	Sample Space Diameter	Status
CRYO 01	Janis helium cryostat	2-600	58 mm	Operational
CRYO 02	Janis “SuperTran” CF cryostat	4-300	60 mm	Operational
CRYO 03	AS orange cryostat	2-300	70 mm	Operational
CCR 03	FERNS[a] auto changer	7-300	Has own vanadium cans: 4,6,8 mm	POWGEN[b] dedicated
CCR 04	Sumitomo bottom load with warm stage	7-400	55 mm	Operational
CCR 05	Top load “Split Head” CCR[c]	10-300	47 mm	available Dec. 08
CCR 06	High-temp top loader	10-500	70 mm	Operational
CCR 07	ARCS[d] goniometer	10-300	>100 mm	ARCS dedicated
CCR 08	Bottom load JT-displex	2-300	70 mm	Operational
CCR 09	Top loading CCR and 1-K pot	1.5-300	50 mm	available Sept. 08
CCR 10	CNCS[e] custom rig	4-300	TBD	Under development
HOT 01	ILL[f] vacuum furnace	300-1900	50 mm	Operational
ULT 01	He^3 insert	0.3-300	30 mm	Operational
ULT 02	Dilution insert for MAG 01	0.03-0.4	30 mm	available Sept. 08
ULT 03	Cryogen-free He^3 system	0.3-320	100 mm	available Sept. 08
MAG 01	5-T vertical field actively shielded	2-300 (compatible with ULT-02)		Operational
MAG 02	16-T vertical field actively shielded	2-300		available Dec. 09
MAG 03	2-T vertical field/ rotating displex	5-300	Special sample holder (contact SE team)	Magnetism reflectometer dedicated
HIP 01	1-kBar TiZr gas pressure cell	2-600		available May 08
HIP 02	2-kBar sapphire cell	To 670 with dedicated furnace		available June 08
HIP 03	100-Bar gas pressure stick	2 to 500 (with CCR)		available Sept. 08
Anvil pressure cells	Consult SE team for details			

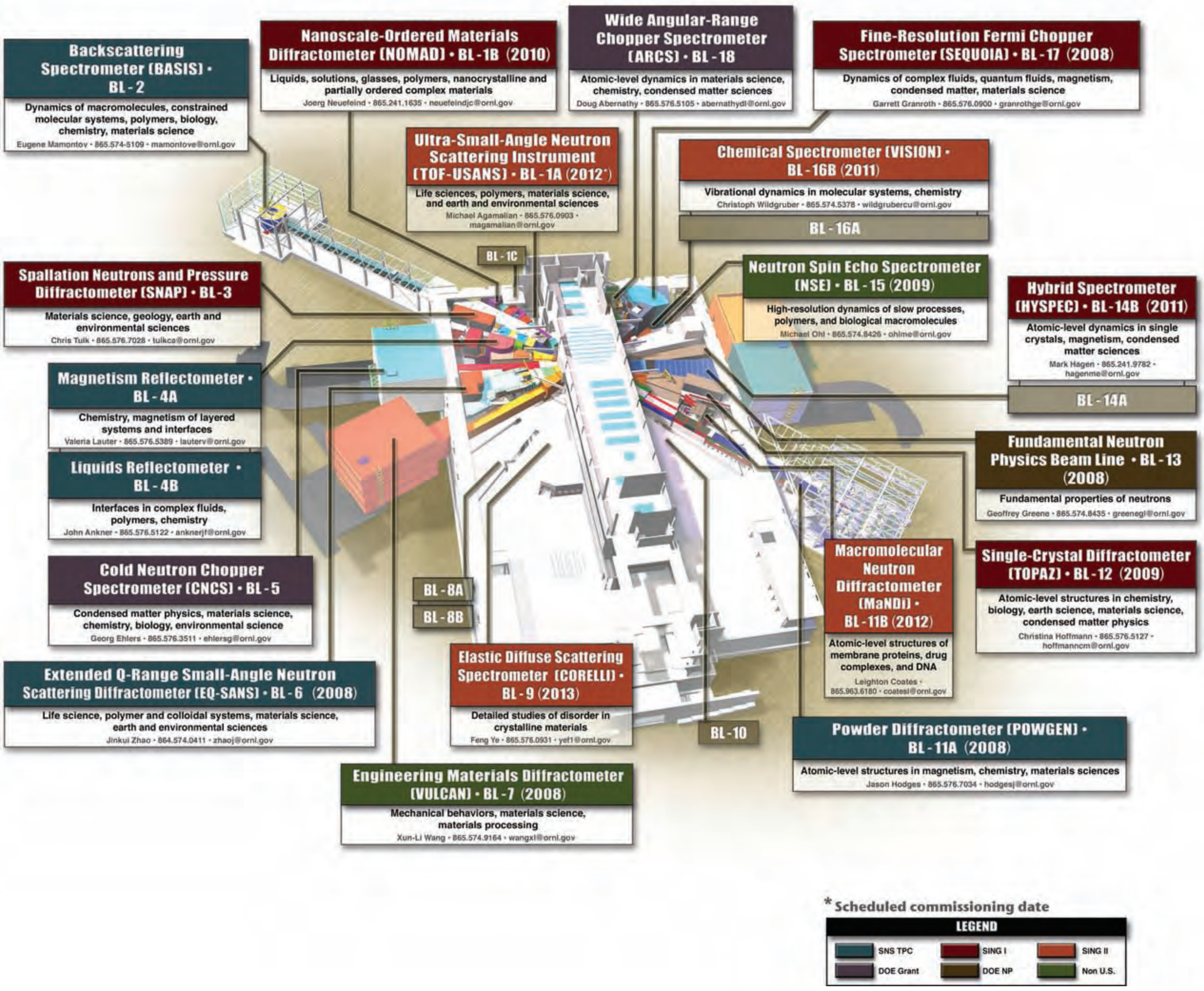
[a]Fast Exchange Refrigerator for Neutron Science.
[b]Powder Diffractometer.
[c]Closed cycle refrigerator.
[d]Wide Angular-Range Chopper Spectometer.
[e]Cold Neutron Chopper Spectometer.
[f]Institut Laue-Langevin.

Conceptual Drawing

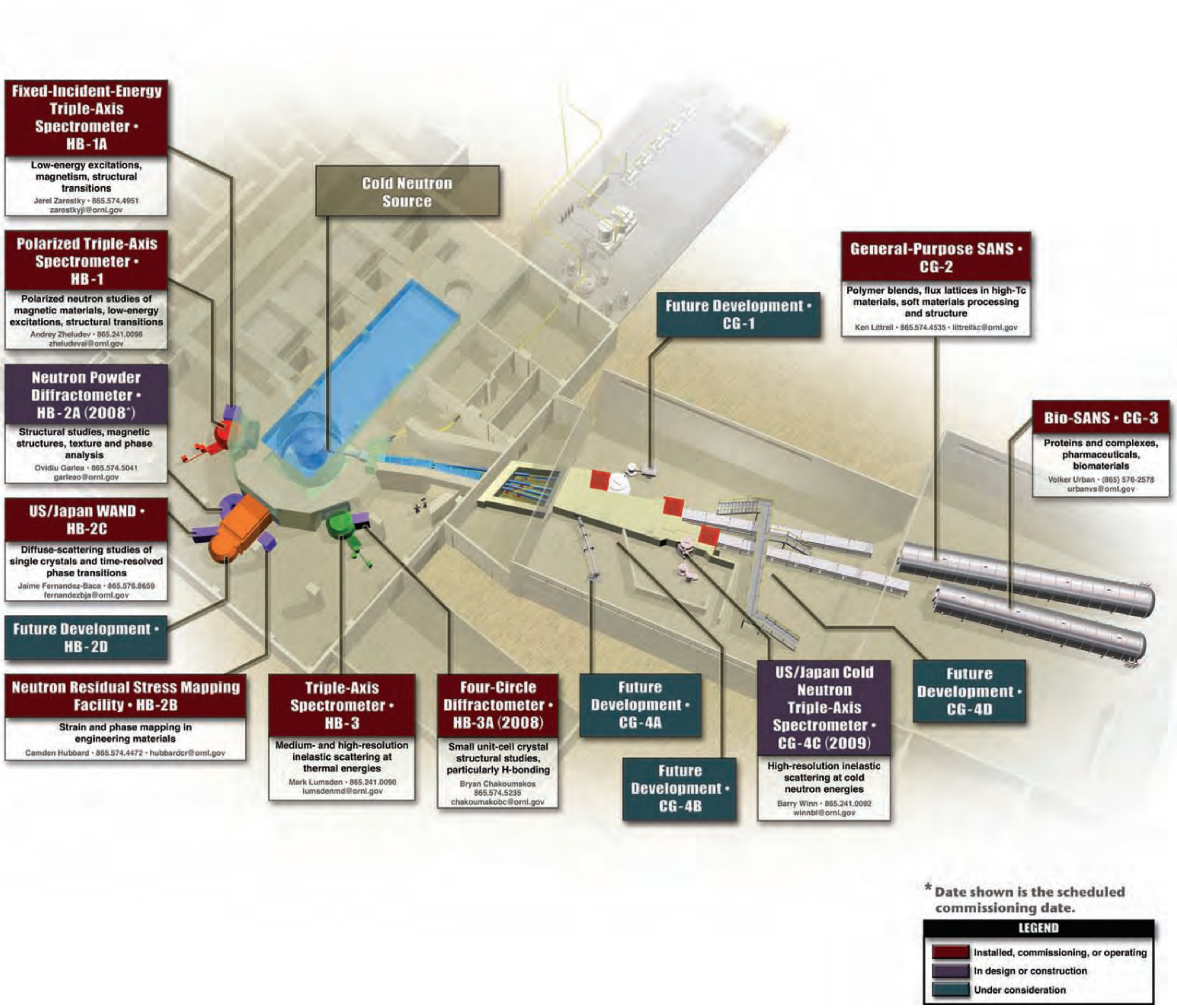
SNS



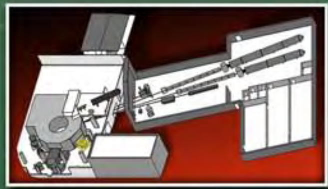
Instrument Layouts SNS



Instrument Layouts *HFIR*



Instrument Fact Sheet



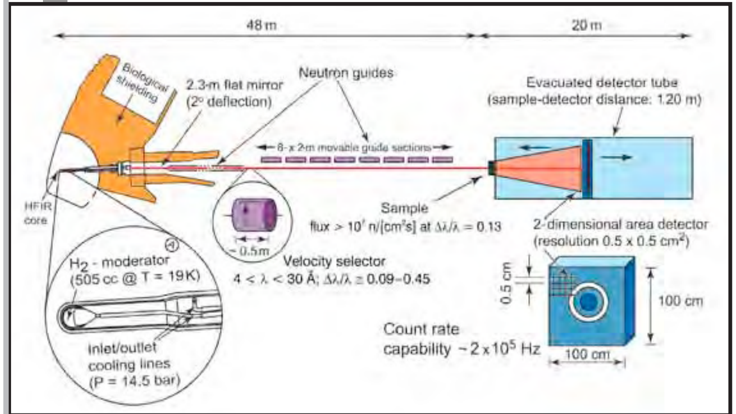
BEAM LINE

CG-2

High Flux Isotope Reactor

General-Purpose SANS – Small-Angle Neutron Scattering Diffractometer

The general-purpose SANS diffractometer is optimized for providing information about structure and interactions in materials in the size range of 0.5–200 nm. It will have cold neutron flux on sample and capabilities comparable to those of the best SANS instruments worldwide, including a wide range of neutron wavelengths λ 5–30 Å, resolution δλ/λ 9.45%, and a 1-m² area detector with 5- × 5-mm² pixel resolution with a maximum counting capability of up to 200 kHz. The sample-to-detector distance can be varied from 1 to 20 m, and the detector can be offset horizontally by up to 45 cm, allowing a total accessible Q range of from <0.001 to 1 Å⁻¹. The 2-m sample environment area will accommodate large, special-purpose sample environments such as cryomagnets, furnaces, mechanical load frames, and shear cells.



Applications

- Soft condensed matter: molecular self-assembly and interactions in complex fluids; intermediate order in glassy systems, polymer solutions, gels and blends, colloids, micelles, and microemulsions
- Hard condensed matter: phase separation, grain growth, and orientation in metallurgical alloys, nanocomposites, advanced ceramics, and porous catalytic and adsorbent materials
- Magnetic systems: flux lattices in superconductors, ferrofluids, and the relationship between structural and magnetic domains and ordering

For more information, contact

Instrument Scientist: Ken Littrell, littrellkc@ornl.gov, 865.574.4535
Instrument Scientist: Yuri Melnichenko, melnichenkoy@ornl.gov, 865.576.7746
Scientific Associate: Katherine Atchley, atchleykm@ornl.gov, 865.574.3989
http://neutrons.ornl.gov/hfir_instrument_systems/CG-2.shtml

Specifications

Beam spectrum	Cold
Monochromator	Helical slot selector
Incident wavelength	$4 < \lambda < 30$ Å
Resolution range	$\Delta\lambda/\lambda$ 0.09–0.45%
Collimation	Eight removable guide sections, each 4 × 4 cm² and 2 m long; 2-m open area at sample stage to mount automatic changers, furnaces, magnets, cryostats, pressure cells, etc.
Q range (Å⁻¹) 1.5-m collimation	$0.038 < Q < 1.0$ Å⁻¹ (5 Å); $0.019 < Q < 0.50$ Å⁻¹ (10 Å)
20-m collimation	$0.004 < Q < 0.074$ Å⁻¹ (5 Å); $0.002 < Q < 0.037$ Å⁻¹ (10 Å)
Sample-detector distances	$1 < D < 20$ m
Detector	2-D (³He) position-sensitive detector with 1-m² active area and 5.1 x 5.1 mm² pixels
Max counting rate	200 kHz

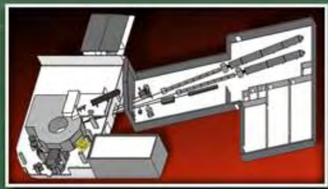
Status: Operational

May 2008

INSTRUMENT Fact Sheet

BEAM LINE **CG-3**

HIGH FLUX ISOTOPE REACTOR



BIO-SANS – BIOLOGICAL SMALL-ANGLE NEUTRON SCATTERING INSTRUMENT

Bio-SANS was designed and optimized for analysis of the structure, function, and dynamics of complex biological systems. Bio-SANS is the cornerstone of the Center for Structural Molecular Biology (CSMB) at Oak Ridge National Laboratory. The Bio-SANS instrument is supported by additional CSMB capabilities that include development of advanced computational tools for neutron analysis and modeling, as well as biophysical characterization and X-ray scattering infrastructure. A dedicated biological sample preparation laboratory is located adjacent to the instrument.

