OAK RIDGE NATIONAL LABORATORY
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The NEUTRON PULSE

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Progress Continues Toward 2006 Completion

By the beginning of FY 06 (October 2005), the Spallation Neutron Source (SNS) will be nearly 95% complete, with less than a year of construction remaining. Commissioning of the entire linac at the full power of 1 GeV begins in August. Equipment installation in the ring tunnel is nearing completion. Commissioning of the high-energy beam transport system and the Ring Accelerator Readiness Review will begin in February 2006.

On the experimental side, general construction of the Target Building and Service Bay are complete, and remote-handling systems are being tested. The first target module has arrived (see right), and target installation and testing are progressing to support full integrated systems testing this winter. Beam lines have been allocated for 17 instruments, 16 of which have received full or partial funding.

First Step in Power Upgrade

In November 2004, Dr. Ray Orbach, director of the U.S. Department of Energy's (DOE's) Office of Science, approved a mission need statement for the SNS Power Upgrade project. This approval initiated conceptual design for an upgrade to take advantage of flexibilities designed into SNS and to maintain its position of worldwide scientific leadership. The power upgrade allows more experiments to be performed and paves the way for a second target station to be built at a later stage.

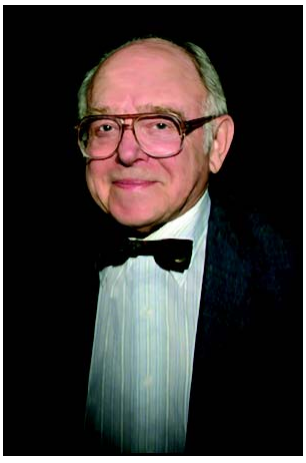
Many technical margins have been built into SNS systems to facilitate a power upgrade to 2 MW, and the proton beam power goal for the upgrade is to achieve at least 3 MW (more than double the initial SNS project goal of 1.4 MW). The preliminary schedule calls for design and long-lead procurements to begin in 2007, with project completion in 2011. Total cost will be $120-160M.

First SNS target module.

In this Issue

Shull Fellowship for Postdoctoral Positions

SNS and Oak Ridge National Laboratory (ORNL) announce establishment of the Clifford G. Shull Fellowship. 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 has been established in recognition of his pioneering work in this field. The goal of the fellowship is to attract new scientific talent to ORNL for the development of its neutron science program. Candidates will have exceptional ability, be capable of developing innovative research programs, and show promise of outstanding leadership. Shull fellows will be sponsored by the SNS and High Flux Isotope Reactor (HFIR) facilities in Oak Ridge. Fellowships will be two-year appointments renewable for a third. Additional information is available at www.sns.gov/shullfellowship.



Clifford Shull.

Director's Comments

Thom Mason
Associate Lab Director
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SNS continues on schedule and on budget. By June 2006, we eagerly anticipate completion of the construction effort with DOE's approval of Critical Decision 4. Although a great deal of work has been accomplished, significant equipment installation and commissioning remains to be done.

In February 2005, DOE's FY 2006 budget request was submitted to Congress and contained three elements related to SNS. The construction portion of the budget was proposed at $75.6M. Because we will be an operating facility during a portion of FY 2006, SNS has a requested operating budget of $73M. In addition, DOE's Office of Basic Energy Sciences has proposed funding design and construction of the five SING instruments (SNS Instruments—Next Generation) at a level of $8.1M. The SING instruments received initial funding in FY 2005 and will be completed at a rate of about one instrument per year beginning in FY 2008.

Main lobby of the SNS CLO.

The state of Tennessee's budget for the fiscal year beginning July 1, 2005, contains $8M for the construction of the Joint Institute for Neutron Sciences (JINS). This new building is proposed for the Chestnut Ridge site near the SNS Central Laboratory and Office Building (CLO) and the Center for Nanophase Materials Sciences (CNMS). JINS is an important element of future collaborative research efforts and will provide strong links to the academic community.

