Oak Ridge National Laboratory — Neutron Sciences

The Neutron Pulse

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SNS Instrument Status

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During the summer and fall of 2006, several significant events occurred on the Spallation Neutron Source (SNS) instrument floor. The Backscattering Spectrometer was joined by the Magnetism and Liquids reflectometers as operating instruments. The two reflectometers opened their shutters for the first time in July 2006. All three instrument teams have been busy with commissioning activities (e.g., calibrating detectors and motors, improving shielding and reducing backgrounds, and testing polarization optics on the Magnetism Reflectometer)

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HFIR Update: Cool Times Ahead

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The High Flux Isotope Reactor (HFIR) cold source project passed a major milestone in September with the successful completion of the "helium" heater test. The cold source maintained vacuum and temperature in situ, while cooling to temperatures below 20 K (see below). This was accomplished with an applied heat load equivalent to that expected in actual operations and fully validated the existing cold source performance models. Helium was used as a cryogen for the test. As of this writing, a second test has been successfully completed using supercritical hydrogen as a cryogen. The next required step is an operational readiness review. Users are looking forward to resumption of HFIR operations, with the anticipated production of cold and thermal neutrons during May 2007.

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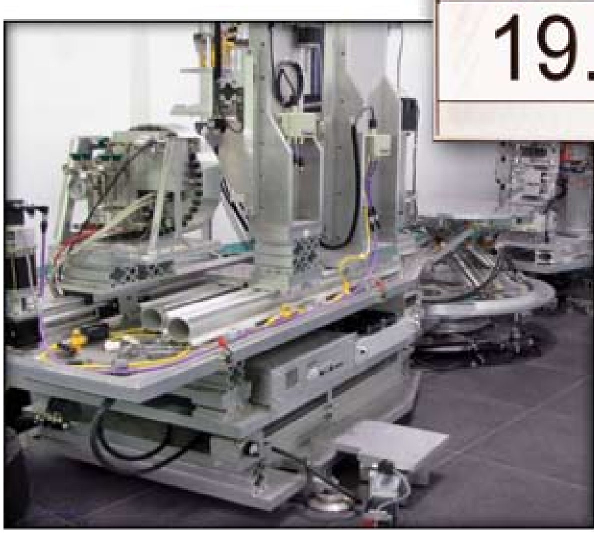
Bottom left: sample stage of the SNS Magnetism Reflectometer. The front left side shows the detector table and spin analysis optics; the middle shows the hexapod sample support and omega rotation table; and the right back shows the incident optics table. Center: the HFIR cold source maintains vacuum and temperature while cooling to below 20 K. Right: interior of the SNS Backscattering Silicon Spectrometer large evacuated flight path.



Associate Laboratory Director's Comments

Thom Mason, masont@ornl.gov

Effective October 1, 2006, HFIR and SNS were combined into a newly formed Neutron Sciences Directorate. This reorganization naturally follows completion of the SNS construction project and the upgrade of HFIR. The purpose of the new organization is to allow the two facilities to more easily share resources and expertise, while developing a unified, world-class neutron science program. Although the past focus of *The Neutron Pulse* has been SNS, we look forward to sharing more news about the exciting activities at HFIR. Other groups within the Neutron Sciences organization will continue to provide dedicated support to both facilities for scientific and technological development.

The budget for 2007 was not approved until February, but it now appears that both SNS and HFIR will receive close to the expected funding. Many users spoke up in support of Office of Science programs, which contributed to the Congressional action to increase science funding over the 2006 levels.

As we prepare for users, we are developing the proposal review and training systems that will provide easy access to ORNL. Our goal is to make doing science in a safe environment as straightforward as possible, with much of the training accomplished online before arrival.

Aerial view of the HFIR complex. The HFIR cold source operational readiness review is scheduled for April 2007.

Over the next several months, I anticipate welcoming returning users to HFIR and initial users at SNS. I'm optimistic that we will soon be seeing the first published results from our new instruments.

SHUG UPDATE

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After many years in the making, SNS is on its way to becoming the most advanced pulsed neutron source in the world. We all know and realize the benefits of such an accomplishment, brought to fruition by the dedicated people at SNS. The user community is looking forward to getting hands-on experience with the state-of-the-art instruments—optimized to operate with the high flux—and to the exciting scientific opportunities they will make possible. The excitement from users continues to grow as approved instruments wait to come on line and as new, innovative instruments are continuously proposed. This anticipation will continue through completion of the planned second target station and beyond as the future of neutron scattering science becomes brighter and brighter. This is also an exciting time for HFIR, with installation of the new cold source, the new SANS instruments, and operations about to resume. The two Oak Ridge sources are highly complementary and vital to the neutron community. Together, under the new neutron sciences organization, both facilities will serve the community well, with the potential of doubling the number of neutron users in North America.

This is an opportune time to establish strong collaborations between academia and ORNL. Such a partnership is absolutely necessary for the steady growth of neutron science in this country. The neutron science program at Oak Ridge should go beyond the regional science community by establishing an infrastructure for a strong, worldwide collaborative program.

