

The
NEUTRON PULSE

Volume 7
Number 1
Spring 2006

SNS on Schedule for June 2006 Completion

The Spallation Neutron Source (SNS) continues to be within budget and on schedule. In the past eight months, the project has passed three highly significant milestones on its way to an official completion date of June 2006.

August 16, 2005, marked the successful transport of a 865.6-MeV H- beam through the superconducting linear accelerator. The energy has since been increased to 910 MeV, and 880-ms-long pulses have been accelerated with intensities up to 8×10^{13} ions per pulse, about one-half of the design parameter for full-power operation.

In October another major milestone was achieved with the installation of the inner reflector plug (IRP) in the target monolith. The IRP contains the target moderators, and completion of this critical piece of equipment was an extremely complex engineering challenge that was successfully met thanks to the hard work and expert skills of the target design and installation teams.

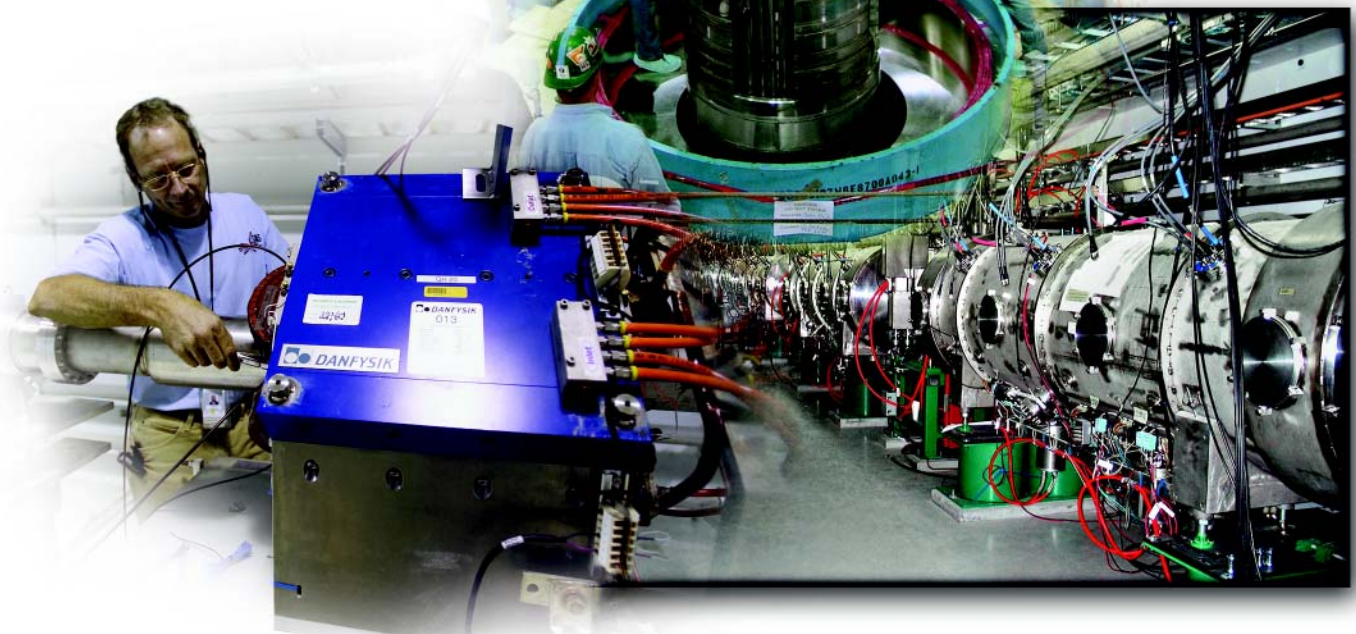
In January 2006, another major milestone was achieved with the successful commissioning of the proton accumulator ring. After only three days of initial operation, the ring accumulated protons, which were then extracted and sent to a point just short of the target. In the words of Accelerator Systems Division Director Norbert Holtkamp, "With this extraordinary success, we are definitely on our way to operating the world's highest intensity proton accelerator."