In October 2005, SNS and HFIR will host an on-site user meeting. Although final preparations are still being made, SNS elements of this meeting will include soliciting input from users for the first experiments on the first three instruments—the backscattering spectrometer and the magnetism and liquids reflectometers. Presentations will be made about the detectors, sample environments, user training, and other elements of the "user experience," and the audience will be encouraged to provide feedback. Instrument advisory teams and instrument development teams (IDTs) will also be meeting. I look forward to seeing you there.

SHUG Update

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With HFIR's user program regaining strength and the first neutrons at SNS just around the corner, it is an exciting time to be involved with the two facilities. It is also an opportune time to assist with the development of the two user programs. The policies and facilities that are put in place over the next few years will play a significant part in ensuring the long-term success of the user programs at both neutron-scattering centers.

I am grateful for an opportunity to serve the neutron user community and am particularly grateful to my colleagues who have been, or are currently, part of the SNS-HFIR User Group (SHUG) Executive Committee for all of their efforts. I would also like to thank the management teams and staff at both SNS and HFIR for their tireless efforts to develop world-class capabilities for us—the users—and for their willingness to partner with the user community through SHUG. Executive Committee members meet on a regular basis (about every other month) by conference call, and users, or potential future users, are invited to peruse our web site (www.sns.gov/shug/) to read announcements and minutes from these meetings and to provide input on issues of concern.

A significant concern of SHUG is the reliability of operations at HFIR. Other issues that are being addressed include (1) monitoring the restarted user program at HFIR and the time line for the addition of instruments to this program, (2) the scientific program for the first SNS and HFIR user meeting (October 2005)—and in particular whether this meeting should include a workshop focused on training new or potential users in some area of neutron scattering, (3) providing user input on the type of ancillary lab space and equipment that is desirable, (4) housing and other quality and cost-of-living issues for users, and (5) stewardship and shipment of samples that are brought to SNS and HFIR for experiments.

Instrument Updates

Liquids Reflectometer

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Liquids reflectometer procurements continue, and installation activities have begun. Bandwidth chopper and neutron guide final factory acceptance tests were completed in early spring. The poured-in-place incident beam line shielding is complete, and we have successfully passed the 50% design milestone for the instrument enclosure.

The final design review for the sample goniostat was successfully completed in early February, and manufacturing has begun. This instrument will control 24 motor axes to enable specular and off-specular reflectivity measurements of liquid ($Q > 0.5$ Å^{-1}) and solid ($Q > 1$ Å^{-1}) surfaces. In addition, the detector arm will be able to swing out of the specular reflectivity plane to carry out grazing-incidence, small-angle scattering studies.

Magnetism Reflectometer

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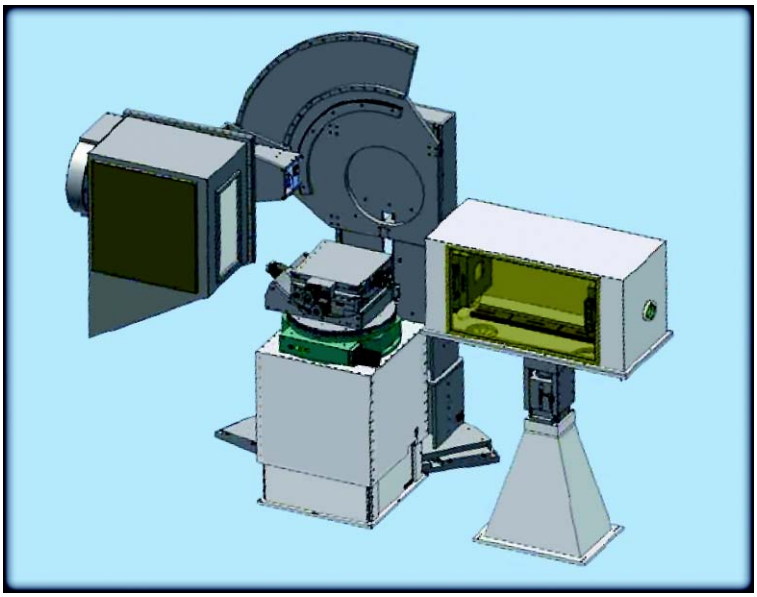
Installation of the magnetism reflectometer is progressing. All of the neutron guide support posts were erected early this year, followed by installation of the permanent "under the guide" concrete shielding sections and the concrete instrument floor. In March, the sample stage was delivered and connected to the data acquisition system for pretesting. The instrument enclosure concrete shielding installation has started and will be completed by mid-July. The main beam line shutter, including the most upstream guide sections, will be installed in September. Manufacturing of the neutron guide system is complete, and installation of technical components (guide, choppers, etc.) is planned throughout the remainder of 2005.