In the past year, the SNS-HFIR User Group (SHUG) Executive Committee has closely monitored neutron activities at Oak Ridge. At the American Conference on Neutron Scattering, potential users had the chance to listen to the latest updates from the two facilities and to make suggestions for improvements. SHUG has also actively participated in Synchrotron and Neutron User Group activities in an effort to bring synchrotron and neutron science activities to the forefront of U.S. federal government budgetary science requirements. The SHUG Executive Committee, along with the Neutron Sciences User Office, is organizing the second SHUG meeting on October 8-10, 2007, at ORNL. This meeting will serve as outreach to the academic community and will feature recent results from some of the first experiments at the HFIR cold source and SNS. The event will be coupled with the nanoscience meeting organized by the ORNL Center for Nanophase Materials Sciences. The nanoscience meeting will follow in the second part of the week, after the SHUG meeting, and will explore opportunities for applying neutron scattering techniques to the characterization of materials at the nanoscale. An outreach program will provide fellowships for select graduate students to participate in a training program for neutron data analysis and experimentation.

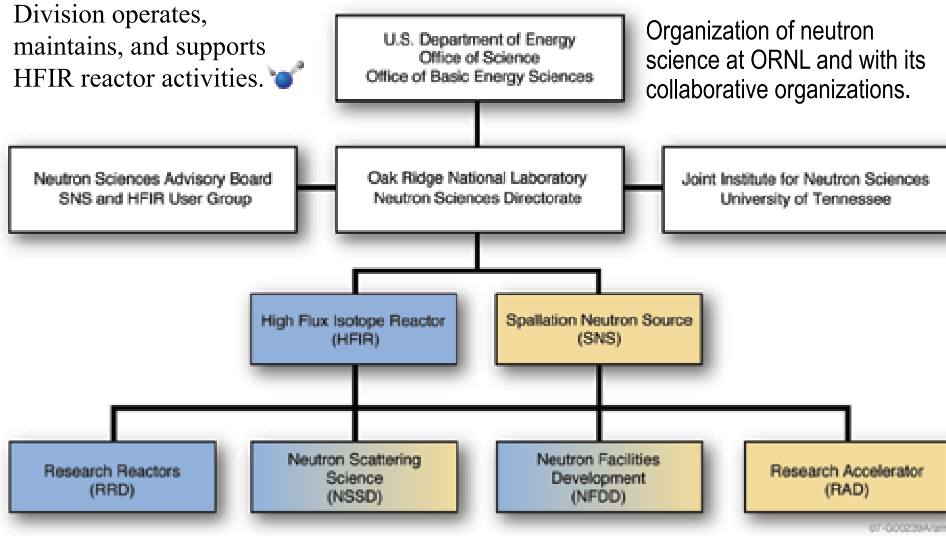
The Executive Committee's primary role is to voice the concerns and needs of the user community to the two neutron scattering facilities. We would like to hear from you so that we can address your concerns and needs. Please visit our web site at www.sns.gov/shug/.index.html.

ORNL's New Neutron Sciences Directorate

For the past several years, ORNL has been undergoing a major transformation that includes a substantial upgrade of HFIR and construction of SNS. These two facilities are now being managed and operated under a single Neutron Sciences Directorate. This new organization was established in October 2006 and is led by Thom Mason, now the Associate Laboratory Director for Neutron Sciences.

Although HFIR and SNS will continue to operate as separate facilities, the new organizational structure is intended to foster scientific integration between the two. Within the directorate, the neutron scattering programs at both HFIR and SNS are part of the Neutron Scattering Science Division, led by Ian Anderson. The goal of this organization is to develop and maintain a world-class neutron scattering program through in-house research and comprehensive support of an international neutron user community. Part of this goal is to operate and maintain a best-in-class suite of instruments and to support development of new instruments that allow neutron methods to be applied to a growing range of multidisciplinary scientific challenges.

Three other Neutron Sciences divisions augment and support neutron scattering science activities. The Neutron Facilities Development Division supports continued development of the facilities and their capabilities through research and development (R&D), such as for new accelerator and neutron techniques, and through management of new projects. The Research Accelerator Division operates and maintains the SNS accelerator systems and supports R&D, construction, and commissioning of new systems. The Research Reactors Division operates, maintains, and supports HFIR reactor activities.



Organization of neutron science at ORNL and with its collaborative organizations.

Initial Users at SNS

Teams supporting the first three SNS instruments (Backscattering Spectrometer and Magnetism and Liquids reflectometers) are making significant commissioning progress. Working closely with members of the instrument advisory teams (IATs) for these instruments, we are almost ready to open our online proposal system.

The "initial user" period will include a call for initial users from the general user population. Again, the IATs will provide scientific evaluation of proposals. Operating procedures and training will be formalized by this time, and instrument predictability will improve.

During the "user" phase, instruments will available for full participation in the general user program. At this stage, proposals will be evaluated by external scientific review committees.

This phased approach will encourage IAT members to become involved in initial user experiments. SNS expects to receive feedback from IATs on all aspects of activities, including instrument performance, the proposal system, site access, training, sample management, and other aspects of the user process.

For the first three instruments, we anticipate entering the initial user phase in summer 2007, with the general user program beginning in fall 2007. For all phases, experiment feasibility and safety reviews will be performed by SNS management.

New Shull Fellows Selected

Two new Shull fellows were recently selected and are expected to begin work at ORNL within the next several months. ORNL established the Clifford G. Shull Fellowship in honor of Shull's pioneering neutron scattering research while at ORNL in the 1940s. Shull was a corecipient of the 1994 Nobel Prize in Physics.

The new fellows are Sylvia McLain and Christopher Stanley. Since 2004, Sylvia McLain has been serving as an academic visitor in the Department of Biochemistry at the University of Oxford and as a U.S. National Science Foundation International Postdoctoral Fellow at ISIS. She received her PhD in chemistry from the University of Tennessee. Recent research has included studies of the atomic structure of amino acids in solution. Christopher Stanley has been a postdoctoral research associate at the NIST National Research Council since 2004. He received his PhD in polymer science and engineering from the University of Massachusetts, Amherst. Christopher's areas of interest include using neutron scattering for studies of osmolytes and biological systems.