In addition, target system tests have been completed, and preparations are under way to deliver the first beam on target in early May. ✨

In this Issue

Director's Comments	2
Open Session of SHUG	2
SNS-HFIR User Meeting	3
First Shull Fellowships Announced	5
User Meeting Technique Sessions	6
User Meeting Instrument Sessions	8
User Meeting Workshops	11

From left to right: fine tuning of magnets in the proton accumulator ring, installation of the inner reflector plug into the target monolith, and a view of the completed superconducting linear accelerator



Director's Comments

Thom Mason

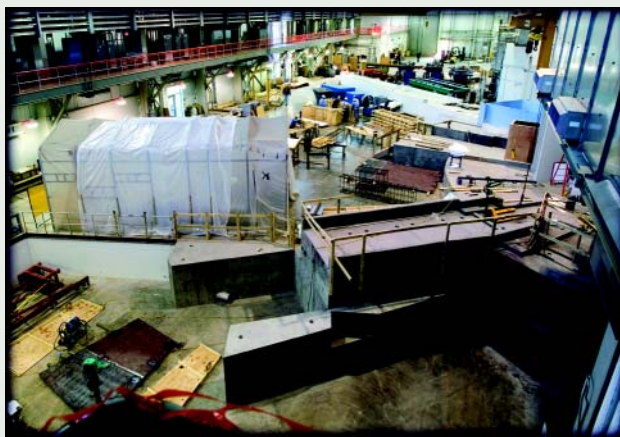
Associate Lab Director for SNS
masont@sns.gov

After seven and one-half years since the formal start of the SNS project, and more than six years of construction, it's difficult to believe that we're in the final few months of completion. The tremendous accomplishments of the dedicated people working on this project are impossible to miss when looking around the site and within its buildings. The SNS site is a very exciting place to be right now!

Last fall, SNS became the world's highest power proton accelerator with the successful commissioning of the superconducting linac. With successful ring commissioning earlier this year, only one major milestone remains: delivery of beam on target. This final commissioning step is expected in early May and will include delivery of neutrons to three instruments.

Formal project completion is expected before the end of June 2006. After that we'll begin the 2- to 3-year rampup to the designed power level, high reliability, and desired predictability of operations for users.

An important element in all of our efforts has been the emphasis on safety. We have now worked well over 7 million hours, with



Most of the SNS construction activity is now in the Target Building, which is filling up fast with instruments. Here you can see the east side of the target monolith and construction on beam lines 11 through 18.

only two lost-workday cases. Although we consider this an achievement, we are still

working hard to maintain our safety focus as we achieve startup and then proceed into operations.

Those attending the October SNS-High Flux Isotope Reactor (HFIR) User Meeting were able to see the progress for themselves by touring the SNS site and through photos in some of the talks. This meeting was the first on-site SNS-

HFIR User Meeting and attracted about 240 attendees from 28 states and more than 50 institutions. Roughly 60% of the attendees were new to SNS and HFIR. To enable new users to attend, Oak Ridge Associated Universities and the Joint Institute for Neutron Sciences sponsored scholarships for about 50 students and faculty. Attendees participated in six technique sessions and seven instrument team meetings and presented 55 science posters. More than 140 people attended three workshops for new users on nanoscience, reflectometry, and small-angle neutron scattering (SANS).

Open Session of SHUG at User Meeting

Angus Wilkinson, Past SHUG Chair
angus.wilkinson@chemistry.gatech.edu

During the October 2005 SNS-HFIR Users Meeting, the SNS-HFIR Users Group (SHUG) held a well-attended open session. After a brief introduction to the purpose of SHUG and to its current Executive Committee members, the discussion leader engaged the audience on a variety of topics. The session went extremely well and continued until lunch intervened!

The first agenda item was a call for volunteers willing to run in the upcoming SHUG Executive Committee elections and for SHUG representatives willing to serve on the recently formed Synchrotron and Neutron Users Group (SNUG) Committee. SNUG is an advocacy organization focused on advertising the importance of U.S. Department of Energy (DOE) Office of Basic Energy Sciences (BES) major user facilities to policy makers.

Additional discussion topics included improving communications between SHUG members and its Executive Committee,

possible program topics for the next users meeting, reaching potential new users of SNS and HFIR, and the cost and nature of on-site housing for SNS. There was a consensus that e-mail is the best method of keeping in touch, and it was suggested that SHUG keep a searchable archive of e-mail messages sent by the Executive Committee. Many suggestions were made on ways to reach out to new users, and SNS and HFIR representatives made it clear that there are funds available to support some activities in this area. ✨

SNS-HFIR User Meeting Features Lively Discussions

The first on-site, combined user meeting of the SNS and HFIR user communities was held at the Oak Ridge National Laboratory (ORNL) Research Support Center on October 11-13, 2005. The organizers had three goals for this meeting. First, we wanted to increase interest and awareness of the important scientific and engineering research challenges that can be tackled successfully by neutron scattering in general and with the instruments at SNS and HFIR in particular. Second, we wanted to receive feedback on user policies and issues. Finally, through targeted workshops, we wanted to acquaint new users with some of the major techniques available at the two facilities. Many of the talks are available at the workshop web site: www.sns.gov/workshops/sns_hfir_users.