Detector tanks for the new SANS instruments at HFIR. The Bio-SANS detector is on the right.

APPLICATIONS

- Bio-macromolecules and their assemblies
  - Protein complexes
  - Protein/DNA complexes
  - Lipids
  - Viruses
  - Carbohydrates
- Biomimetic and bio-inspired systems
- Hierarchical biological structures
  - Gels
  - Fibers and fibrils
  - Vesicles
  - Microemulsions
- Membrane diffraction

USER ACCESS

Bio-SANS is operated as a user facility and is sponsored by DOE's Office of Biological and Environmental Research. The instrument is managed under the CSMB User Program. For information about the CSMB rapid access proposal process, go to www.csmb.ornl.gov.

FOR MORE INFORMATION, CONTACT

Instrument Scientist: Volker Urban, urbanvs@ornl.gov, 865.576.2578
Instrument Scientist: William Heller, hellerwt@ornl.gov, 865.241.5694
Center Director: Dean Myles, mylesda@ornl.gov, 865.574.5662

http://neutrons.ornl.gov/hfir_instrument_systems/factsheet_pdf/Instrument_cg3.pdf

SPECIFICATIONS

Wavelength	$6 < \lambda < 30$ Å
Wavelength resolution	$\Delta\lambda / \lambda$ = 12–45%
Q range	0.002–1 $Å^{-1}$
Sample-to-detector distance	1–15 m
Detector	2–D ^3He
Detector size	1 x 1 m
Detector resolution/ pixel size	5.1 x 5.1 mm^2
Max count rate	200 kHz

CENTER CAPABILITIES

X-ray scattering
Light scattering
Computational tools
Bio-support lab
Protein production + analysis
Bio-deuteration lab

Status: Operational

May 2008

Instrument Fact Sheet

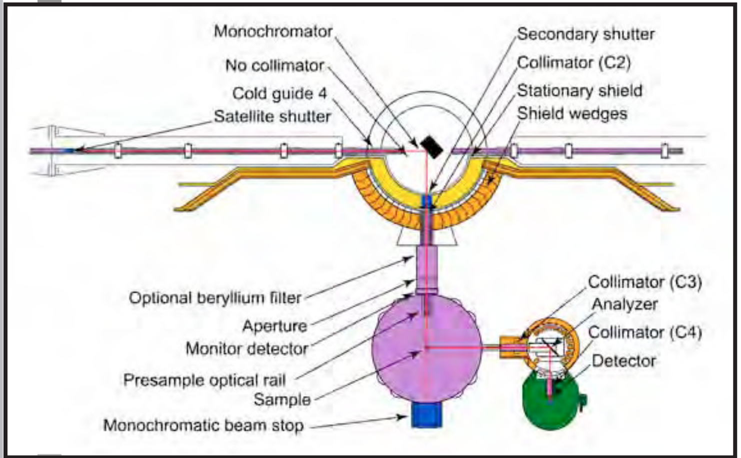
BEAM LINE

CG-4C

High Flux Isotope Reactor

US/Japan Cold Neutron Triple-Axis Spectrometer

The US/Japan Cold Neutron Triple-Axis Spectrometer is a conventional triple-axis spectrometer with variable incident energy and variable monochromator-sample and sample-analyzer distances. The cold guide 4 bender and guide hall shielding reduce background levels at CG-4C, and the 15-cm-tall guide profile is well exploited by CG-4C's vertically focusing monochromator (PG 002). To enhance accommodation of strong magnetic fields at the sample position and to simplify future polarization analysis, the amount of ferromagnetic material has been minimized in the construction of this instrument.



CG-4C is a collaboration of the Neutron Scattering Science Division at Oak Ridge National Laboratory, the Neutron Scattering Group at Brookhaven National Laboratory, and the Neutron Science Laboratory, Institute for Solid State Physics, at the University of Tokyo.

Applications

- High-resolution measurement of low-energy excitations with high signal-to-noise ratios due to the low background
- Studies of magnetic phenomena, exploiting the energy range that matches achievable applied field at sample

For more information, contact

Principal Investigator: Steve Shapiro, shapiro@bnl.gov, 631.344.3822
Principal Investigator: Hideki Yoshizawa, yoshi@issp.u-tokyo.ac.jp
Instrument Scientist: Barry Winn, bwinn@bnl.gov, 865.241.0092
http://neutrons.ornl.gov/hfir_instrument_systems/CG-4C.shtml

Specifications

Incident energy range (PG 002)	2–20 meV
Final energy range (PG 002)	>2.8 meV
Sample scatter angular range	Geometry dependent (<160°)
Collimation before mono-chromator	Guide dependent (40' at 2 meV, 20' at 20 meV)
Collimation after mono-chromator	10', 20', 40', 80'

Status:
To be commissioned in 2008

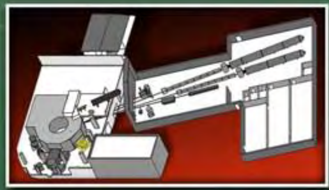
May 2008

Instrument Fact Sheet

BEAM LINE

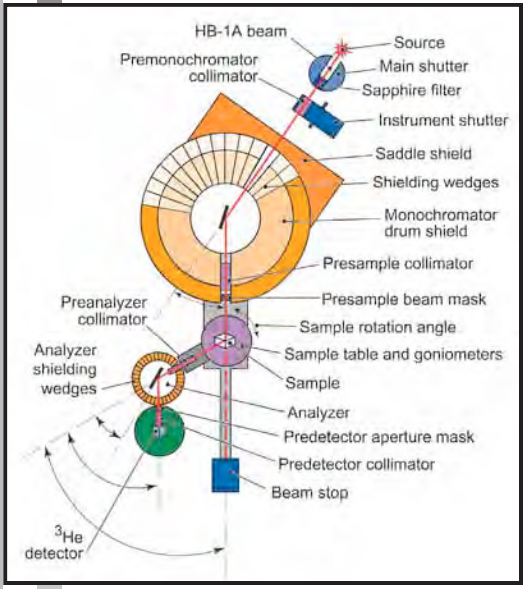
HB-1

High Flux Isotope Reactor



Triple-Axis Spectrometer

The HB-1 Triple-Axis Spectrometer is designed primarily for the study of excitations in crystalline solids at intermediate energies. Thanks to the vertical beam focusing and the very high time-averaged flux at HFIR, its geometry is optimal for investigating small samples and weak scattering in specific areas of energy-momentum space. The sample goniometers and a full software implementation of the three-dimensional sample orientation matrix allow measurements outside the traditional single-scattering plane. The unique capability of HB-1 is the polarized configuration for studies of excitations, phase transitions, structures, and density distributions in magnetic materials.



Applications

The following are some of the scientific applications for which the Triple-Axis Spectrometer is particularly well suited.

- Spin waves in ordered magnetic materials
- Exotic excitations in low-dimensional, molecular, itinerate, and other "quantum" magnets
- Spin and lattice excitations in high-T_c superconductivity, colossal magnetoresistance materials, and multiferroic systems
- Spin density distributions in magnetic compounds
- Phonon dispersion curves in alloys and phonon-driven phase transitions

For more information, contact

Instrument Scientist: Andrey Zheludev, zheludevai@ornl.gov, 865.241.0098

http://neutrons.ornl.gov/hfir_instrument_systems/HB-1.shtml

Specifications

Beam spectrum	Thermal
Monochromators	Unpolarized PG(002) Polarized (not currently available)
Analyzers	Unpolarized PG(002), Be(101), Be(002) horizontally focused PG(002) Polarized (not currently available)
Monochromator angle	18 to 75°
Sample angles	0 to 360°
Scattering angle	–90 to 140°
Analyzer angles	–40 to 140°
Collimations (FWHM)	C1: 0.25, 0.5, 0.8° C2: 0.166, 0.333, 0.666, 1, 1.333° C3: 0.166, 0.333, 0.666, 1, 1.333° C4: 0.333, 0.666. 1, 2°

Status: Operational

HFIR

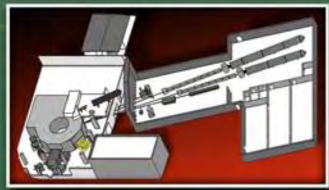
May 2008

Instrument Fact Sheet

BEAM LINE

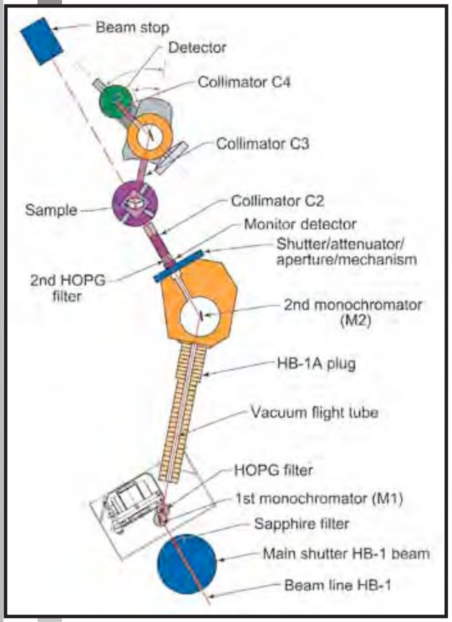
HB-1A

High Flux Isotope Reactor



Fixed-Incident-Energy Triple-Axis Spectrometer

The Fixed-Incident-Energy (14.6 meV) Triple-Axis Spectrometer uses a double pyrolitic graphite monochromator system. The first monochromator is vertically focused, and the second can be either a vertically or doubly focused unit. Two highly oriented pyrolytic graphic filters (HOPG), one after each monochromator, are used to reduce λ/2 contamination. These filters, together with the double monochromator system, provide HB-1A with an exceptionally clean beam in terms of higher-order contamination neutrons: $I_{\lambda/2} \approx 10^{-4} \times I_{\lambda}$. This spectometer also has one of the most intense beams at this energy at the HFIR, as well as a very low γ and fast neutron background. Typical energy resolution is ~1 meV, but, using the beryllium analyzer, the energy resolution width can be reduced to ~0.5 meV.



HB-1A development and operation is a collaborative effort of the Oak Ridge National Laboratory and Ames Laboratory neutron scattering groups.

Applications

- Excitation spectra to ~35 meV using neutron energy gain and low-lying excitations, 1–9 meV, using neutron energy loss
- Elastic studies on crystallographic and magnetic structures and transitions in a Q range of 0.2 to 4.9 $Å^{-1}$
- Elastic studies and excitations in thin films and other small-volume samples where high flux and very low higher-order contamination of the beam are critical

Recent experiments on this instrument include measurement of phonon dispersion curves in martensitic, shape-memory, and magnetostrictive alloys; crystallographic and magnetic structure determinations in giant magnetocaloric, magnetoresistive, and intermetallic alloys; magnetic structures and spin-density waves in thin films; magnetism in low-dimensional systems; and spin waves and magnetic structures in magnetoelectric materials.

For more information, contact

Instrument Scientist: Jerel Zarestky, zarestkyjl@ornl.gov, 865.574.4951

http://neutrons.ornl.gov/hfir_instrument_systems/HB-1A.shtml

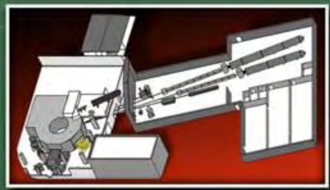
Specifications

Beam spectrum	Thermal
Monochromator	PG(002) double crystal
Monochromator angle	$2\Theta_M = 41.3°$ E_i = 14.6 meV
Analyzers	PG(002) Be(101) Be(002) Si(111) Ge(111)
Sample angles	0° < s1 < 360°
Scattering angle	-5° < s2 < 135°
Analyzer angles	-60° < a2 < 120°
Collimations (FWHM)	C1: open (48' effective) C2: open (40' effective) (30', 20', 10') C3: 40', 30', 20',10' (sample analyzer) C4: 34', 68', 136' (analyzer-detector)
Beam size	40 × 150 mm max
Filters	Sapphire pre-monochromator-1 2-HOPG; after M-1 and M-2 ($I_{\lambda/2} \approx 10^{-4} I_{\lambda}$)
Flux at sample	~ 2 × 10^7 n/cm^2/s (est.)
Momentum range	0.2 to 4.9 $Å^{-1}$ (elastic configuration)
Energy transfer	~-35 meV to ~+11 meV at q = 3 $Å^{-1}$

Status: Operational

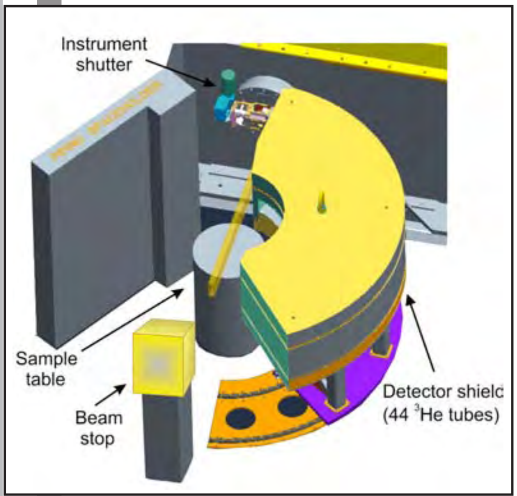
May 2008

Instrument Fact Sheet
BEAM LINE
HB-2A
High Flux Isotope Reactor



Neutron Powder Diffractometer

The Neutron Powder Diffractometer has a Debye-Scherrer geometry. The detector bank has 44 ^{3}He tubes, each with 6’ Soller collimators. A germanium wafer-stack monochromator is vertically focusing and provides one of three principal wavelengths, depending on which reflection is in the diffracting condition: (113) 2.41 Å, (115) 1.54 Å, and (117) 1.12 Å. The takeoff angle from the monochromator is fixed at 90°, and the minimum peak full width at half maximum (FWHM) is 0.2°. There are two choices of premonochromator collimation (α_1 = 12’ or open) and three choices of presample collimation (α_2 = 16’, 21’, or 31’) that allow the operation of the instrument in high-resolution or high-intensity modes.



Applications

The HB-2A Neutron Powder Diffractometer is a workhorse instrument used to conduct crystal structural and magnetic structural studies of powdered and ceramic samples, particularly as a function of intensive conditions (T, P, H, etc.). Technologically important materials amenable to study by neutron powder diffraction include (but are not limited to) catalysts, ionic conductors, superconductors, alloys, intermetallic compounds, ceramics, cements, colossal magnetoresistance perovskites, magnets, minerals, waste forms, H-storage, thermoelectrics, zeolites, and pharmaceuticals. Powder diffraction data collected on this instrument are ideally suited for the Rietveld method. In addition to traditional crystal structural refinements, studies of phase transitions, thermal expansion, quantitative analysis, residual stress, and ab initio structure solution can be undertaken from the powder data. A full range of ancillary sample environments can be used, including cryofurnaces (4–800 K), furnaces (to 1800 K), cryostats (to 0.3 K), and cryomagnets (to 7 T).