We welcome these two new fellows to the neutron scattering community at ORNL.

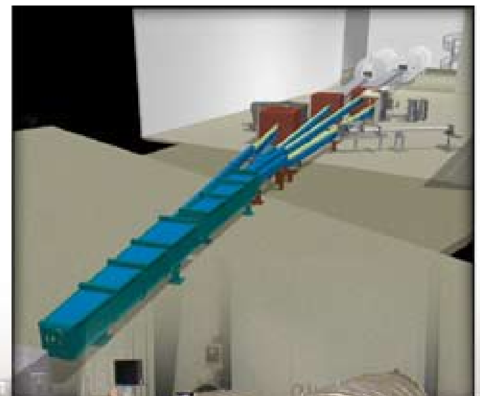
HFIR Update

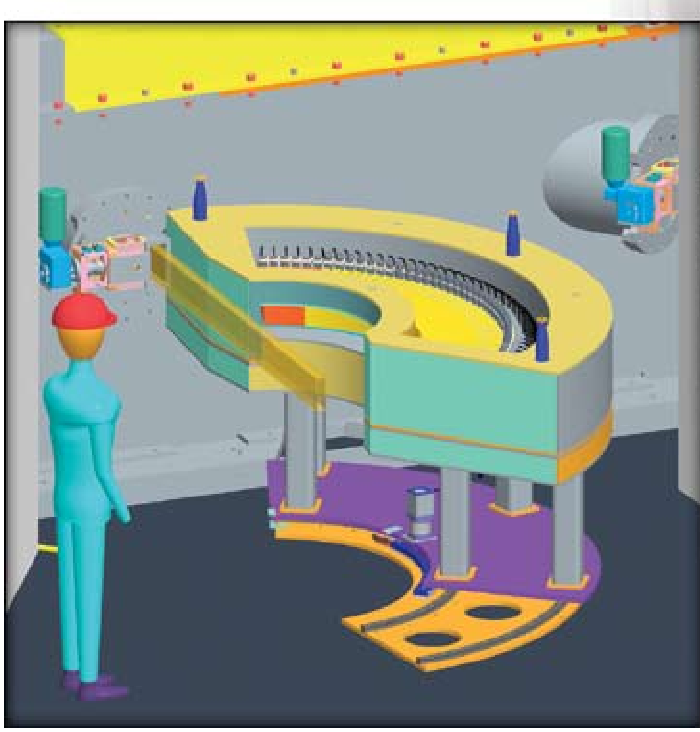
Continued from page 1

The HFIR instrument configuration is shown on page 6. The red boxes indicate instruments that are actually on the facility floor. For the past few years, the three thermal triple-axis spectrometers (HB-1, HB-1A, and HB-3) have been available to experimenters and have been running the highly popular SPICE software developed at Oak Ridge National Laboratory (ORNL). The Residual Stress Spectrometer (HB-2B) is also ready to accept users as soon as the reactor runs. Both the Wide-Angle Neutron Diffractometer (WAND, HB-2C) and the Single-Crystal, Four-Circle Diffractometer (HB-3A) are installed and are undergoing commissioning. Perhaps the most exciting new development for many users is the construction of two new small-angle neutron scattering (SANS) spectrometers. The detector tanks for these instruments are shown below on the right. The instrument on the left (CG-2) is a general-purpose, high-resolution SANS instrument. The one on the right (CG-3) was constructed especially for biological studies. SPICE software configured for small-angle scattering will be used on both spectrometers. The SANS instruments will be commissioned with cold neutrons as soon as possible, ushering in a new era of research at HFIR. As this happens, the adjacent laboratories will be equipped for users, and plans are afoot to improve the overall HFIR facilities.

Development of other instruments at HFIR is continuing, with two near-term priority instruments, as indicated on page 6 by the gray boxes. The U.S./Japan triple-axis spectrometer (CG-4C) is under construction, and initial commissioning of the Powder Diffractometer on HB-2A is scheduled for this fall. Beam lines are available to add other instruments, based on the needs of the scientific community (page 6). With the current beam configuration, HFIR can support eight thermal instruments and seven cold instruments, with the possibility of adding one additional beam in the position of the old 12-m SANS.

For the last year, HFIR has been shutdown for installation and relicensing with the cold source. We anticipate that steady-state operations will eventually provide neutron beams for eight to ten reactor cycles per year and that, with regular operations, the next major shutdown for a beryllium reflector replacement will not be necessary until after 2020. In principle, it is possible to install a cold source in radial beam tube HB-2, which would provide an unparalleled flux of cold neutrons feeding instruments in a new guide hall. In the meantime, ORNL neutron users will soon be able to access thermal and cold neutron beams of world-class brightness at HFIR, as well as the most intense pulsed source in the world at SNS. Exciting, cool times indeed.





Left: schematic of the Powder Diffractometer at HFIR, which is scheduled for initial commissioning by fall 2007. Center: detector tanks for the new SANS instruments. On the left is the general-purpose, high-resolution instrument; on the right is the SANS instrument constructed specifically for biological research. Top right: schematic of the guide tubes leading into the SANS instrument detector tanks.