Liquids reflectometer goniostat.

Ultra-High Resolution Spin-Echo Spectrometer (USESpec)

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Neutron spin-echo (NSE) instruments offer the highest energy resolution of all neutron instruments and cover a broad range of applications in dynamics of soft condensed matter, polymer, and glassy materials, as well as disordered magnetic systems and transport phenomena. The most striking feature of NSE is the "energy" resolution given in terms of the Fourier time τ. The Fourier time is directly proportional to the magnetic field integral J. USESpec will be equipped with magnetic solenoids and correctors that enable a resolution exceeding the state of the art by a factor of ~5, thereby being able to cover the time range of 1 ps $< \tau <$ 1 ms. This is achieved by the use of large-bore stray field compensated superconducting coil sets with a magnetic field integral up to $J_{max} = 1.5$ Tm. In addition, high-precision correction elements in the neutron path are required to reach a field integral homogeneity of about $\Delta J < 10^{-6}$ Tm.

For the superconducting coils, the winding geometry has been fixed and technical design studies have been conducted in collaboration with possible manufacturers. A superconducting NbTi wire with minimum hysteresis effects has been identified and selected. Also, the correction elements ("Fresnel coils") for the most demanding task—correcting the divergent wide beam close to the area detector—have been developed. These correction coils have to be neutron transparent, carry radial current densities up to 150A/mm, be cooled with a resulting negligible effect of thermal expansion, and be equipped with a three-dimensional position control with an accuracy of a few microns (so called Hexapods™). During the last three months, a prototype was made that is able to correct the field integral of $J = 1$ Tm within the current limits set by the cooling. We expect that optimization of the bonding techniques and design will yield further improvements.

In addition, the full detailed specifications for the guide system, chopper, and superconducting coils, as well as for the Hexapods™, have been prepared. The radiation shielding has been assessed by DORT calculations and awaits approval. To summarize, in 2004 the research and development work was successfully completed up to a stage where detailed construction, commissioning, and manufacture can start.

Backscattering spectrometer large evacuated final flight path (right) and (below) first section of beam line 2 neutron guide (outside the bulk shield).

Backscattering Spectrometer

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The main focus of the backscattering spectrometer instrument team is installation. Several major components have been installed recently, including guide sections from the moderator through the shutter region and the primary shutter. Installation of the remaining guide sections began the last week of April, with completion expected in early July. Polyethylene shielding has been installed around the large, evacuated final flight path, with a protective steel cover installed over it. Analyzer crystal mounting/adjusting system and support panels are in fabrication, and some of the support columns are complete. Contracts for the major portion of the stackable concrete and steel incident beam line shielding have been awarded, and initial delivery of the steel components began in March. The remaining shielding components are scheduled to arrive by the end of June. In addition, planning is under way for initial commissioning measurements.