For more information, contact

Instrument Scientist: Ovidiu Garlea, garleao@ornl.gov, 865.574.5041

http://neutrons.ornl.gov/hfir_instrument_systems/HB-2A.shtml

Specifications

Beam spectrum	Thermal
Monochromator	Vertically focusing Ge (115) 20
Monochromator angle	$2\Theta_m = 90°$
Wavelengths	λ=1.54 Å(115) 2.41 Å(113) 1.12 Å(117)
Sample angles	$0° < \omega < 360°$
Scattering angle	$-5° < 2\Theta < 165°$
Collimations (FWHM)	α_1=12’ or open α_2=16’, 21’, or 31’
Detector bank	44 ^{3}He detectors
Beam size	25 x 25 mm^2 at sample position
Resolution	2 x 10^{-3} $\Delta d/d$

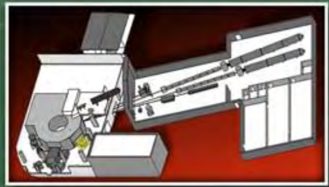
Status:
To be commissioned in 2008

May 2008

Instrument Fact Sheet

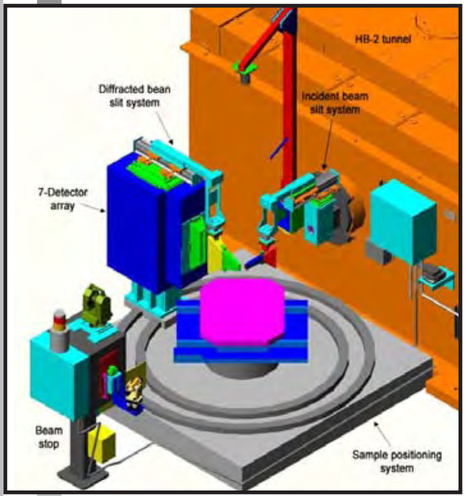
Beam Line HB-2B

High Flux Isotope Reactor



NRSF2 – Neutron Residual Stress Mapping Facility

NRSF2 at the HFIR HB-2B beam port is optimized for strain measurement and determination of residual stress in engineering materials. The large-specimen "XYZ" instrument is designed for spatial scanning of strains at depths from submillimeters to centimeters. The sample orienter can be used to determine the stress tensor and texture mapping and to study strains in large-grained materials and single crystals. The high flux and detector coverage allow real-time, in situ studies or high-resolution mapping. Ancillary equipment available for use at NRSF2 includes a 2,267-kg uniaxial (tension or compression) load frame, a Huber Eulerian cradle, high-temperature furnaces (vacuum or air), and a 5-T superconducting magnet with an induction furnace insert. Custom-built sample environment systems can be installed on the XYZ sample positioning system.



Applications

The penetrating power of neutrons is useful in mapping residual stresses in engineering materials. Examples of applications include residual stress maps of welds, heat-treated samples, forgings, extrusions, bearings and races, fasteners, and composites. Neutron diffraction studies of materials under applied stress reveal phase- and grain-level knowledge of deformation processes, which is fundamental for developing finite-element method and self-consistent field models of materials behavior. Also characterized are strains in functional materials, such as piezoelectrics under the influence of electrical fields, shape memory alloys, and hydrogen storage materials.

User Access

NRSF2 is operated as a user facility sponsored by DOE's Office of FreedomCAR and Vehicle Technologies. The NRSF2 instrument is managed under the High Temperature Materials Laboratory (HTML) User Program. Information about the HTML rapid access proposal process can be obtained from http://html.ornl.gov.

For more information, contact

Instrument Scientist: Camden Hubbard, hubbardcr@ornl.gov, 865.574.4472
http://neutrons.ornl.gov/hfir_instrument_systems/HB-2B.shtml

Specifications

Beam spectrum	Thermal
Monochromator	Stacked Si wafers with vertical and horizontal focusing
Monochromator takeoff angle	88° (fixed), λ= 1.452 Å (Si 511); 1.540 Å (Si 422); 1.731 Å (Si 331); 1.886 Å (Si 400); 2.275 Å (Si 311); 2.667 Å (Si 220)
Flux on sample	3 x 10^7 n/cm²/s (Si 331 and Si 400)
Detector angle range	70–100° optimal
Detection system	7 linear position-sensitive detectors
Position-sensitive detector coverage	5° 2Θ ±17° out of plane
Sample positioner Z elevator Z translation	Ω ± 180° X ± 200 mm Y ± 100 mm Z ± 100 mm, 500 Kg Z ± 200 mm, 50 Kg
Nominal gage volume	Width: 0.3–5 mm; Height: 0.3–20 mm
Peak location precision	0.003° 2Θ
Sample environments	• Load frame for tension and compression (2,267-kg) • Huber Eulerian cradle for tensor and texture • Vacuum and environmental furnaces • 5-T superconducting magnet with induction heater

Status: Operational

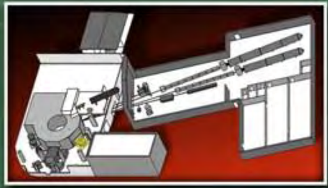
May 2008

Instrument Fact Sheet

BEAM LINE

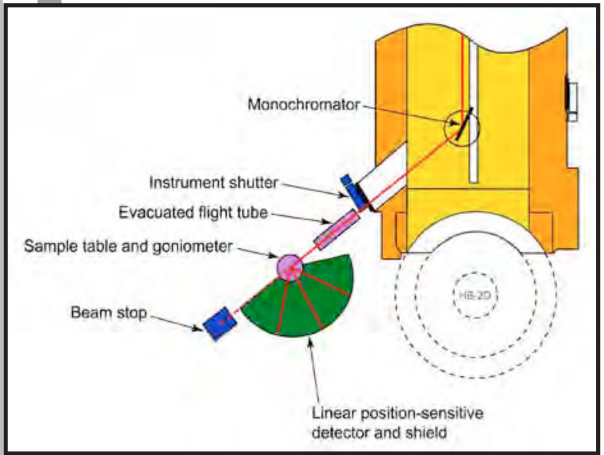
HB-2C

High Flux Isotope Reactor



WAND – US/Japan Wide-Angle Neutron Diffractometer

The US/Japan WAND at the HFIR HB-2C beam tube was designed to provide two specialized data-collection capabilities: (1) fast measurements of medium-resolution powder-diffraction patterns and (2) measurements of diffuse scattering in single crystals using flat-cone geometry. For these purposes, this instrument is equipped with a curved, one-dimensional ^{3}He position-sensitive detector covering 125º of the scattering angle with the focal distance of 71 cm.



The sample and detector can be tilted in the flat-cone geometry mode. These features enable measurement of single-crystal diffraction patterns in a short time over a wide range of the reciprocal space, as well as performance of time-resolved experiments for structural transformations having short time constants. The WAND detector (ORDELA 1410N) is a multianode type (624 anodes and a 0.2° pitch) ^{3}He gas counter specially designed for this instrument. This detector has an intrinsic angular resolution of 0.25° and a maximum counting rate per anode of 10^5 counts/s.

Specifications

Beam spectrum	Thermal
Monochromator	Vertically focused Ge(113). Ge(115) is also available to provide λ=0.95 Å
Monochromator angle	$2\Theta_M = 52.0°$
Wavelength	$\lambda = 1.5$ Å
Scattering angles	10° < 2Θ < 135°
Sample angles	0° < Ω < 135°
Detector	Multiwire (624 anodes, 0.2° pitch) He^3 curved PSD

Status: Operational

Applications

WAND is ideal for the study of time-resolved phenomena and for the study of diffuse scattering in single crystals. Research performed at WAND includes studies of the growth of ferroelectric ice-XI, hole and charge ordering in colossal magnetoresistance materials, and studies of magnetic structures and correlations in low-dimensional magnetic systems and other magnetic materials.

WAND is operated in collaboration with the Japan Atomic Energy Research Institute under the US/Japan Cooperative Program on Neutron Scattering Research.

For more information, contact

Instrument Scientist: Jaime Fernandez-Baca, fernandezbja@ornl.gov, 865.576.8659

http://neutrons.ornl.gov/hfir_instrument_systems/HB-2C.shtml

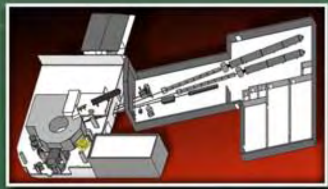
May 2008

Instrument Fact Sheet

BEAM LINE

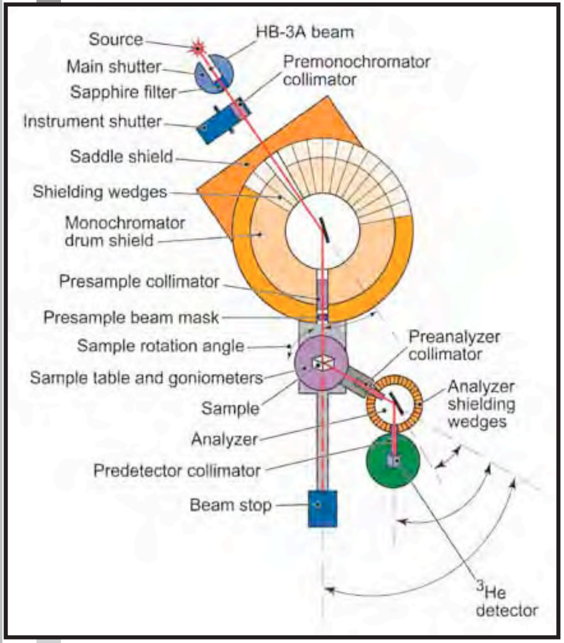
HB-3

High Flux Isotope Reactor



Triple-Axis Spectrometer

HB-3 is a high-flux thermal neutron three-axis spectrometer designed for inelastic measurements on single crystals over a wide range of energy and momentum transfers. Although the energy and momentum range for measurements is quite large at HB-3, the instrument is the ideal location for performing experiments at high-energy transfers (up to about 100 meV). This is due to a combination of its location directly at the end of the beam tube and the availability of a beryllium monochromator. The HB-3 monchromator provides three crystal choices (PG 002, Be 002, and Si 111) with variable vertical focus. This focus is calibrated to maintain the smallest beam size at the sample position, thus optimizing incident neutron flux as the incident energy varies. Of the three monochromators, pyrolitic graphite provides the highest neutron intensity as a result of its very high neutron reflectivity. The high-quality beryllium monochromator allows measurements with good energy resolution at higher energy transfers, whereas the silicon 111 monochromator has the advantage of an absent second-order reflection, providing a higher order contamination-free beam.



Specifications

Beam spectrum	Thermal
Monochromators	PG (002), Be (002), Si (111)
Analyzer	PG (002)
Monochromator angle	12–88°
Sample angle	-180–180°
Scattering angle	Up to 115°
Analyzer angle	-120–120°
Collimations (FWHM)	Premonochromator: 15', 30', 48' Monochromator - sample: 20', 40', 60' Sample - analyzer: 20', 40', 60', 80' Analyzer - detector: 70', 120', 240'

Status: Operational

Applications

The availability of three different monochromator crystals makes HB-3 an extremely versatile instrument for studies of excitations in materials with energies ranging from 2 to 100 meV. Typical applications include spin and lattice dynamics in high-temperature superconductors and related compounds; low-dimensional magnetic model systems; magnetic excitations and phonons in colossal magnetoresistive materials, multiferroics, and ruthenates; and spin waves in magnetically ordered materials. The high incident neutron flux makes HB-3 well suited to studying samples that have a small volume or weak scattering characteristics.

For more information, contact

Instrument Scientist: Mark Lumsden, lumsdenmd@ornl.gov, 865.241.0090
http://neutrons.ornl.gov/hfir_instrument_systems/HB-3.shtml

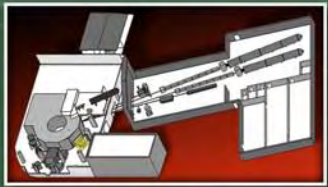
HFIR

May 2008

INSTRUMENT Fact Sheet

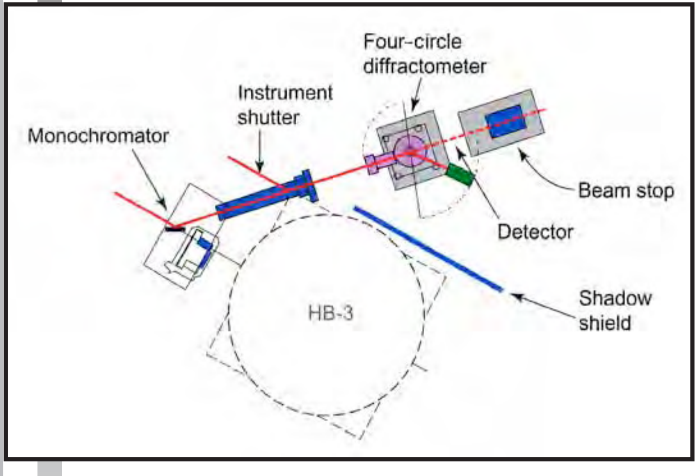
BEAM LINE **HB-3A**

HIGH FLUX ISOTOPE REACTOR



FOUR-CIRCLE DIFFRACTOMETER

The Four-Circle Diffractometer goniometer has a full χ circle with a 10-K closed-cycle helium refrigerator. The detector is ^{3}He with a 7-anode array in a honeycomb pattern. The upper 2Θ limit is 100°. A multilayer-[110]-wafer silicon monochromator with the reflection from planes of the <011> zone ensures sharp diffraction peaks in specified ranges of detector angles by control of the horizontal radius of curvature. Any plane from the <011> zone can be set in Bragg position, but only the (155), (133), (022) with (044), and (111) with (333) reflections are of practical interest. For the fixed monochromator angle of 48°, these reflections provide principal incident wavelengths of 0.618, 1.01, 1.56, and 2.55 Å, respectively. A PC-based LabView system provides user-friendly diffractometer control and data acquisition. The beam size is 5 × 5 mm^2, and the minimum crystal size is 1 mm^3. The maximum crystal dimension is about 4 mm. The flux on the sample is estimated to be greater than 5 × 10^6 n/cm^2/s.