SNS Instrument Status

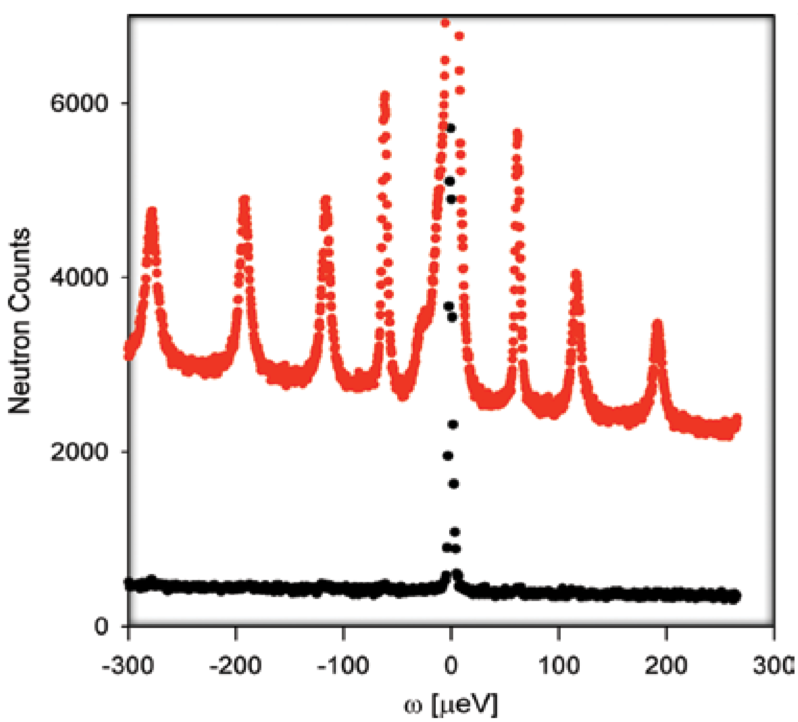
Continued from page 1

and with getting the instruments ready to reliably produce world-class science. The progress in both instrument performance and accelerator power is truly remarkable and is illustrated in data collected on the Backscattering Spectrometer (see below). These three instrument teams should be ready for initial science measurements this summer. The SNS web site includes the near-term operations schedule (www.sns.gov/calendar/operations_schedule.shtml).

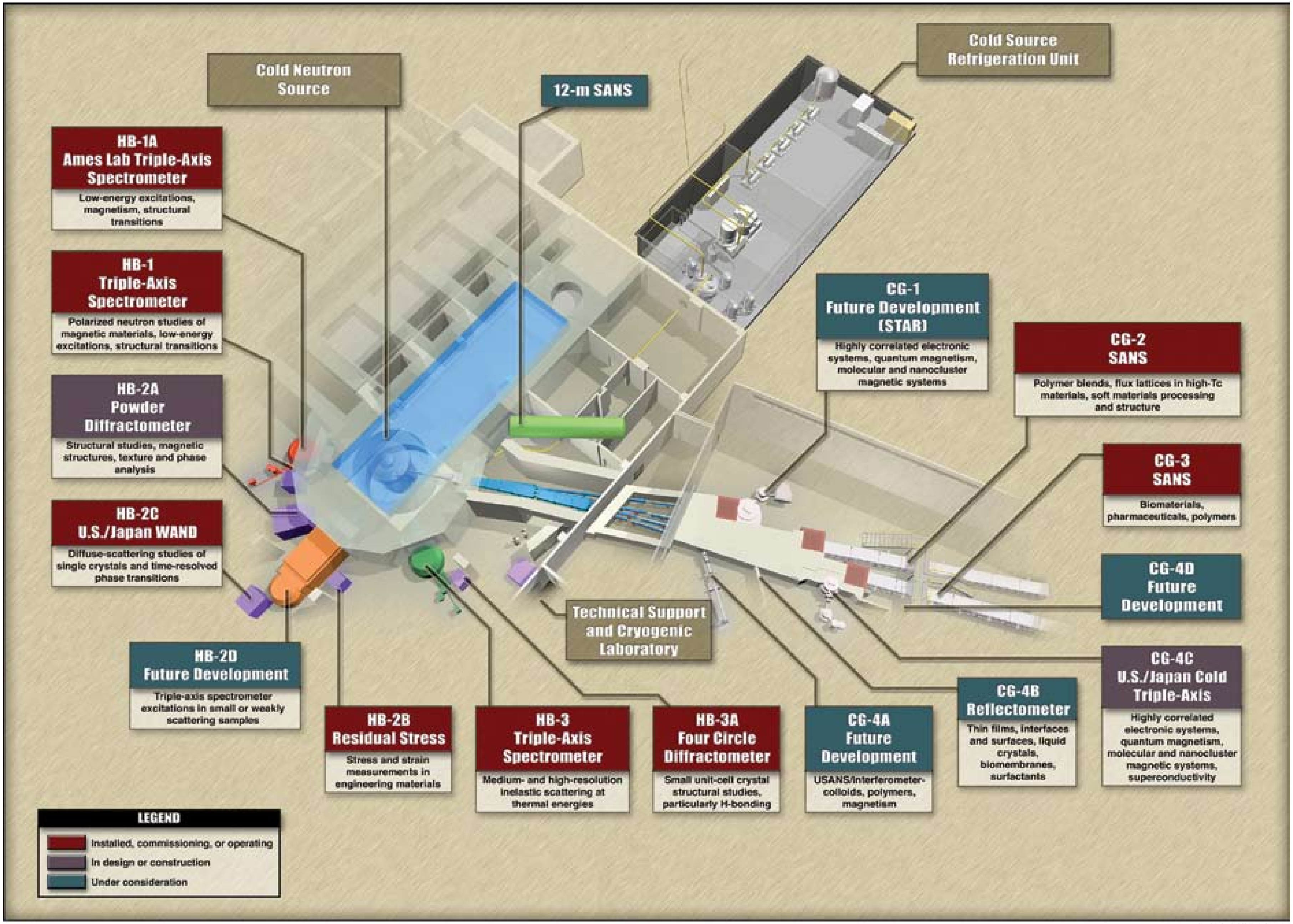
Instrument installation will continue to be a major part of SNS activities for the foreseeable future. The next instrument scheduled for commissioning is the Wide Angular-Range Chopper Spectrometer (ARCS), to be closely followed by the Powder Diffractometer (POWGEN3), Extended Q-Range Small-Angle Diffractometer, and the Cold Neutron Chopper Spectrometer (CNCS). Installation activities on these instruments are in full swing. The complete SNS instrument configuration is shown on page 7.