Macromolecular Neutron Diffractometer (MaNDi)

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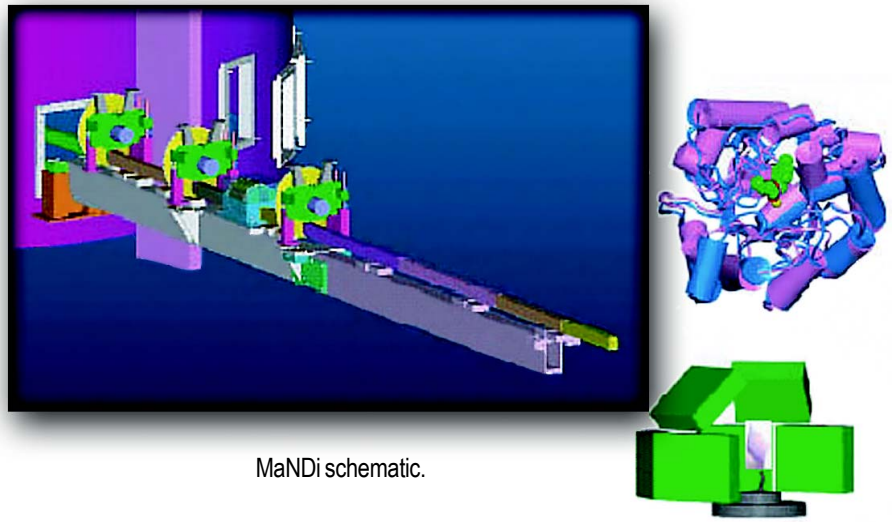
MaNDi is a single-crystal diffractometer proposed for determining high-resolution neutron structures of macromolecules. The conceptual design of MaNDi, agreed upon at an IDT workshop at the Intense Pulsed Neutron Source in October 2003, was optimized with financial support from Oak Ridge Associated Universities (ORAU), and a full scientific proposal was submitted in July 2004. An external peer-review panel was highly enthusiastic of both the instrument design and the new science that would result from MaNDi. The proposal received Experimental Facilities Advisory Committee approval for the instrument in October 2004, and MaNDi has been assigned beam line 11B at SNS. The next major step is to secure ~$14M in funding for construction and support facilities. Towards this goal, Reinhold Mann (ORNL) and Richard Swaja [National Institutes of Health (NIH)] organized a meeting with program managers from NIH, the National Science Foundation, and DOE. The meeting was held on February 15 at NIH, and the MaNDi team presented the state-of-the-art developments in macromolecular neutron crystallography and ultrahigh resolution X-ray crystallography, the predicted performance of MaNDi, and its potential impact on structural genomics and drug development research. The scientific case for MaNDi was well received, and the team was encouraged to proceed further. We are currently organizing a two-day conference for July 12-13, 2005, at SNS on "New Frontiers in Neutron Macromolecular Crystallography." We believe that this is an excellent opportunity for the scientific community to participate and learn more about the scientific need and impact of neutron macromolecular crystallography at SNS.



MaNDi schematic.