SPECIFICATIONS

Beam spectrum	Thermal
Monochromators	Vertically focusing silicon
Monochromator angle	48°
Incident wavelength	0.618 Å (155), 1.01 Å (133), 1.56 Å (022), 2.55 Å (111)
Goniometer	Huber, full chi circle, with 10 K CCR
Scattering angle	-110° < 2θ < -110°
Detector	7 anode ^{3}He (honeycomb pattern)
Crystal size requirement	>1 mm^3
Unit-cell size	<15,000 Å^3
Flux at sample	>5 × 10^6 n cm^{-1} s^{-1} (est.)

Status:
To be commissioned in 2008

APPLICATIONS

This instrument is suitable for a wide range of small-unit-cell crystallography studies, from structure refinement and solution to charge and nuclear density mapping. Problems from chemistry, physics, materials science, and mineralogy have been addressed. Specific areas of study include hydrogen bonding and weak interactions, organometallics, supramolecular chemistry and crystal engineering, metal hydrides, charge density, pharmaceuticals, and magnetic structures. More general solid-state physics problems in magnetism, diffuse scattering, and ordering phenomena can also be addressed.

FOR MORE INFORMATION, CONTACT

Instrument Scientist: Bryan Chakoumakos, chakoumakobc@ornl.gov, 865.574.5235

http://neutrons.ornl.gov/hfir_instrument_systems/HB-3A.shtml

HFIR

May 2008

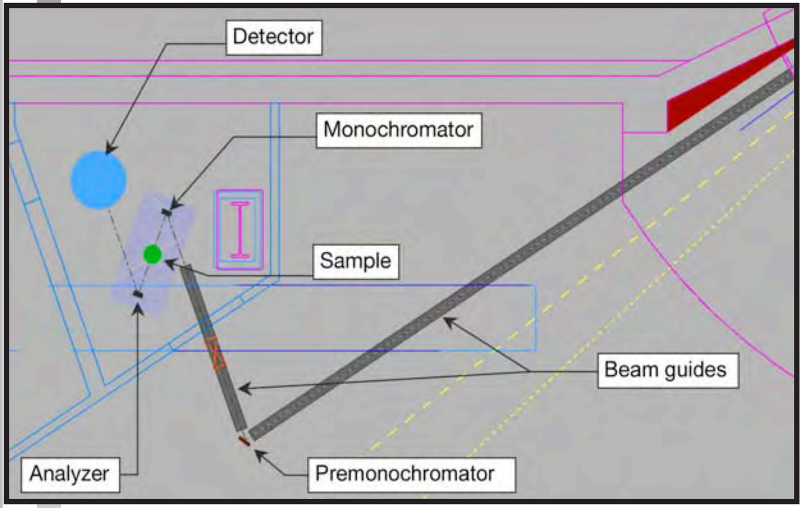
INSTRUMENT Fact Sheet

BEAM LINE 1A

SPALLATION NEUTRON SOURCE

TOF-USANS – TIME-OF-FLIGHT ULTRA-SMALL-ANGLE NEUTRON SCATTERING INSTRUMENT

The TOF-USANS instrument is designed for the study of hierarchical structures in natural and man-made materials. It can be considered an advanced version of the classical Bonse-Hart Double-Crystal Diffractometer (DCD), which, in contrast with its single-wavelength reactor-based analog, will operate with the discrete multiwavelength spectrum of Bragg reflections. The optical scheme of the TOF-USANS instrument is similar to that of the conventional Bonse-Hart DCD; however, the pulsed nature of SNS offers an opportunity to separate the orders of Bragg reflection in time space using the time-of-flight technique. Thus, the concept of the TOF-USANS technique allows optimization of the neutron flux and the Q resolution, following the principles of dynamical diffraction theory.



Discrete multiwavelength spectrum created by a family of Bragg reflections.

SPECIFICATIONS

Moderator	Decoupled poisoned hydrogen
Source detector distance	25 m
Focusing premonochromator	Bent sapphire (1120) crystal
Monochromator and analyzer	Si(220) channel-cut, triple-bounce crystals
Bragg angle	70°
Wavelength spectrum	7 Bragg reflections at 3.6, 1.8, 1.2, 0.9, 0.72, 0.6, 0.51 Å
Q range	2 10^{-6} Å^{-1} < Q < 5 10^{-3} Å^{-1}

Status:
To be commissioned in 2013

FOR MORE INFORMATION, CONTACT

Instrument Scientist: Michael Agamalian, magamalian@ornl.gov, 865.576.0903

May 2008

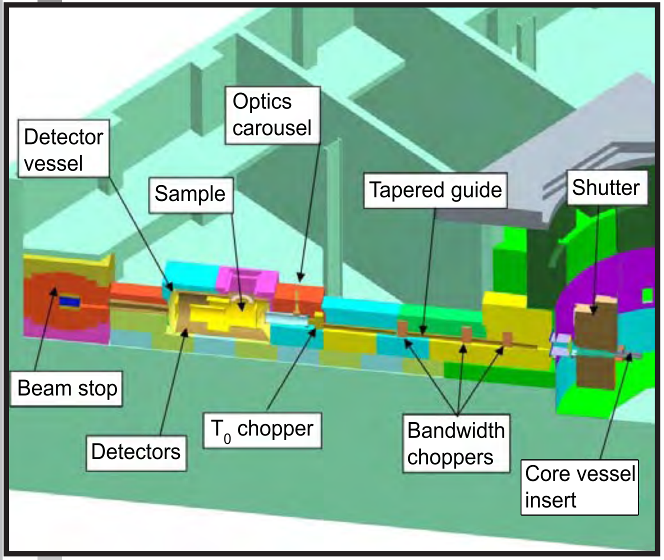
INSTRUMENT Fact Sheet

BEAM LINE 1B

SPALLATION NEUTRON SOURCE

NOMAD – NANOSCALE-ORDERED MATERIALS DIFFRACTOMETER

NOMAD is a high-flux, medium-resolution diffractometer that uses a large bandwidth of neutron energies and extensive detector coverage to carry out structural determinations of local order in crystalline and amorphous materials.The instrument enables studies of a large variety of samples, ranging from liquids and solutions, glasses, and nanocrystalline materials to long-range-ordered crystals. The enhanced neutron flux at SNS, coupled with the advanced neutron optics and detector features, allows for unprecedented access to high-resolution pair distribution functions, small-contrast isotope substitution experiments, small sample sizes, and parametric studies.



APPLICATIONS

- Environmental (e.g., solvent) effects on and direction of nanoscale structure formation
- In situ structural changes in nanoscale oxide catalysts used in automobile catalytic converters
- Structure of hydrogen storage materials under in situ conditions
- Transient structures of materials under extreme conditions (e.g., at high temperature or high pressure under the influence of transient fields or in metastable states)

FOR MORE INFORMATION, CONTACT

Instrument Scientist: Jörg Neuefeind, neuefeindjc@ornl.gov, 865.241.1635

http://neutrons.ornl.gov/instrument_systems/beamline_01b_nomad

SPECIFICATIONS

Moderator	Decoupled poisoned supercritical hydrogen
Moderator-to-sample distance	19.5 m
Sample-to-detector distance	0.5–3 m
Wavelength range	0.1–3 Å
Momentum transfer range	0.04–100 $Å^{-1}$
Detector angular range	1–175° scattering angle
Detector coverage	~10.5 sr
Flux on sample	~1 x 10^8 neutrons cm^{-2} sec^{-1}

Status:
To be commissioned in 2010

May 2008

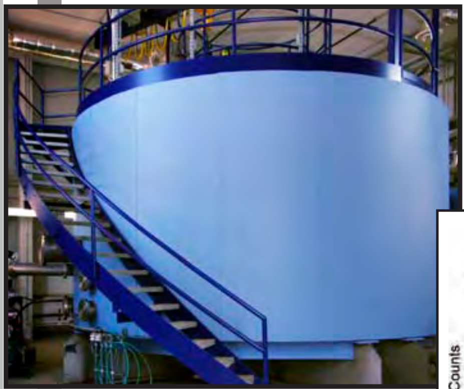
Instrument Fact Sheet

BEAM LINE 2

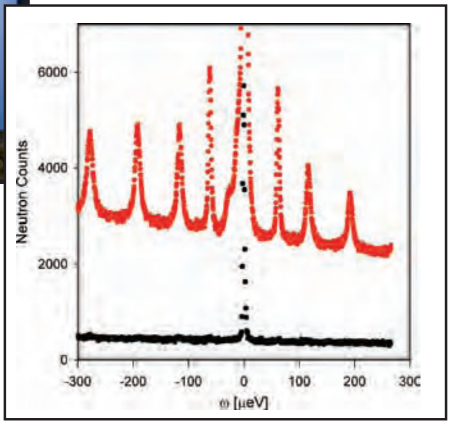
Spallation Neutron Source

BASIS – Backscattering Spectrometer

BASIS is designed to provide extremely high-energy resolution near the elastic peak, enabling studies of the diffusive dynamics of molecules on the atomic length scale (quasi-elastic neutron scattering). This instrument features very high flux and a dynamic range in energy transfer that is approximately five times greater than what is available on comparable instruments today. In addition, this instrument provides the unique capability of shifting the incident neutron bandwidth, enabling inelastic scattering to 18 meV of energy transfer, with a resolution of 0.1% of the energy transfer.



Backscattering spectrometer large evacuated final flight path.



Measurement of the quantum tunneling peaks in 4-methyl pyridine N-oxide (N-oxy gamma-picoline, C_6H_7NO) at 4 K.

Applications

BASIS can be used to probe dynamic processes in various systems on the pico- to nanosecond time scale. It is well suited for probing diffusive and relaxational motions but can also be effectively used for studying some types of collective excitations in condensed matter. Applicable fields of study include, but are not limited to, biology, polymers, small molecules, complex fluids, magnetism, and materials science.

Specifications

Si 111	
Elastic energy	2.08 meV
Bandwidth	±250 μeV
Resolution (elastic)	3.5 μeV
Q range (elastic)	0.2 Å^{-1} < Q < 2.0 Å^{-1}
Solid angle	1.2 sr 2.4 sr (upgrade)

Si 311 (upgrade)	
Elastic energy	7.64 meV
Bandwidth	±1700 μeV
Resolution (elastic)	10 μeV
Q range (elastic)	0.38 Å^{-1} < Q < 3.8 Å^{-1}
Solid angle	1.2 sr

Status: Operational

For more information, contact

Instrument Scientist: Eugene Mamontov, mamontove@ornl.gov, 865.574.5109

Instrument Scientist: Michaela Zamponi, zamponimm@ornl.gov, 865.576.5119

Scientific Associate: Stephanie Hammons, hammonsse@ornl.gov, 865.300.8100

http://neutrons.ornl.gov/instrument_systems/beamline_02_basis

SNS

May 2008

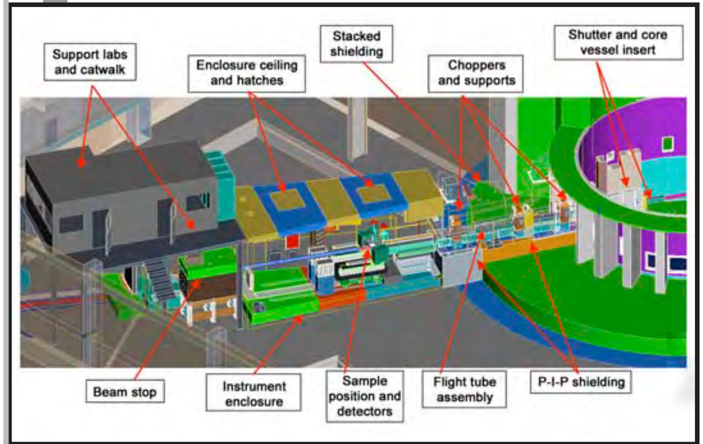
INSTRUMENT Fact Sheet

BEAM LINE 3

SPALLATION NEUTRON SOURCE

SNAP – SPALLATION NEUTRONS AND PRESSURE DIFFRACTOMETER

The SNAP Diffractometer allows studies of a variety of powdered and single-crystal samples under extreme conditions of pressure and temperature. The increased neutron flux, coupled with large-volume pressuring cells using large synthetic single-crystal opposed anvils, allows significant advances in the pressure range accessible to neutron diffraction. The pressure goal is 50 to 100 GPa on an ~1-mm^3 sample on a routine basis. In addition, recent advances in next-generation detectors will allow the incident beam-focusing optics, pressure chamber, and detector array to be highly integrated, providing a highly flexible facility for materials studies under extreme conditions.



APPLICATIONS

SNAP offers new opportunities for scientific studies involving the following:

- Hydrogen under extreme conditions
- Elastic anisotropy of ε-iron at Earth core conditions
- Real-time in situ monitoring of “real rocks” as an analogue to the down-going slab in the subduction context
- Planetary ices—structure and strength of ices under pressure
- Silicate melts—glasses at high pressure and temperature and the dynamical changes occurring during heating and pressurization
- Strength and rheology of materials and the relationship to brittle and ductile failure, including stress release as a function of time
- Structural changes accompanying transitions in Fullerenes and their derivatives
- Hydrogen bonding in organic and inorganic systems as a function of pressure and temperature, including liquids

SPECIFICATIONS

Moderator	Decoupled poisoned supercritical hydrogen
Source-to-sample distance	15 m
Sample-to-detector distance	50 cm
Angular coverage	381–42º \ 981–50º horizontal ±34º vertical
Wavelength range (bandwidth)	
Frame 1	0.5–3.65 Å
Frame 2	3.7–6.5 Å
Pressure range	From ambient pressure to >50 GPa (500 kbar)
Focused beam size	From 1 cm to <100 μm

Status: Operational

FOR MORE INFORMATION, CONTACT

Instrument Scientist: Chris Tulk, tulkca@ornl.gov, 865.576.7028
Scientific Associate: Jamie Molaison, molaisonjj@ornl.gov, 865.206.0478

http://neutrons.ornl.gov/instrument_systems/snap.shtml

SNS

May 2008

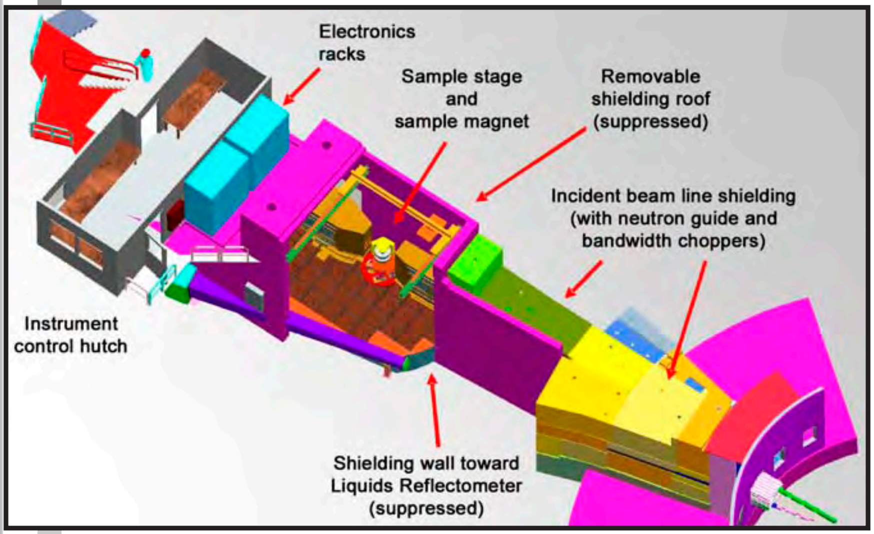
Instrument Fact Sheet

Beam Line 4A

Spallation Neutron Source

Magnetism Reflectometer

The Magnetism Reflectometer is designed for reflectometry and high-angle diffraction studies of magnetic thin films, superlattices, and surfaces. The combination of the high-power SNS and the use of advanced neutron optics allows for off-specular diffraction studies of in-plane structures. Today, even at the world's most advanced neutron sources, such experiments are extremely difficult to perform. The availability of polarized neutrons and polarization analysis suggests that this instrument can also be used for specific studies of nonmagnetic thin-film samples. Examples of the latter include contrast variation, incoherent background reduction, and phase determination for direct inversion of reflectivity data into real-space scattering-length density profiles.