The Sample Environment Team has expanded to six members and has been gaining operations experience by supporting low-temperature equipment mounted on the Backscattering Spectrometer. The Sample Environment equipment inventory has also been growing rapidly with the recent arrival of a 1600ºC furnace and a cryogenic sample changer (Fast Exchange Refrigerator for Neutron Science), initially designed for use on POWGEN3. Delivery of a 5-T, self-shielded superconducting magnet and a 0.03-K dilution refrigerator insert is expected in September 2007.

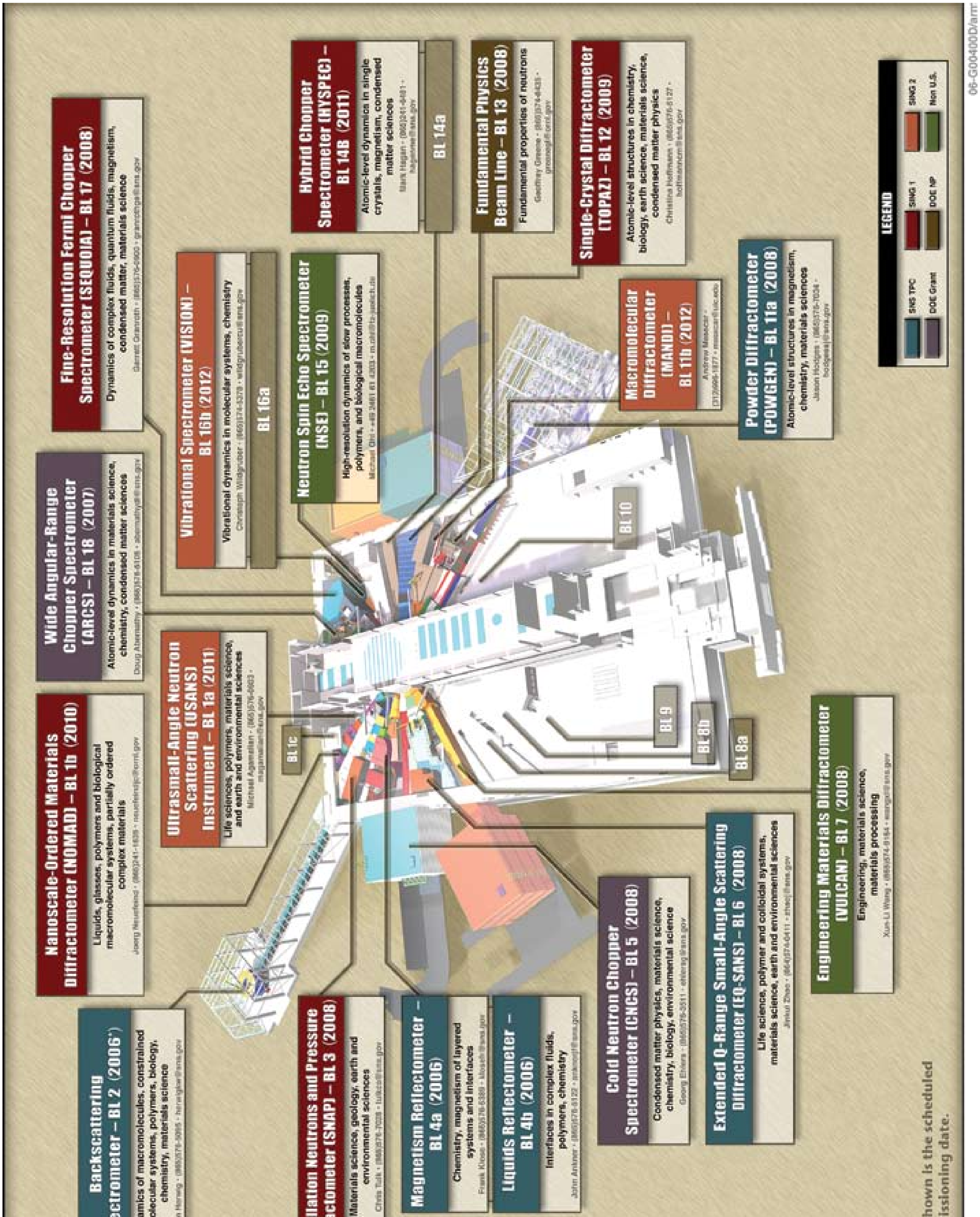
Top left: cryogenic sample changer for the Fast Exchange Refrigerator for Neutron Science. Top right: 1600ºC niobium furnace. Bottom left: future CNCS sample area. Bottom right: test fit of the ARCS scattering chamber.