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

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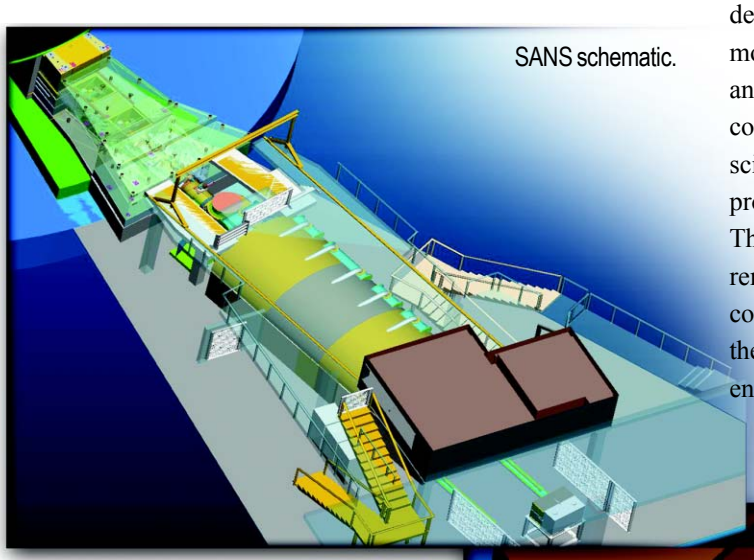
The EQ-SANS diffractometer is optimized towards extending SANS studies into multilength scales. The instrument is located on beam line 6, which faces the cold, coupled LH_2 moderator. The neutron optics use a true-curved beam bender to avoid the direct line-of-sight of the moderator, with the provision for a future T_0 chopper. The true-curved bender was chosen to better preserve the beam divergence. The three bandwidth limiting choppers, located at 5.7, 7.8, and 9.5 m from the moderator, will also allow for pulse-rejection operations. The sample stage is centered at 14 m from the source. The main, low-angle detector is movable from ~1 to ~8 m away from the sample within the scattering tank. In addition, a large-angle detector bank is located at 1 m around the sample. All detectors will be ^{3}He-tube based, which offers the benefits of a higher count rate, higher counting efficiency, and lower parallax than other detectors we have evaluated. The ^{3}He tubes will be arranged in easily serviceable modules. Beam-line shielding design has been optimized with the guidance of systematic neutronic calculations. Emphasis is given to reducing both the radiation dosage around the instrument and the background at the detector.

Major instrument design work has been completed, and the first section of the neutron guide has been installed in the core vessel insert. The steel shielding for the shutter bender insert has been delivered, and the bender itself is being manufactured by the vendor. All instrument procurements will be placed before spring 2006, and full instrument installation is expected to be later in 2006.

As a part of the concerted efforts to reach out to potential users, a "BioMaterials and Neutrons (BioMaN)" symposium is being organized as part of the 52nd American Vacuum Society Meeting this fall. For more information, see www.neutron-eu.net/bioman and www2.avs.org/call/2005/bi.html.



SANS schematic.

Powder Diffractometer (POWGEN3)

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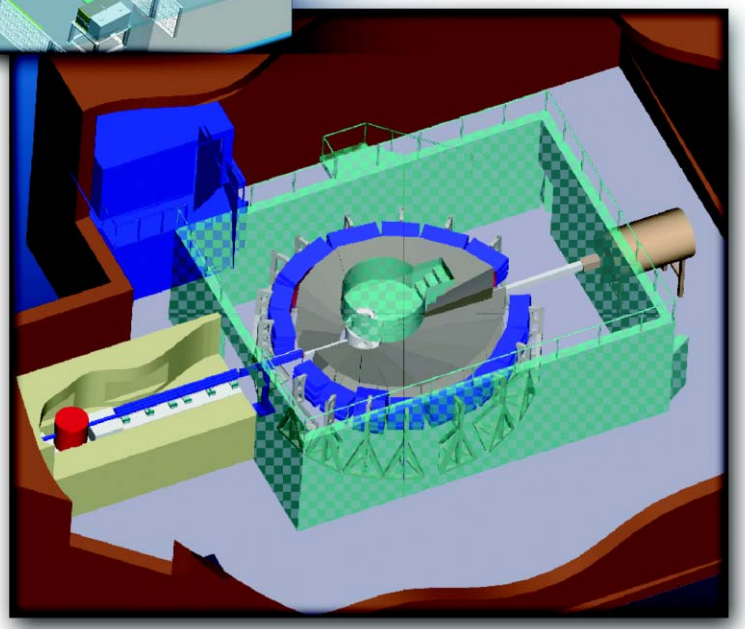
The 100% design and associated instrument safety reviews for POWGEN3 were completed in October 2004. Installation of the core vessel insert and poured-in-place concrete shielding has also been completed. The three sections comprising the wide shutter and double channel shutter insert will be installed in June 2005. In addition, the first 42 m of the supermirror neutron guide and associated steel shielding has been delivered. The integration of the supermirror guide with steel shielding to eliminate streaming paths along the sides of the glass guide was developed for POWGEN3. Mechanical design of the rectangular-shaped detector modules, for use on both the POWGEN3 and VULCAN instruments, has been completed. Work on developing a new scintillator screen for these modules is proceeding with encouraging results so far. The first two detector modules are currently under fabrication and will be completed in the summer. In March 2005, the POWGEN3 project welcomed a new engineer, Robert Whippel, to the team.