Specifications

Source-to-sample distance	18.64 m
Sample-to-detector distance	0.5–6 m
Detector size	18 x 18 cm^2
Detector resolution	1.5 mm
Moderator	Coupled supercritical hydrogen
Bandwidth	$\Delta\lambda$ = 3.1 Å
Wavelength range	1.8 Å < λ < 14.0 Å
Q range	0 $Å^{-1}$ < Q < 7.0 $Å^{-1}$
Minimum reflectivity	10^{-9}–10^{-10}

Status: Operational

Applications

The Magnetism Reflectometer is applicable primarily to studies with thin magnetic films, an increasingly important area of solid-state physics. Experiments could also benefit engineering, metallurgy, or biological problems. Instrument capabilities allow, for example, studies of magnetic recording media and magnetic sensors, as well as depth-dependent studies of structural/magnetic nanoparticles or domains. The instrument's unique capabilities provide for multilength-scale experiments, and it has sufficient beam intensity for detailed structural/magnetic phase-diagram determinations. In situ studies on ultrathin films in an ultrahigh-vacuum environment are planned as a future upgrade capability.

For more information, contact

Instrument Scientist: Valeria Lauter, lauterv@ornl.gov, 865.576.5389
Scientific Associate: Richard J. Goyette Jr., goyetterj@ornl.gov, 865.241.9991

http://neutrons.ornl.gov/instrument_systems/beamline_04a_mr

SNS

May 2008

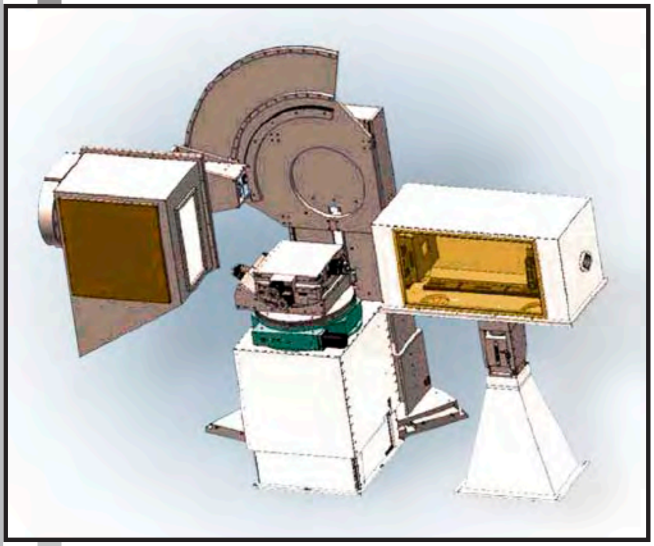
Instrument Fact Sheet

BEAM LINE 4B

SPALLATION NEUTRON SOURCE

LIQUIDS REFLECTOMETER

The Liquids Reflectometer features a horizontal sample geometry and thus can accommodate air/liquid surfaces in addition to air/solid and liquid/solid interfaces. Active vibration isolation minimizes capillary-wave production by the external environment. Data rates and Q range covered at a single scattering angle setting will be sufficiently high to permit "real-time" kinetic studies on many systems. Time-resolved experiments include investigations of chemical kinetics, solid-state reactions, phase transitions, and chemical reactions in general.



Liquids Reflectometer goniostat.

APPLICATIONS

The Liquids Reflectometer is useful for a wide range of science. Current areas of interest include biomaterials, polymers, and chemistry involving thin layers of surfactants or other materials on the surfaces of liquids, such as cell-membrane analogs. These systems provide a flexible platform to study structure-property relationships at the boundary between hard and soft matter, with applications in biomimetics, bio-sensing, and bio-compatible films; hydrogen storage and fuel cells; and polymers.

FOR MORE INFORMATION, CONTACT

Instrument Scientist: John Ankner, anknerjf@ornl.gov, 865.576.5122

Instrument Scientist: Jim Browning, browningjf@ornl.gov, 865.241.3905

Scientific Associate: Candice Halbert, halbertce@ornl.gov, 865.574.9255

http://neutrons.ornl.gov/instrument_systems/beamline_04b_lr

SPECIFICATIONS

Source-to-sample distance	13.6 m
Sample-to-detector distance	1.5 m
Detector size	20 x 20 cm^2
Detector resolution	1.3 x 1.3 mm^2
Moderator	Coupled supercritical hydrogen
Bandwidth	$\Delta\lambda$ = 3.5 Å
Wavelength range	2.5 Å < λ < 17.5 Å
Q range (air/liquid)	0 $Å^{-1}$ < Q < 0.5 $Å^{-1}$
Q range (air/solid)	0 $Å^{-1}$ < Q < 1.5 $Å^{-1}$
Minimum reflectivity	1 x 10^{-7}

Status: Operational

SNS

May 2008

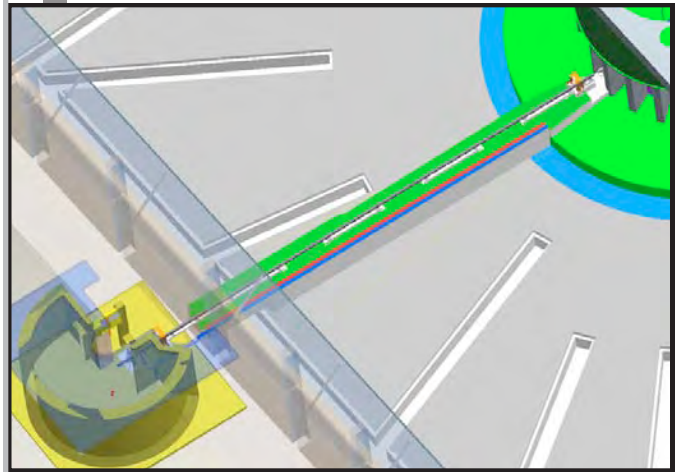
Instrument Fact Sheet

BEAM LINE 5

SPALLATION NEUTRON SOURCE

CNCS – Cold Neutron Chopper Spectrometer

CNCS is a high-resolution, direct-geometry, multichopper inelastic spectrometer designed to provide flexibility in choice of energy resolution and to perform best at low-incident energies (2–50 meV). Although the initial detector coverage around the sample is 1 sr, a later upgrade to 3 sr is possible. CNCS experiments typically use an energy resolution between 10 and 500 μeV. A broad variety of scientific problems, ranging from complex and quantum fluids to magnetism and chemical spectroscopy, can be addressed through experiments on the CNCS.



Engineering design of the CNCS beam line from the target monolith to the instrument satellite building.

Specifications

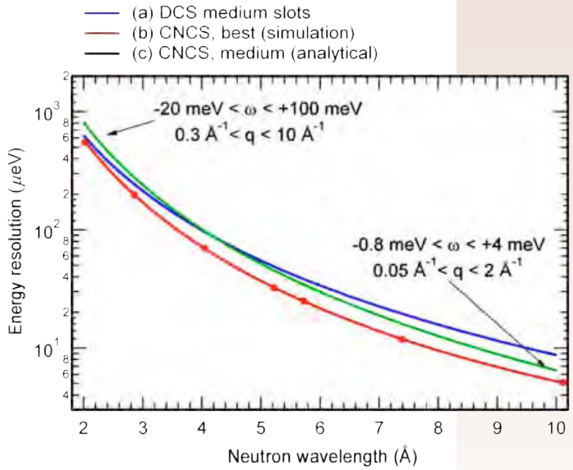
Source-to-sample distance	36.2 m
Sample-to-detector distance	3.5 m
Angular coverage	-90 … +140° horizontally ± 25° vertically
Energy resolution	10-500 μeV
Incident energy range	2–50 meV
Momentum transfer range	0.05–10 Å^{-1}

Status:
To be commissioned in 2008

Applications

CNCS is applicable primarily to studies in the following:

- Complex fluids: dilute protein solutions, biological gels, selective absorption of molecules on surfaces
- Dynamics in confined geometries
- Magnetism: low-dimensional systems; non-Fermi liquids; frustrated, disordered, or molecular magnets



For more information, contact

Instrument Scientist: Georg Ehlers, ehlersg@ornl.gov, 865.576.3511
Scientific Associate: Jennifer Niedziela, niedzielajl@ornl.gov, 413.478.1621

http://neutrons.ornl.gov/instrument_systems/beamline_05_cncs

SNS

May 2008

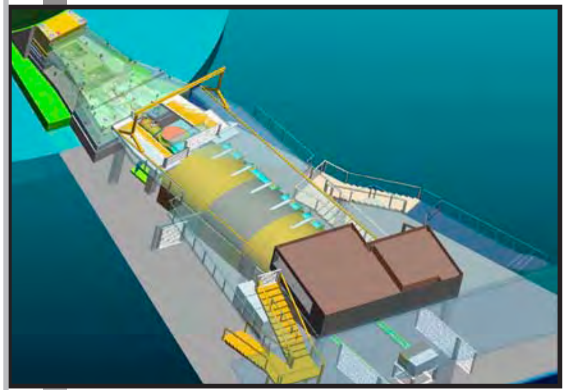
INSTRUMENT Fact Sheet

BEAM LINE 6

SPALLATION NEUTRON SOURCE

EQ-SANS — EXTENDED Q-RANGE SMALL-ANGLE NEUTRON SCATTERING DIFFRACTOMETER

The EQ-SANS Diffractometer is designed to study noncrystalline, nanosized materials in solid, liquid, or gas forms such as polymers, proteins in solution, and micelles. EQ-SANS has very high intensity and wavelength resolution. It also has a wide Q coverage, allowing simultaneous data collection in both low-and high-Q regions. Scattering from nanomaterials is concentrated mostly in a forward direction, or small angles. These scattering data yield information about the size and shape of the nanoparticles. Applications include the study of polymers, better detergents and soaps from improved micelles, proteins for better drug design, and materials of interest to the oil industry.



APPLICATIONS

The unique capabilities of the EQ-SANS offer new opportunities for scientific studies in the following:

Life science

- Solution structures of proteins, DNA, and other biological molecules and molecular complexes
- Protein-protein and protein-ligand interactions, kinase regulation
- Protein-membrane interaction

Polymer and colloidal systems

- Block copolymers and dendrimers
- Micelles, aerosols, and emulsions
- Polyelectrolytes and electric double-layer and ion distribution at solid-liquid interfaces

Materials science

- Simultaneous study of domain and crystalline structures
- Crystallization and precipitation
- Nanoparticles

Earth and environmental sciences

- Pore structure in soil
- Absorption of contaminants by soil
- Fractal structure of rocks

FOR MORE INFORMATION, CONTACT

Instrument Scientist: J. K. Zhao, zhaoj@ornl.gov, 865.574.0411

http://neutrons.ornl.gov/instrument_systems/beamline_06_eqsans

SPECIFICATIONS

Source-to-sample distance	14 m
Bandwidth	3–4.3 Å
Moderator	Coupled supercritical hydrogen
Integrated flux on sample	~10^7–10^9 n/cm^2/s
Q range	0.004 $Å^{-1}$ < Q < 10 $Å^{-1}$

Low-Angle Detector	
Sample-to-detector distance	1–8 m
Detector size	1 x 1 m
Detector resolution	8 mm

High-Angle Detector	
Sample-to-detector distance	1 m
Angular coverage	~35–150°
Detector resolution	8 mm

Status:
To be commissioned in 2008

May 2008

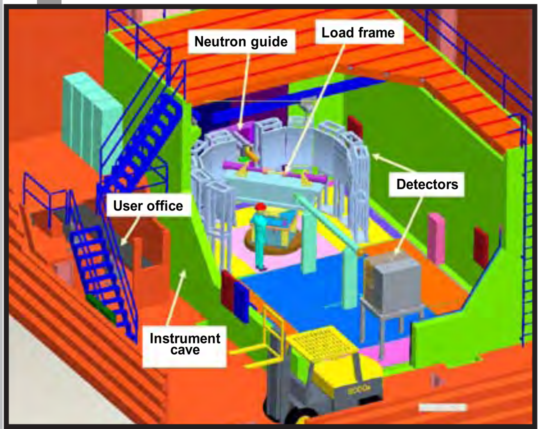
Instrument Fact Sheet

Beam Line 7

Spallation Neutron Source

Vulcan – Engineering Materials Diffractometer

VULCAN helps users understand a broad range of engineering and materials science problems. Characteristics of the instrument include stress mapping of engineering components with a 1-mm³ sampling volume, in situ loading with 10 to 20 reflections, and real-time studies of the kinetics of materials on subsecond time scales. The basic design allows users to determine stress distribution in engineering components and to understand more about the deformation of materials under multiaxial loading. VULCAN can help scientists and engineers test the reliability of structural components and better understand how materials deform. The flux on sample will reach 1 x 10^8 neutrons/cm^2/s, providing a high intensity for fast kinetic studies. The instrument team plans to have a small-angle detector to allow users to conduct simultaneous measurements of small-angle scattering, thereby enabling studies of the evolution of material structures at multiple-length scales.