Inelastic data collected on the Backscattering Spectrometer from a quantum tunneling sample, 4-methyl pyridine N-oxide, at 4 K. The tunneling peaks that were just visible in data collected when the instrument was first operational in May 2006 (shown by black circles) are now clearly seen in data collected from the same sample in November (shown by red circles). For comparison, the data have been scaled to equivalent collection times.



HFIR instrument configuration.



SNS instrument configuration.

Array of Cray supercomputers at ORNL's National Center for Computational Sciences.

Neutron Science: Experiment and Simulation

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ORNL's National Center for Computational Sciences (NCCS) is to simulation researchers what HFIR and SNS are to neutron scientists: one of the world's best resources for delving into challenging scientific questions. The computing resources of NCCS, the restart of HFIR, and the opening of SNS present a perfect opportunity for researchers to couple their experiments with computational simulations.

Running codes on supercomputers is serious business. In the words of Julia White, group leader for NCCS User Assistance and Outreach, "An idea is emerging to allocate time to groups of researchers with moderate levels of simulation experience on high-performance computers and to help them make the transition to very large supercomputers. . . . We want to gauge the interest of SNS and HFIR users in tapping the computational resources of the center." Researchers are invited to submit one- to two-page outlines demonstrating how they would use the advanced computing capability of NCCS, including current simulations, plans for future simulations, and a brief description of their research.

Researchers should have some idea of how well their codes might scale up, for instance, or how effectively additional CPUs could be used. Just a few of the questions to think about: Are there memory issues to consider? Will file input/output become a bottleneck past a certain number of processors? What is the impact to the science being explored? NCCS staff have considerable experience assisting users and will help HFIR and SNS users as they venture into using supercomputing simulation to enhance their experiments.

Questions or replies to this request for interest should be submitted to help@nccs.gov or to Steve Miller, Neutron Sciences Scientific Computing group leader (millersd@ornl.gov). For more information regarding NCCS, see www.nccs.gov.

Probing Matter in High Magnetic Fields (>30 T) Using Neutron Scattering

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The National Science Foundation (NSF) has funded a project for conceptual and engineering design of SNS instrumentation to enable neutron scattering experiments in ultrahigh magnetic fields. The proposed facility would provide magnetic fields more than twice as large as those now possible.

High magnetic fields are of interest to a wide range of materials scientists because they offer a controlled means of altering materials properties. Over the last decade, experiments at the National High Magnetic Field Laboratory show that by studying the response of materials to high magnetic fields it is possible to derive unique insight into the origin of useful or interesting materials properties. Neutron scattering, on the other hand, provides a time-resolved window on the nanoscale, which is of growing importance to advanced technologies. By combining these techniques, the proposed facility could make it possible to probe nanoscale structure and dynamics while tuning materials properties in magnetic fields that exceed 30 T.

The proposed facility would provide unique materials research capabilities in areas such as quantum magnetism, correlated metals, molecular magnetism, nanostructured magnets, superconductivity, metallurgy, macromolecular crystallography, hydride structure determination, and neutron-excited nuclear and electronic magnetic resonance. This basic research has the potential to impact technological areas such as high-density magnetic information storage, quantum computing, superconducting power transmission, steel processing, pharmacology, and hydrogen-based energy distribution. By involving students and postdocs in design of the facility and development of the research program, this project will also build new expertise in high-field technology and instrumentation development for materials science.

Two recent technical advances make the project feasible now. First, the increased brightness of SNS enables experiments on small samples under extreme thermodynamic conditions. Second, a new series-connected hybrid magnet technology developed at the National High Magnetic Field Laboratory makes it feasible to bring a neutron beam into a >30-T DC magnet and operate it cost effectively at SNS.

This project is being funded as an NSF Instrumentation for Materials Research—Major Instrumentation Project. Assuming a successful conceptual design phase and continued funding support, construction could start in FY 2009.

Tennessee Structural Biology Symposium

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Attendees at the Tennessee Structural Biology Symposium.

The annual meeting of the Tennessee Structural Biology Symposium was hosted jointly by The University of Tennessee (UT) and ORNL on September 29-30, 2006. The meeting was attended by more than 140 PhD students, postdocs, and mentors from UT, St. Jude Children's Research Hospital, Vanderbilt University, ORNL, and other institutes in Tennessee and neighboring states. This meeting provides a forum for the presentation and discussion of project work by young researchers and postdocs working in the complementary fields of computational and structural molecular biology. The 2006 meeting included more than 20 talks and 35 posters. Day one was spent at UT, with presentations on a wide range of topics such as state-of-the-art work on protein structure and function using nuclear magnetic resonance and X-ray techniques, structural analysis of protein complex systems using electron microscopy, and computational analysis of genomic data. Day two was hosted at SNS and began with an introduction on ORNL neutron scattering sciences and capabilities, presented by Ian Anderson, director of the ORNL Neutron Scattering Science Division. Following that was a presentation on small-angle neutron scattering of protein complexes in solution and neutron diffraction analysis of enzyme structure and function. The keynote address was given by UT/ORNL's first Governor's Chair, Jeremy Smith, who presented work on the neutron and molecular dynamical analysis of complex biological systems.

The meeting was supported by the Joint Institute for Neutron Sciences.

IAN2006

The Imaging and Neutrons 2006 (IAN2006) Workshop was held on October 23-25, 2006, at SNS. More than 200 people from 14 countries participated. In addition to neutron scattering, presentations included information on a wide range of other imaging techniques and scientific disciplines. The goal of the interdisciplinary meeting was to promote understanding of the effectiveness, as well as limitations, of different imaging tools and to provide a forum for sharing knowledge in these areas.