POWGEN3 schematic.

Center for Nanophase Materials Sciences Update

Linda Horton, hortonll@ornl.gov

CNMS, April 2005.

Conventional construction on CNMS, SNS's sister facility on Chestnut Ridge, was completed in April of this year. CNMS is one of the five DOE nanoscale science user facilities under construction at national laboratories across the country. The first of these facilities to be completed, CNMS will open for on-site users in October 2005. To date, the interim "jump start" user program, under way for the past two years using existing ORNL capabilities, has accepted more than 70 user proposals for research on macromolecular materials, functional nanomaterials, and nanomaterials theory, as well as for use of ORNL's interim Nanofabrication Research Laboratory and advanced tools for imaging and characterization.

The Inaugural User Meeting was held on May 23-25, 2005. This meeting showcased the new facility and research areas for CNMS. The focus of the meeting was on how to become a user at CNMS and included discussions of a new call for proposals beginning in Fall 2005. The meeting also included time for individual discussions with CNMS scientific leaders and tours of related ORNL facilities, including SNS and the microscopy facilities located in the new Advanced Microscopy Laboratory (which houses aberration-corrected electron microscopes from the High Temperature Materials Laboratory and the Basic Energy Sciences Microscopy Research Program).

Bio-Deuteration Laboratory

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The Center for Structural Molecular Biology and the Life Sciences Division at ORNL are establishing a Bio-Deuteration Laboratory for in vivo production of H/D-labeled bio-macromolecules to support the user research programs at HFIR and SNS. Neutron scattering provides a unique, nondestructive probe of delicate biological materials and higher-order assemblies, and the design and production of H/D-labeled material permits selected parts of macromolecular structures to be highlighted and analyzed in situ. The Bio-Deuteration Laboratory, which is supported through ORNL's Laboratory Directors Research and Development Program, will provide the user communities at HFIR and SNS with the support, expertise, and facilities required to produce specific, selective, and randomly H/D-labeled proteins and other macromolecules for neutron analysis. As a central training and user facility, we will train researchers, students, and staff from academia and industry in the use and application of these powerful techniques and, with ORAU support, have now launched a first-user access program for the facility. The development of the Bio-Deuteration Laboratory will leave ORNL, its scientists, and facility users uniquely equipped for neutron analysis of large macromolecular complexes and assemblies, ensuring broader community access and innovative use of Oak Ridge's world-leading, neutron-scattering facilities. For more information, contact Dean Myles (mylesda@ornl.gov, 865-576-5230).

Greetings from the JINS Director

Takeshi Egami, egami@utk.edu

For some time, JINS has been operating without a permanent home, but this is going to change very soon. Earlier than expected, Tennessee Governor Phil Bredesen sent a budget proposal to the state House and Senate that included a line item for $8M to build JINS next to the SNS CLO and CNMS. The Tennessee General Assembly recently approved this budget plan. Since the design and the construction plan for the JINS building is already finished, construction can begin as early as this fall. The JINS building will be two-stories high, with a medium-size lecture hall, several small meeting rooms, and offices for staff, visitors, and students. We will even have a coffee shop with a sumptuous menu! The JINS building will be a focal point for neutron research for visitors from all over the world. Isn't it great to have a governor with a physics degree from Harvard?