Applications

VULCAN is designed to tackle a variety of problems in materials science and engineering, ranging from determining residual stress in engineering components to understanding the fundamental aspects of materials behaviors during processing and use. Although it is difficult to predict the kinds of new science that will be enabled by instruments like VULCAN, some research areas that VULCAN could benefit include the following:

- In situ studies of materials behavior during processing: temperature distribution, texture changes, stress development, precipitation
- In situ loading studies at high or cryogenic temperatures: fatigue damage, deformation in nanostructured materials, creep behaviors, piezoelectric and shape-memory alloys
- Residual stress and microstructure changes in surface-engineered materials
- Deformation in amorphous materials
- Phase transformation kinetics

For more information, contact

Instrument Scientist: Xun-Li Wang, wangxl@ornl.gov, 865.574.9164
Scientific Associate: Harley Skorpenske, skorpenskehd@ornl.gov, 865.228.8460

http://neutrons.ornl.gov/instrument_systems/beamline_07_vulcan

Specifications

Moderator	Decoupled poisoned water
Source-to-sample distance	43.5 m
Sample-to-detector distance	1.5–2 m
Detector angular coverage	60° < 2θ < 150°
Wavelength bandwidth	~1.3 Å
Resolution	0.2% in high-resolution mode
Flux on sample (n/s/cm²)	3 x 10^7 in high-resolution mode 1.2 x 10^8 in high-intensity mode
Gauge volume	3D strain mapping: 1 mm³ 1D strain mapping: 0.1 mm
SANS Q range	0.01–0.2 (Å^{-1})

Status:
To be commissioned in 2008

May 2008

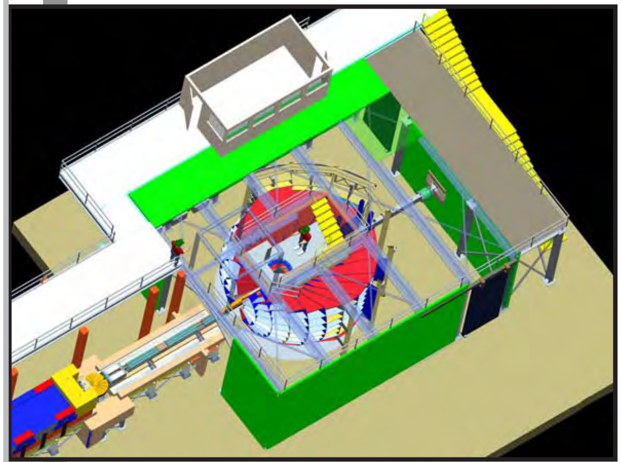
INSTRUMENT Fact Sheet

BEAM LINE 11A

SPALLATION NEUTRON SOURCE

POWGEN – POWDER DIFFRACTOMETER

POWGEN is designed to study polycrystalline materials. This versatile diffractometer enables users to collect typical Rietveld statistics in ~20 minutes from a 0.6-cm^3 sample with <0.1% resolution at short d-spacings and <1% resolution for nearly all d-spacings of interest. Adjustment of the phase of the bandwidth choppers in this instrument also allows collection of diffraction data for d-spacings as large as 66 Å. Because of the third-generation conceptual design of POWGEN, users can choose the wavelengths for data collection and have complete freedom in selecting the subset of data to be included in analysis. These alternatives allow greater flexibility than most existing neutron diffractometers. In addition, this standard tool provides faster and higher precision than other diffractometers in the United States.



Secondary flight path for the Powder Diffractometer. The sample is 60 m from the moderator, necessitating a satellite building outside the Target Building for the secondary flight path.

APPLICATIONS

Scientific studies at this instrument encompass a wide range of novel materials. These include, but are not limited to, structural studies of magnetic materials such as high-Tc superconductors, metal-insulator phase transitions, charge and orbital ordering transitions, and molecular magnets. Additional possibilities include nonmagnetic materials such as Zeolite and aluminophosphate frameworks; metals and semiconductors; dielectrics, ferroelectrics, and thermoelectrics; and ab initio structure solutions of polycrystalline materials such as pharmaceutical compounds. In addition, POWGEN is capable of acquiring refineable data sets in rapid data collection mode, making it an ideal instrument for parametric studies and time-resolved in situ studies of the electrochemistry of catalysts, ceramic membranes, hydrogen storage materials, and charging and discharging of battery materials.

FOR MORE INFORMATION, CONTACT

Instrument Scientist: Jason Hodges, hodgesj@ornl.gov, 865.576.7034
Instrument Scientist: Ashfia Huq, huqa@ornl.gov, 865.574.7923
Scientific Associate: Luke Heroux, herouxla@ornl.gov, 865.241.8673

http://neutrons.ornl.gov/instrument_systems/beamline_11a_powgen

SPECIFICATIONS

Moderator	Decoupled poisoned supercritical hydrogen
Source-to-sample distance	60 m
Sample-to-detector distance	1–6 m
Detector angular coverage	$6 < 2\theta < 170°$
Wavelength bandwidth	~1 Å
Frame 1	0.3 Å < d < 10 Å
Frame 6	3 Å < d < 66 Å
Resolution	$0.001 < \Delta d/d < 0.016$
Resolution at 90°	$\Delta d/d = 0.0015$

Status:
To be commissioned in 2008

May 2008

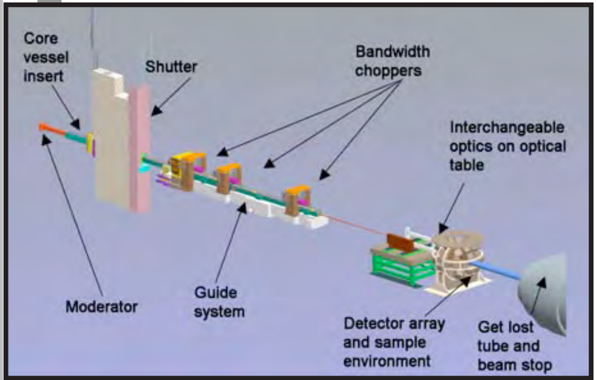
INSTRUMENT Fact Sheet

BEAM LINE **11B**

SPALLATION NEUTRON SOURCE

MaNDi – Macromolecular Neutron Diffractometer

MaNDi allows the study of single crystals and is optimized for rapid data collection from large macromolecular structures. MaNDi will achieve 1.5-Å resolution from crystal volumes between 0.1 and 1.0 mm^3, with lattice repeats on the order of 150 Å. With larger crystals (>1 mm^3), it will be possible to obtain useful data in the resolution range of 2.0 to 2.5 Å for unit-cell repeats of up to 300 Å, a revolution in neutron macromolecular crystallography (NMC). Experimental duration times are to be between one and seven days, which will revolutionize NMC for applications in the fields of structural biology, enzymology, and computational chemistry.



The MaNDi detectors are designed to cover a large solid angle to record most of the neutrons scattered from a single-crystal sample, regardless of the reflection angle. This capability is accomplished through the instrument design, which places the detectors approximately spherically around the sample. The detector design follows a modular approach. A spherical detector mount will be constructed to accommodate the appropriate number of individual modules of two-dimensional, time-sensitive detectors with front face dimensions of 150 × 150 mm, leaving openings for the sample orienter/environment (top) and the incident and exiting direct neutron beam (horizontal plane). The spatial resolution of the detector is 1 mm, with a minimal sensitivity to gamma rays, hence preserving the signal-to-noise ratio of the Bragg peaks. The efficiency of this type of detector using a 1.5-mm-thick scintillator is 78% for neutrons with a wavelength of 1 Å. An increase in neutron wavelength is coupled with an increase in detection efficiency.

Precision mounting will place the 0.1-mm^3 crystals within the neutron beam, and the sample-positioning system will allow translation and rotation in x, y, and z to precisely align the sample. These operations will be remotely controlled and motor driven by a user-friendly graphical user interface.

Applications

MaNDi offers radical new opportunities for scientific studies involving the following:

- Protein studies to provide better drug molecules for the treatment of cancer and HIV
- Studies of enzyme mechanisms to accelerate important industrial reactions
- Mechanisms used by plants to convert light into energy

For more information, contact

Instrument Scientist: Leighton Coates, coatesl@ornl.gov, 865.241.3427

http://neutrons.ornl.gov/instrument_systems/beamline_11b_mandi

Specifications

Moderator	Decoupled hydrogen
Source-to-sample distance	24 m
Sample-to-detector distance	0.5 m
Initial angular detector coverage	4 sr
Optional angular detector coverage	9 sr
Detector pixel size	6.2 x 10^{-6} sr (1 mm)
Detector angles	0–180°
Wavelength bandwidth	2.69 Å
Frame 1	1.5–4.2 Å
Resolution	1.5%
Sample size	0.1 mm^3
Divergence	4.0–9.8 mrad

Status:
To be commissioned in 2012

SNS

May 2008

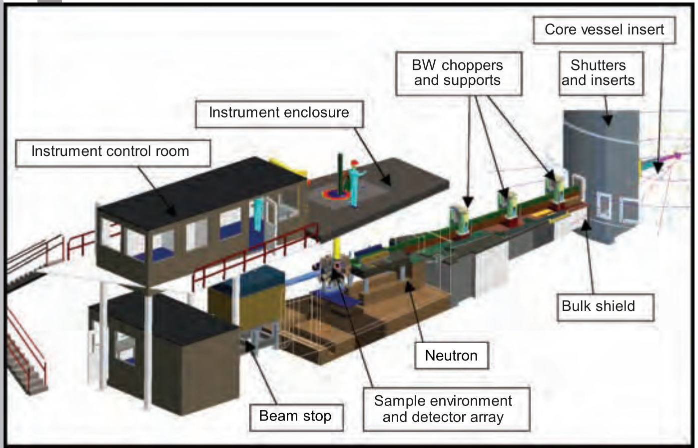
INSTRUMENT Fact Sheet

BEAM LINE 12

SPALLATION NEUTRON SOURCE

TOPAZ – SINGLE-CRYSTAL DIFFRACTOMETER

The TOPAZ Single-Crystal Diffractometer (SCD) is designed to perform elastic scattering experiments under controlled environmental conditions to probe material structures and responses. Use of the same single-crystal sample for X-ray and neutron diffraction was the guiding design principle of TOPAZ, a versatile and variable-environment SCD for neutron scattering. Data are collected on samples of between 0.001 and 0.1 mm^3, and expected average unit cell sizes are around 50 Å^3 for compounds of moderate complexity. The goal for TOPAZ is the capability to collect data in a matter of hours rather than days. Materials investigated include functional materials of the high-Tc superconductor perovskite family; magnetic superstructures in perovskites and spinels; the molecular basis of future high-density, three-dimensional storage materials; and catalytic precursors, metalhydrides, and organometallics. Options to polarize the neutron beam for magnetic scattering experiments are included, as well as the ability to record Bragg intensities and diffuse scattering at cryogenic and elevated temperatures. A polarized incident neutron beam and magnetic field option on the sample help scientists decipher complex and directional magnetism and magnetic transitions.



APPLICATIONS

TOPAZ can address problems and greatly expand the range of materials explored in chemistry, earth sciences, materials science and engineering, solid-state physics, and biology. It can also assist in studies of therapeutics and medical compounds, such as aspirin and paracetamol, to show differences in hydrogen locations and bonding, helping scientists better understand a material's individual effectiveness.

FOR MORE INFORMATION, CONTACT

Instrument Scientist: Christina Hoffmann, hoffmanncm@ornl.gov, 865.576.5127
Scientific Associate: Matthew Frost, frostmj@ornl.gov, 865.576.2033

http://neutrons.ornl.gov/instrument_systems/beamline_12_topaz

SPECIFICATIONS

Moderator	Decoupled poisoned hydrogen
Source-to-sample distance	18 m
Sample-to-detector distance, evacuated	39–45 cm
Sample-to-detector distance in air	39–45 cm, 60–80 cm
Initial angular detector coverage	4 sr
Optional angular detector coverage	9 sr
Detector pixel size	6.2 x 10^{-6} sr (1 mm)
Detector angles	0–180°
Wavelength bandwidth	3.35 Å
Frame 1	0.5–3.85 Å
Resolution	0.1%
Sample size	0.001 mm^3 < S < 1 mm^3
Divergence on sample	10 mrad < d < 25 mrad

Status:
To be commissioned in 2009

SNS

May 2008

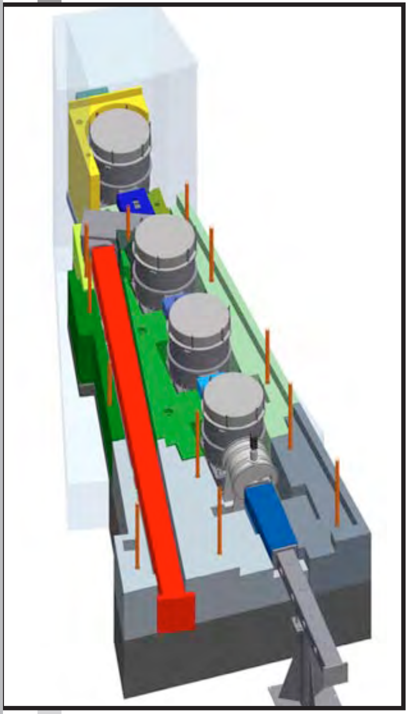
Instrument Fact Sheet

Beam Line 13

Spallation Neutron Source

FNPB – Fundamental Neutron Physics Beam Line

The FNPB provides neutron beams for a variety of experiments in nuclear and particle physics. This facility is designed to accommodate two classes of experiments: (1) cold neutron experiments that require intense, broad-spectrum beams and (2) ultracold neutron experiments in which neutrons of ~1 meV are "down-converted" to near zero energy in superfluid liquid helium. Experiments at the FNPB include precise measurements of the parameters that describe neutron beta decay, studies of the weak interaction between quarks, and a search for a non-zero neutron electric dipole moment. Each of the experiments at the FNPB requires the development, construction, and installation of major pieces of experimental equipment, and each experiment could take beams for periods of several months to a few years.



Design model of the FNPB guide system showing the curved cold beam with four frame overlap choppers, as well as the monochromator housing and the ballistic ultracold neutron guide. The cold guide and choppers share a common vacuum to reduce window losses.

Applications

The FNPB is designed to address questions of interest in cosmology, nuclear and particle physics, and astrophysics. Among the questions that will be addressed are the origin of the light elements (big bang nuclear synthesis), the source of the cosmic matter-antimatter asymmetry, and the origin of parity violation.