Talks identified the current needs and potential contributions of imaging with neutrons in a wide range of applications. Planned as a follow-up to the 8th World Conference on Neutron Radiography, IAN2006 was directed at a broad-based international scientific community interested in the potential application of novel imaging techniques using neutrons, with a particular emphasis on the capabilities provided by next-generation neutron sources.

The program included 40 speakers and was divided into two parts. On Monday, the focus was on current neutron techniques and related challenges and opportunities. Tuesday and Wednesday sessions were oriented to applications and included other techniques, such as X rays and magnetic resonance imaging.

On the opening night of IAN2006, in a presentation open to the public, Philippe Walter of the Centre de Recherche et de Restauration des Musées de France spoke on the various investigative techniques used in cultural heritage. In his talk, "Neutrons for Mona Lisa," he discussed activities at the Ion Beam Analysis Facility of Le Louvre in Paris, including scientific imaging and analysis of Leonardo Da Vinci's Mona Lisa and other works of art and artifacts.

Sponsors of IAN2006 included ORNL's Neutron Scattering Science Division, the Joint Institute for Neutron Sciences, Oak Ridge Associated Universities, and NSF, in collaboration with the International Atomic Energy Agency.

Preceding IAN2006 was the Progress in Electron Volt Neutron Spectroscopy Workshop. Objectives of the workshop included identifying the needs and potential contributions of electron-volt neutron spectrometers and identifying new techniques that will be made possible by next-generation neutron sources. The 45 attendees of the workshop reviewed the latest progress in field and instrument

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Set Your Calendars for User Meetings in 2007

ORNL will host two user meetings this October. The SNS-HFIR User Group will meet on October 8-10. This will be followed by a meeting of the Center for Nanophase Materials Sciences User Group on October 10-12. See www.sns.gov for more details.

Neutronics Overview

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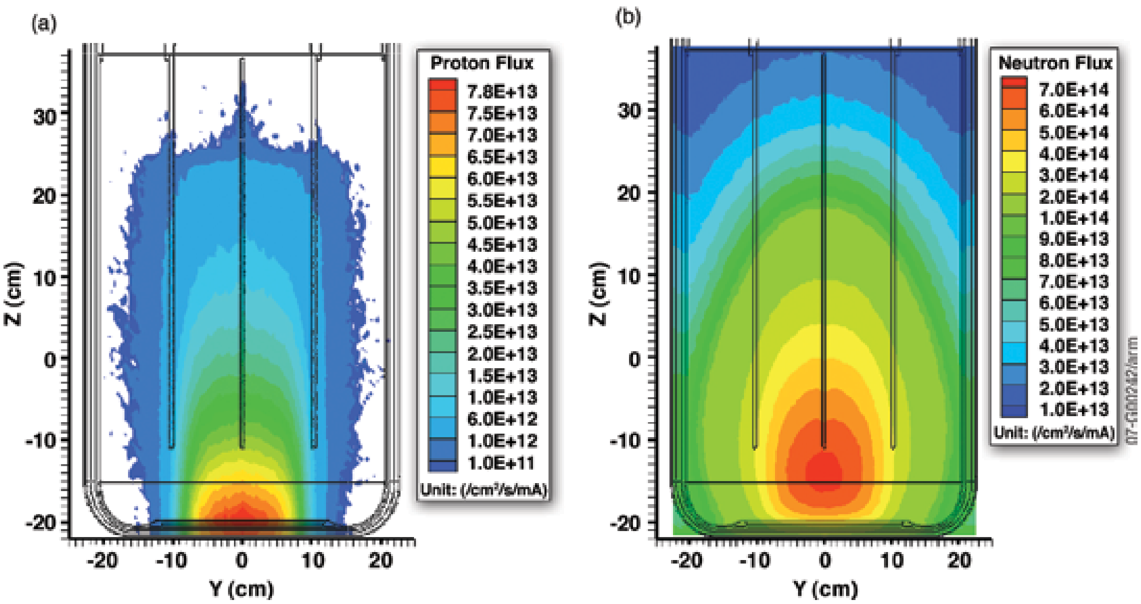
Detailed Monte Carlo models have been used to simulate the interaction of the SNS proton beam with the mercury target. From these simulations, we gain important information on the neutron production and energy deposition in the target system. This information has led to the thermal hydraulics design of the target, placement of moderators, choice of reflector materials and geometry, etc. Results from these calculations are being used to simulate and optimize the design of neutron scattering instruments for SNS. Here we summarize the simulation results to give users a better understanding of the SNS target system.