Neutron Scattering at High Magnetic Fields

To minimize problems from magnetic interference between instruments, SNS has been developing high-field magnets with active compensation to reduce stray fields. Several systems are being developed.

The extensive science case for a 30- to 40-T magnet instrument was detailed at the workshop on "Probing Matter at High Magnetic Fields with X-Rays and Neutrons," held in Tallahassee, Florida, in May of this year. To determine the need for dedicated high-magnetic field instruments at SNS and the Advanced Photon Source (APS) at Argonne National Laboratory, the science case examined areas such as high-temperature superconductors, heavy fermion materials, quantum magnets, magnetic nanoparticles and multilayers, novel metallurgical material processing, and chemistry. Both SNS and APS demonstrated that, in cooperation with the expertise of the National High Magnetic Field Laboratory, world-class instruments can be built that can meet the ever-growing challenges of the community. SNS contacts for this endeavor are Frank Klose (klosefr@sns.gov) and Garrett Granroth (granrothge@ornl.gov). For more information, see www.xraysandneutrons.magnet.fsu.edu.

At the bottom end of the scale, an actively shielded 10-Tesla magnet is under development in a collaboration between SNS and a local vendor. This vertical split coil will provide maximum performance for both polarized and unpolarized beams by operating in either symmetric or asymmetric mode. A design study is being funded through a small business innovation research proposal. SNS contacts are Lou Santodonato (santodonatol@sns.gov), Hal Lee (leewt@sns.gov), and Andre Parizzi (parizziad@sns.gov).

A 15-Tesla, self-shielded magnet system is also under development. The proposed magnet uses an actively shielded vertical split coil, with advantages similar to those for the 10-T magnet. Design and construction are being funded by a grant from the Swiss government, the Paul Scherrer Institute, and SNS. The SNS contact is Frank Klose (klosefr@sns.gov).

SNS and HFIR User Meeting October 12-13, 2005

Mark your calendars for the first on-site meeting for SNS and HFIR users, to be held at the ORNL Research Support Center. This meeting will provide an ideal opportunity for experienced and new users to interact directly with facility staff; learn about the capabilities and status of instrumentation; and provide feedback on the science, instrumentation, sample environment equipment, and user processes. We will be providing information on

- instrument capabilities;
- time lines for instrument readiness and power rampup at SNS;
- the proposal system;
- collaboration among the two facilities, the Center for Nanophase Materials Sciences, and groups focusing on theory and modeling;
- and who to contact for more information.

We will also be soliciting feedback about policies and procedures, including access, training, data management, sample management, and the proposal system. In particular, we will be looking for input on specialized sample environments, which are not included in the facility inventory and could require collaboration between several user teams to be funded and developed. Plenty of opportunities will be available for participants to discuss ideas for initial experiments and to propose directions for future development.

Tours of HFIR and SNS are planned, along with opportunities for individual discussions with instrument scientists and staff. JINS is expected to propose a short course related to neutron scattering, which would follow the user meeting. More information will be available soon at www.sns.gov.

Upcoming SNS/HFIR Events for 2005

- *VULCAN Instrument Development Team Meeting, Oak Ridge, Tennessee, July 11-12*
- *Macromolecular Biology Workshop, Oak Ridge, Tennessee, July 12-13*
- *SNAP Instrument Development Team Meeting, Oak Ridge, Tennessee, July 18-19*
- *Probing Complex Fluid Membranes and Films with Neutron Spin-Echo, Bloomington, Indiana, August 14-17*
- *SNS and HFIR User Meeting, Oak Ridge, Tennessee, October 12-13*
- *BioMaN–BioMaterials and Neutrons, Boston, Massachusetts, October 30-November 4*

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Westward view of the SNS site, April 2005. The CNMS is the curved building in the foreground that extends to the right of the SNS CLO. For more photos, see the SNS Photo Gallery at web.ornl.gov/sci/iris/search_sns.shtml.

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