For more information, contact

Project Manager: Geoff Greene, greenegl@ornl.gov, 865.574.8435

http://neutrons.ornl.gov/instrument_systems/beamline_13_fnpb

Specifications

Cold Neutron Beam Line	
Supermirror guide	Curved, m = 3.6
Beam area	100 x 120 mm
Choppers	4 frame overlap
Peak wavelength	3.5 Å
Independent secondary shutter	
Floor pit for superconducting magnet	

Ultracold Neutron Beam Line	
Guide	33 m ballistic
Wavelength	8.9 Å
Monochromator	Double-crystal alkalai intercalated graphite
External building experimental area	

Status:
To be commissioned in 2008

May 2008

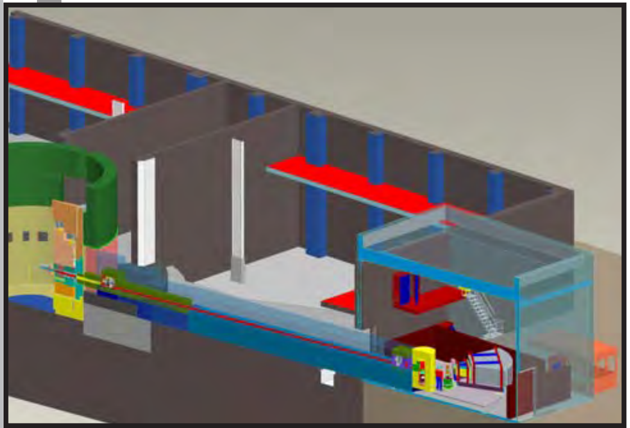
Instrument Fact Sheet

BEAM LINE **14B**

SPALLATION NEUTRON SOURCE

HYSPEC – Hybrid Spectrometer

HYSPEC is a high-intensity, direct-geometry instrument optimized for measurement of excitations in small single-crystal specimens. The incident neutron beam is monochromated using a Fermi chopper with short, straight blades and is then focused onto the sample using Bragg scattering optics. Neutrons are detected in a bank of position-sensitive detector tubes that can be positioned over a wide range of scattering angles about the sample axis. This combination of Fermi chopper and Bragg focusing optics, plus a position-sensitive detector bank, leads to a highly flexible instrument in which the energy and wave vector resolution can be independently varied by nearly an order of magnitude. Either full or partial neutron polarization analysis can be deployed on HYSPEC. This is accomplished by using a Heusler crystal array to polarize the incident beam and either a ^{3}He spin filter or supermirror wide-angle polarization analyzers for the scattered beam.



Applications

HYSPEC is applicable primarily to studies in the following:

- Superconductors
- Strongly correlated electron materials
- Ferroelectrics
- Lattice and magnetic dynamics
- Phase transitions
- Quantum critical points
- Complex phases in intermetallic compounds
- Frustrated magnets
- Low-dimensional magnetic excitations
- Transition metal oxides
- Spin and lattice dynamics in nanostructures

For more information, contact

Instrument Scientist: Mark Hagen, hagenme@ornl.gov, 865.241.9782

http://neutrons.ornl.gov/instrument_systems/hyspec.shtml

Specifications

Moderator	Coupled cryogenic hydrogen
Moderator-to-Fermi chopper distance	37.2 m
Chopper - to-sample distance	3.2 m
Focusing crystals-to-sample distance	1.4–1.8 m
Sample-to-detector distance	4.5 m
Incident energy range	3.6–90 meV
Energy resolution (elastic scattering)	$0.02 < (\Delta E/E_I) < 0.2$
Scattering-angle range	$2° < 2\theta_S < 135°$

Status:
To be commissioned in 2011

May 2008

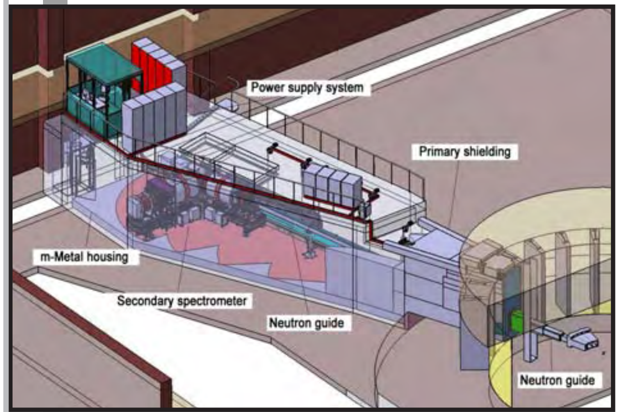
Instrument Fact Sheet

Beam Line 15

Spallation Neutron Source

NSE – Neutron Spin Echo Spectrometer

NSE is the best spectrometer of its class in both resolution and dynamical range. Exploiting superconducting technology and developing novel field correction elements, the maximum achievable Fourier time will be extended to at least 1 μs. Using wavelengths of $0.25 < \lambda/\text{nm} < 2.0$, an unprecedented dynamical range of six decades from 1 ps $< \tau$ to $\tau <$ 1 μs can be achieved. The design of the spectrometer takes advantage of recent progress in neutron optics and polarizing supermirror microbenders, resulting in considerable gains in polarized neutron flux over a wide wavelength range. Performance is also extended by a position-sensitive, two-dimensional detector with a broad detection region. As a result, the effective data rate will gain an additional factor of 5 in addition to the estimated time-averaged sample flux of 10^7 n/cm^{2}s around $\lambda = 1$ nm. This yields the highest available data accumulation rate. In addition, the wavelength distribution width at any time is well below 0.5%, causing the resolution in momentum transfer to increase significantly compared with reactor instruments with 10% or more wavelength distribution width.



Specifications

Moderator	Cold-coupled hydrogen
Neutron guide $h \times b$	^{58}Ni coated, 4×8 cm^2, m = 1.2
Wavelength selection	Chopper system consisting of four choppers and selecting a wave length band up to 3.66 Å
Accessible wavelength frame	2 Å < λ < 20 Å
Declination angle	3.5°
Maximum scattering angle	≅80°
Q range	0.0025–3.6 Å^{-1}
Maximum field integral	J = 1.8 Tm
Dynamic range	1 ps < τ < 1 μs
Typical sample size	30 × 30 mm
Analyzer	m=3 rotatable supermirror
Detector	^{3}He counter (300 × 300 mm^2)
Typical scanning time with 10% scatterer	5 hours/ spectrum

Status:
To be commissioned in 2009

May 2008

Applications

Although the NSE spectrometer is designed primarily for soft-matter research, its capabilities also make it useful for all fields of modern condensed matter and materials science. This instrument is especially suited for analyzing slow dynamical processes and thereby unraveling molecular motions and mobilities at nanoscopic and mesoscopic levels. This feature is highly relevant to soft-matter problems in research on the molecular rheology of polymer melts, related phenomena in networks and rubbers, interface fluctuations in complex fluids and polyelectrolytes, and transport in polymeric electrolytes and gel systems. NSE could also aid studies in biophysics and magnetism.

For more information, contact

Instrument Scientist: Michael Ohl, ohlme@ornl.gov, 865.574.8426

http://neutrons.ornl.gov/instrument_systems/nse.shtml

Instrument Fact Sheet

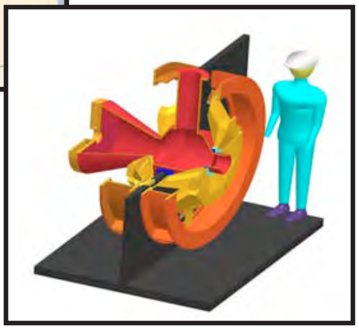
Beam Line **16B**

Spallation Neutron Source

VISION – Chemical Spectrometer

VISION is best thought of as the neutron analogue of an infrared-Raman spectrometer. It is optimized to characterize molecular vibrations in a wide range of crystalline and disordered materials over a broad energy range (<5 to >500 meV), while simultaneously recording structural changes using diffraction detectors in the backscattering position and at 90°. This inverted-geometry instrument offers enhanced performance by coupling a white beam of incident neutrons with two banks of eight analyzer modules, equipped with double-focusing crystal arrays, that focus the desired neutrons on a small detector. This arrangement leads to improved signal noise, and the overall count rate in the inelastic signal is at least two orders of magnitude beyond that of similar spectrometers that are currently available.

Engineering model of VISION, including T_0 chopper, bandwidth chopper, secondary spectrometer, and utility rooms.



Secondary spectrometer with detector and analyzer modules.

Applications

Leading-edge studies involving scientific disciplines such as nanotechnology, catalysis, biochemistry, geochemistry, and condensed/soft-matter science will all benefit from the enhanced performance and properties of VISION.

For more information contact

Principal Investigator: John Larese, jzl@utk.edu, 865.974.3141

Instrument Scientist: Christoph Wildgruber, wildgrubercu@ornl.gov, 865.574.5378

http://neutrons.ornl.gov/instrument_systems/beamline_16b_vision

Specifications

Moderator	Decoupled ambient water
Source-to-T_0 chopper distance	7 m
T_0 chopper-to-sample distance (primary flight path)	17 m
Sample-to-detector distance (secondary flight path)	0.7 m
Incident energy range	3.5–500 meV
Analyzer Bragg angle	45°
Total analyzer area (in 14 identical units)	0.5 m^2
Energy resolution	Exceeds 1.5% (>5 meV) – 5% (<5 meV)
Elastic line width	90 meV
Annular diffraction detector	1.3–14 Å^{-1}
Backscattering diffraction detector	1.5–30 Å^{-1}
delta-d/d	0.001

Status:
To be commissioned in 2012

May 2008

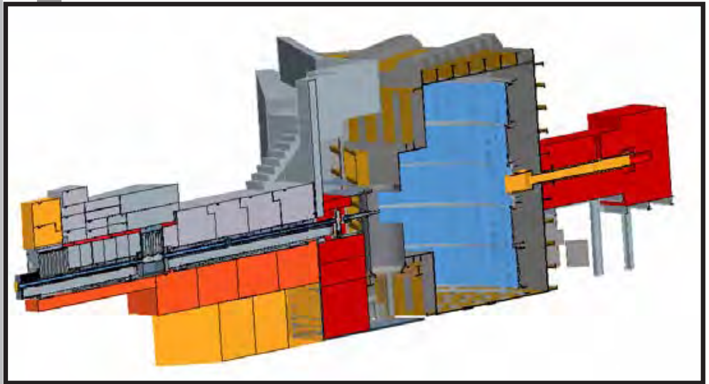
Instrument Fact Sheet

Beam Line 17

Spallation Neutron Source

SEQUOIA – Fine-Resolution Fermi Chopper Spectrometer

SEQUOIA is a fine-resolution Fermi chopper spectrometer optimized to provide a high neutron flux at the sample and fine energy resolution. The spectrometer is capable of selecting neutrons with incident energies from a few hundredths of an electron volt to a couple of electron volts and thus can study excitations over this wide energy scale. An elliptically shaped supermirror guide in the incident flight path boosts the performance at the lower end of this range. The sample and detector vacuum chambers provide a window-free final flight path and incorporate a large gate valve to allow rapid sample changeout. A new T_0 neutron chopper is being developed not only to block the prompt radiation from the source but also to eliminate unwanted neutrons from the incident beam line. SEQUOIA can help scientists understand excitations in many materials, for example, magnetic materials, novel oxides, and high-temperature superconductors. SEQUOIA is a collaboration between Oak Ridge National Laboratory and the Canadian Institute for Neutron Scattering.



Applications

With its capability to acquire data quickly and relate them to three-dimensional momentum transfers, SEQUOIA allows new studies of single crystals and novel systems such as the following:

- High-temperature superconductivity: spin dynamics in superconductors and precursor compounds, incommensurate spin fluctuations at varying doping levels
- Model magnetic systems, such as one-dimensional spin chains and spin ladders, and crossover effects from one- to three-dimensional magnetism
- Excitations in quantum fluids, quantum critical phenomena, and non-Fermi liquid systems
- High-resolution crystal field spectroscopy reaching into the 1-eV range
- Coupling of electronic and spin systems in correlated-electron materials
- Colossal magnetoresistive materials

For more information, contact

Instrument Scientist: Garrett Granroth, granrothge@ornl.gov, 865.576.0900
Scientific Associate: Todd Sherline, sherlinete@ornl.gov, 865.773.3157

http://neutrons.ornl.gov/instrument_systems/hrcs.shtml

Specifications

Moderator	Decoupled ambient water
Source-to-Fermi chopper distance	18 m
Chopper-to-sample distance	2.0 m
Sample-to-detector distance	5.5–6.3 m cylindrical geometry
Incident energy range	10–2000 meV
Resolution (elastic)	1–5% E_i
Vertical detector coverage	-30–30°
Horizontal detector coverage	-30–60°
Minimum detector angle	3°

Status:
To be commissioned in 2008

May 2008

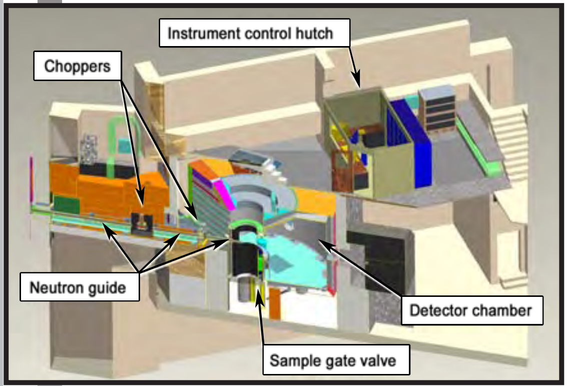
Instrument Fact Sheet

BEAM LINE 18

SPALLATION NEUTRON SOURCE

ARCS – Wide Angular-Range Chopper Spectrometer

ARCS is optimized to provide a high neutron flux at the sample and a large solid angle of detector coverage. This spectrometer is capable of selecting incident energies over the full energy spectrum of neutrons, making it useful for studies of excitations from a few to several hundred milli-electron volts. An elliptically shaped supermirror guide in the incident flight path boosts the performance at the lower end of this range. The sample and detector vacuum chambers provide a window-free final flightpath and incorporate a large gate valve to allow rapid sample changeout. A new T_0 neutron chopper is being developed not only to block the prompt radiation from the source but also to eliminate unwanted neutrons from the incident beam line. In addition to the instrument hardware, the ARCS project includes a significant effort for software development.



Cutaway view of the engineering model of the ARCS instrument showing the incident beam line components, sample and detector chamber, and control area.