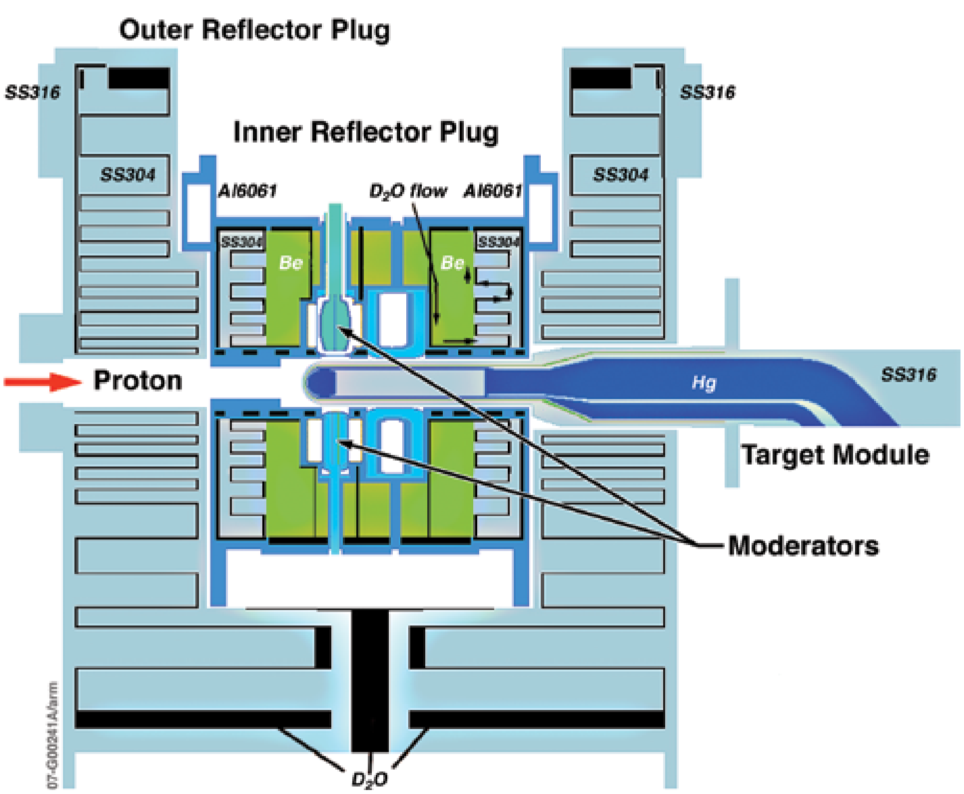


Proton (a) and neutron (b) fluxes at the center plane of the SNS target module.

An elevation view of the Monte Carlo model of the SNS target system used for the calculation is shown below. The SNS target system consists of a flowing mercury target, three hydrogen moderators and one water moderator, an "inner plug" formed of beryllium and steel reflectors, and an "outer plug" formed of steel. The figure above shows a horizontal slice through the mercury target, indicating the proton and neutron flux during operations. The flux plots are normalized to 1 MW but can be scaled to the appropriate power. As can be seen from the plots, the neutron flux is about one order of magnitude higher than the proton flux and peaks ~5 cm downstream of the peak proton flux.

For each 1-GeV proton incident on the target, just under 26 neutrons are liberated, with 85% being freed in the target and 9% being freed in the inner reflector plug. Of the ~26 neutrons per proton, only 5% leave the moderators and make it to the edge of the outer reflector plug at a radius of 1 m. An even smaller percentage of the neutrons make it through the beam lines to the edge of the bulk shield at 5.3 m, depending on the size of the beam extracted, whether or not the beam line uses neutron guides, etc. A safe assumption is that less than 0.1% of the source neutrons actually make it down a beam line to a sample.

So if the majority of neutrons do not make it to a sample, what happens to them? Approximately 20% of the neutrons are absorbed in the target, 34% are captured in the inner reflector plug,



Elevation view of the SNS target system as modeled by MCNPX software. Materials are indicated in italics. For reference, the diameter of the outer cylinder is 1.9 m.

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and 23% are absorbed in the outer reflector plug. Roughly 8% of the neutrons are absorbed in the moderators, including the cadmium and gadolinium used to shape the neutron pulses. The remainder of the neutrons, ~15% of the total, escape from the outer reflector plug into the surrounding shielding, both radially and vertically.

When a 1-GeV proton is incident on the SNS target, it deposits ~62% of its energy in the target, ~15% in the inner reflector plug, and ~8% in the outer reflector plug. A small amount of energy is deposited in the moderators and the proton beam window. The remainder of the energy either escapes the outer reflector plug as neutron kinetic energy or is used to overcome the binding energy of the neutrons, which are freed during the interaction process.

ORNL Nanoscience Center Wraps Up Successful First Year of Operation

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ORNL's new centerpiece for nanoscience research, the Center for Nanophase Materials Sciences (CNMS), was completed—on scope, under budget, and one month ahead of schedule—during 2006. CNMS was the first of the U.S. Department of Energy's (DOE's) five nanoscale research centers to achieve this milestone.

With initial operations and completion of the facility progressing simultaneously over the last year, CNMS was able to host 139 new users. Although the center attracts researchers from around the world, it is also proving to be an important regional research center, drawing many scientists from the southeastern and eastern United States.

Construction on the $65M center began in August 2003. With completion of the building in 2005, activities in 2006 focused on installation of world-class lasers and scanning probes and other instruments for materials synthesis and characterization, as well as outfitting a 10,000 ft^2 clean room.

Designated by DOE as a user facility, the center integrates nanoscale science with neutron science, synthesis science, and theory, modeling, and simulation. With the center's proximity to SNS and HFIR, users will be able to access neutron beams for characterization of materials from CNMS. ORNL's Leadership Computing Facility is also a partner in CNMS research, bringing the high-end capabilities of some of the world's most powerful supercomputers to assist in understanding the complex phenomena controlling nanoscale behavior.

Top: Laura Buchanan, a summer student, and CNMS staff member Joe Pickel perform polymer synthesis at the center. Right: Synthesis of deuterated polymers.

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IAN2006 attendees.

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developments. As a result of the workshop, the attendees agreed to explore options for an instrument at SNS. George Rieter (greiter@uh.edu) is coordinating this activity.

A summary of IAN2006 is being drafted to identify potentially valuable imaging techniques, as well as directions for additional research and investment to realize this potential worldwide. The IAN2006 draft report and presentations from both workshops are available at www.sns.gov/workshops/ian2006.

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For the latest user updates, see the users web site at www.sns.gov/users/users.htm.