Applications

Compared with current instruments, the increased sensitivity of ARCS offers new opportunities for scientific studies in the following:

Lattice Dynamics

- Entropy and the effects of vibrational modes on stability and phase transitions of solids
- Excitations in disordered materials; effects of nanoscale features on vibrational entropy and thermodynamic stability
- Equations-of-state from the measured phonon density-of-states versus temperature and pressure
- Phonons in correlated-electron materials; coupling of lattice and electronic degrees of freedom in high-Tc, heavy-fermion, and mixed-valence materials

Magnetic Dynamics

- High-temperature superconductivity—spin dynamics in superconductors and precursor compounds and crystal field spectroscopy
- Low-dimensional systems; one-dimensional quantum magnets and low-dimensional conductors
- Magnetism in actinide materials; heavy-fermion magnetism and superconductivity

Chemical Physics

- Deep inelastic neutron scattering studies of hydrogen

For more information, contact

Instrument Scientist: Doug Abernathy, abernathydl@ornl.gov, 865.576.5105
Instrument Scientist: Matthew B. Stone, stonemb@ornl.gov, 865.241.0483
Scientific Associate: Mark Loguillo, loguillomj@ornl.gov, 865.235.9000

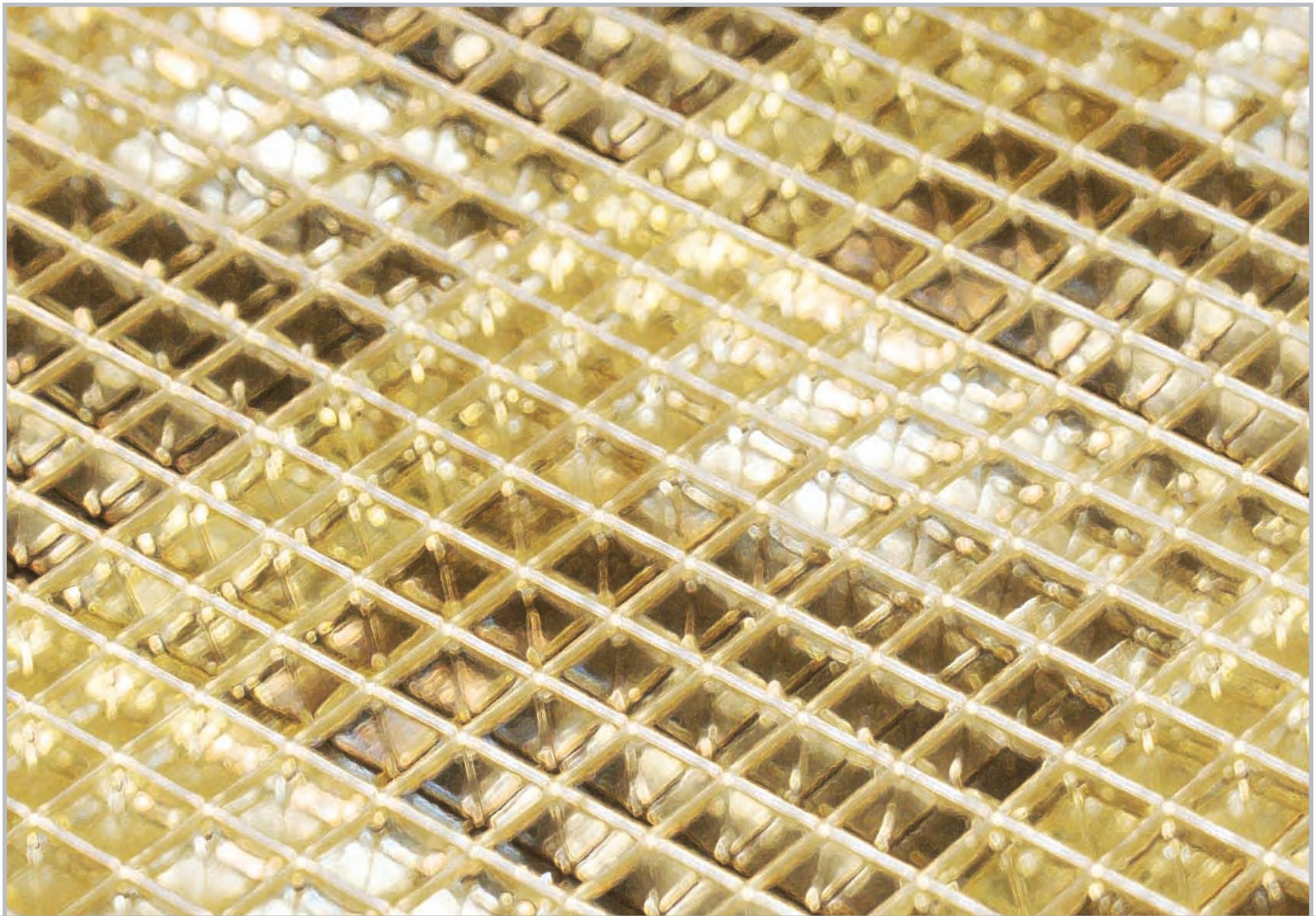
http://neutrons.ornl.gov/instrument_systems/beamline_18_arcs

Specifications

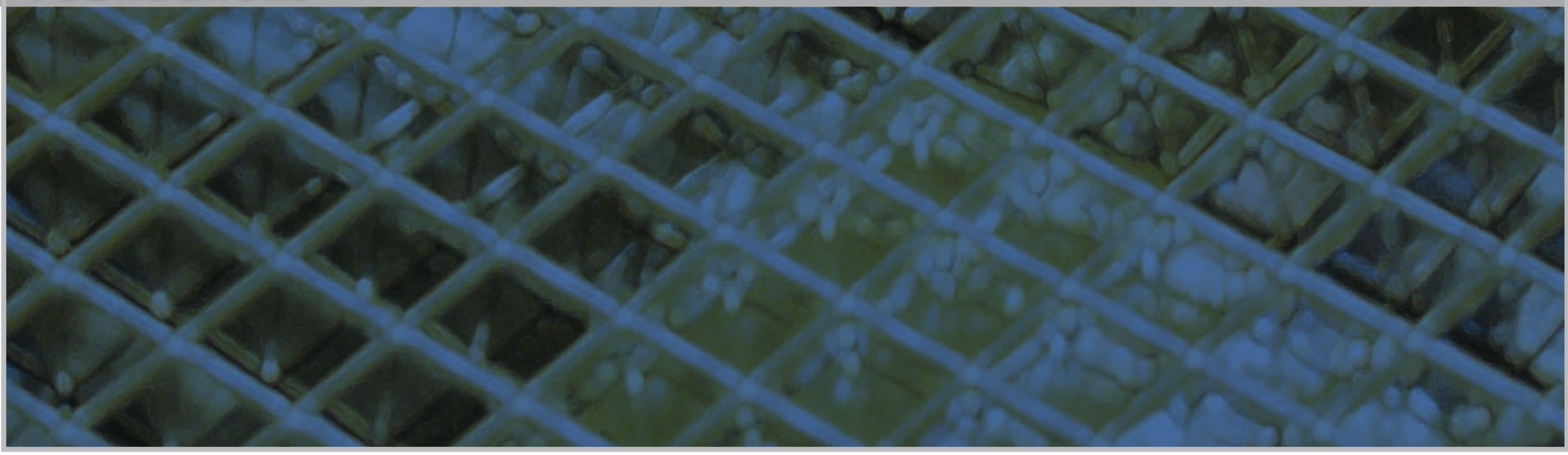
Moderator	Decoupled ambient water
Source-to-Fermi chopper distance	11.6 m
Chopper-to-sample distance	2.0 m
Sample-to-detector distance	3.0 to 3.4 m cylindrical geometry
Incident energy range	10–1500 meV
Resolution (elastic)	2–5% E_i
Detector coverage horizontal	-28–135°
Detector coverage vertical	-27–26°
Minimum detector angle	3°

Status: Operational

May 2008



Publications



The following publications document the results of studies enabled at least in part by use of SNS and HFIR during 2007.

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M. Ando, M. Li, H. Tanigawa, M. L. Grossbeck, S. Kim, T. Sawai, K. Shiba, Y. Kohno, and A. Kohyama, "Creep behavior of reduced activation ferritic/martensitic steels irradiated at 573 and 773 K up to 5 dpa," *Journal of Nuclear Materials* **367**, 122–126 (August 2007).

M. Ando, H. Tanigawa, K. Shiba, S. Jitsukawa, Y. Kohno, A. Kohyarna, M. Li, and R. E. Stoller, "Irradiation creep behavior of reduced activation ferritic/martensitic steel irradiated in HFIR," *Journal of the Japan Institute of Metals* **71**, 559–562 (July 2007).

H. N. Bordallo, D. N. Argyriou, M. Barthes, W. Kalceff, S. Rols, K. W. Herwig, C. Fehr, F. Juranyi, and T. Seydel, "Hydrogen in N-methylacetamide: Positions and dynamics of the hydrogen atoms using neutron scattering," *Journal of Physical Chemistry B* **111**, 7725–7734 (July 2007).

M. D. Brown, B. M. Law, S. Satija, W. A. Hamilton, E. Watkins, J. H. J. Cho, and J. Majewski, "Comparison of critical adsorption scaling functions obtained from neutron reflectometry and ellipsometry," *Journal of Chemical Physics* **126** (May 2007).

T. D. Burchell and L. L. Snead, "The effect of neutron irradiation damage on the properties of grade NBG-10 graphite," *Journal of Nuclear Materials* **371**, 18–27 (September 2007).

J. T. Busby, K. J. Leonard, and S. J. Zinkle, "Radiation-damage in molybdenum-rhenium alloys for space reactor applications," *Journal of Nuclear Materials* **366**, 388–406 (July 2007).

T. S. Byun, "Dose dependence of true stress parameters in irradiated bcc, fcc, and hcp metals," *Journal of Nuclear Material* **361**(2–3), 239–247, (April 2007).

B. C. Chakoumakos, R. Custelcean, T. Kamlyama, K. Oikawa, B. C. Sales, and M. D. Lumsden, "Structural modulation in K_2V_3O8," *Journal of Solid State Chemistry* **180**, 812–817 (March 2007).

W. R. Chen, L. Porcar, Y. Liu, P. D. Butler, and L. J. Magid, "Small angle neutron scattering studies of the counterion effects on the molecular conformation and structure of charged g4 PAMAM dendrimers in aqueous solutions," *Macromolecules* **40**, 5887–98 (August 2007).

Y. Chen, M. B. Stone, M. Kenzelmann, C. D. Batista, D. H. Reich, and C. Broholm, "Phase diagram and spin Hamiltonian of weakly-coupled anisotropic S=1/2 chains in $CuCl_2$ (2((CD3)2SO)," *Physical Review B* **75** (June 2007).

G. Cheng, Y. B. Melnichenko, G. D. Wignall, F. J. Hua, K. L. Hong, and J. W. Mays, "Conformation of oligo(ethylene glycol) grafted polystyrene in dilute aqueous solutions," *Polymer* **48**, 4108–4113 (June 2007).

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Contact Information

Office of the ORNL Associate Laboratory Director for Neutron Sciences
Ian Anderson (andersonian@ornl.gov)
865.574.0558

High Flux Isotope Reactor
Oak Ridge National Laboratory
P.O. Box 2008 MS-6398
Oak Ridge, TN 37831-6398
Phone: 865.574.1301

Spallation Neutron Source
Oak Ridge National Laboratory
P.O. Box 2008 MS-6477
Oak Ridge, TN 37831-6477
Phone: 865.574.0558

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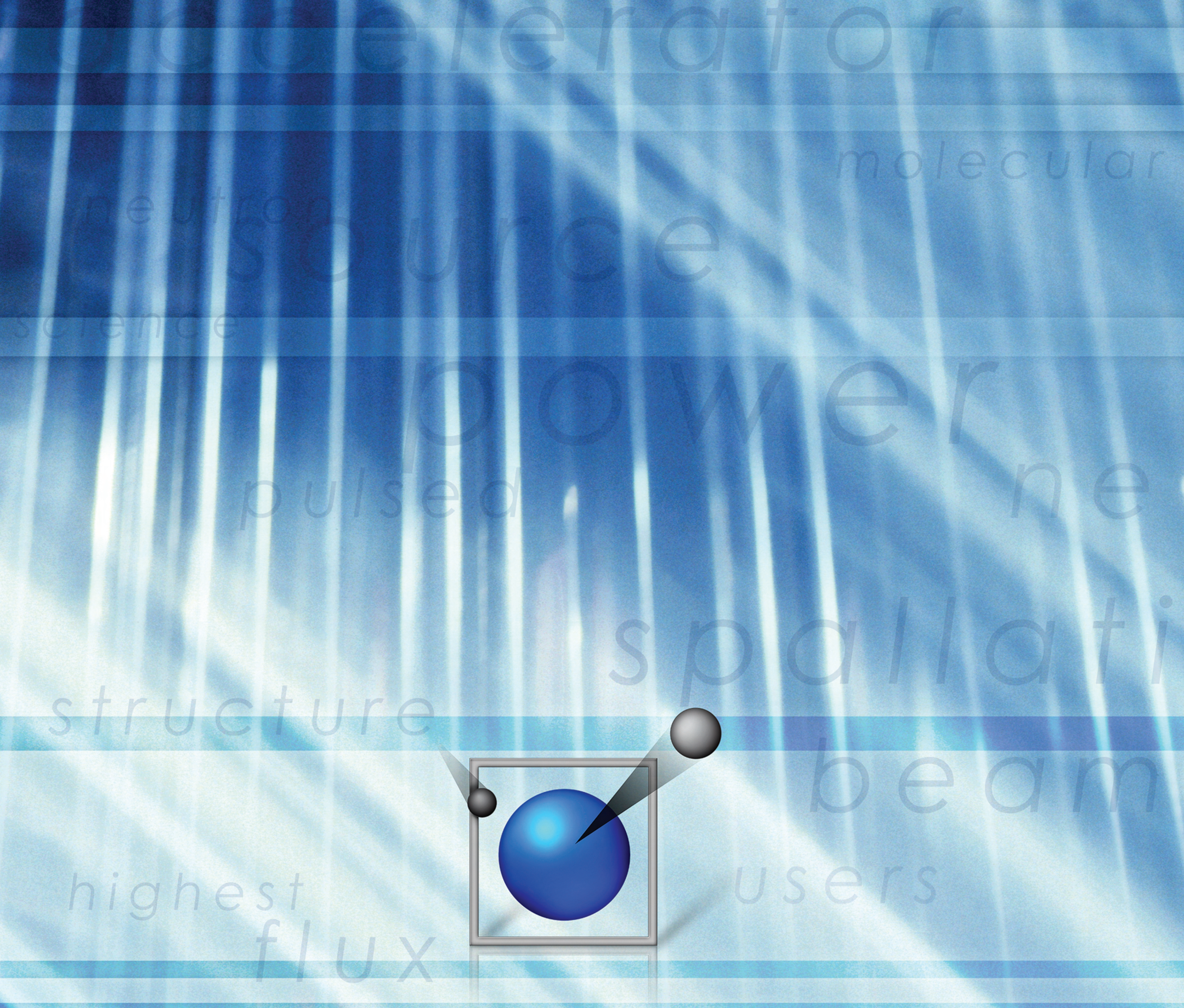

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