Technique sessions on the exciting new science being performed, along with a look forward to the new HFIR and SNS instruments, featured invited speakers on the following topics: diffraction, engineering materials behavior, inelastic and quasi-elastic neutron scattering, reflectivity, and SANS. These sessions were followed by meetings of seven SNS instrument teams, during which questions were answered on status and capabilities and initial experiments were proposed. Tours of HFIR, SNS, and the Center for Nanophase Materials Sciences (CNMS) were also provided.

Information was also provided on the sample environments proposed for these facilities, including staff support. Philosophies of general user policies, sample management, and the proposal system were

discussed, and helpful feedback was received. A SHUG meeting was held, during which the goals and function of the group were explained. Lively discussions followed on the nature of overall policies that should benefit the user, including inexpensive, convenient housing.

The last day of the meeting featured an impressive combination of workshops devoted to the new user. Nanoscience, reflectometry, and SANS were the focus.

Summaries of all the meeting sessions follow in this issue.

SNS and HFIR: A Look Ahead

In his welcoming remarks, ORNL Deputy Director Jim Roberto described ORNL's intent to become the world's foremost center for neutron scattering. In addition to CNMS, SNS, and the upgraded HFIR, Roberto identified the Joint Institute for Neutron Sciences and a guest housing facility as other future facilities that would interest users. DOE's Pedro Montano described BES's role as one of the nation's largest sponsors of basic research, including its world-class scientific user facilities. SNS

Director Thom Mason identified recent project progress and outlined the goal for both SNS and HFIR to operate seamlessly from the user point of view. He also presented a time line of SNS early operations, which will ramp up to scientific productivity within several years.

The directors of the HFIR, CNMS, and SNS experimental facilities provided their views of the path ahead for the user community. Steve Nagler, director of HFIR's Center for Neutron Scattering, described 2006 as a key year for HFIR because the reactor will soon have new and upgraded instruments, a cold source brightness comparable to the world's best, and improved thermal neutron intensity. In addition, new policies are being implemented to significantly improve HFIR's availability. CNMS Director Linda Horton described the center's scientific themes and its integration of nanoscale science with complementary research needs. The center has been accepting research proposals for the last two years through its Jump Start Program. Horton said she anticipates the acceptance of some 100 proposals for FY 2006—the first year of operations in the new facility, adjacent to SNS. CNMS is a research partner with SNS and HFIR, Horton explained, as she described the



SNS-HFIR User Meeting participants.



From top: user meeting participants Yinan Sun (University of Tennessee), John Budai (ORNL), Harold Smith (Oak Ridge), Eliot Specht (ORNL), Rosa Barabash (ORNL), Steve Nagler (ORNL), and Young Lee (MIT).

integration of the user communities. The director of SNS Experimental Facilities, Ian Anderson, provided additional details on the 17 approved SNS instruments and the time line of their commissioning. He described a philosophy of operations that combines the goals of excellence in science, reliable operations, and continual development. Users can expect a combined facility proposal system, full support for experiments and data treatment and analysis software, and a friendly welcome, Anderson added.

In her plenary lecture, Shenda Baker (Harvey Mudd College) described her vision of collaboration among facilities and people and sharing of data. For this cooperation to work, it takes, at a minimum, access, availability, proximity, user support staff, technicians, data management, modern equipment, and feedback mechanisms. The driver for all of this cooperation is science. A significant opportunity for developing collaboration lies with data visualization; this includes visualization between theory and experiment, between raw data and the physical world, and between science and society and public perception.

Preparing for Users

Lou Santodonato of the SNS Sample Environment group noted that the needs of the user community have been expressed during several workshops and instrument team meetings. There is always a strong call for excellent sample environment support, Santodonato said. SNS is responding to this challenge, starting with the formation of a dedicated sample environment team that will grow from its current level of 3 people to 12 in 2008. The members of this team, and their colleagues among the instrument scientists and scientific associates, will ensure reliable

operation of the versatile equipment inventory that is rapidly arriving at SNS.

Greg Smith of HFIR's Center for Neutron Scattering described a developing web-based proposal submission system that will integrate HFIR, CNMS, and SNS. A presentation was also given summarizing modes of facility access, including general and partner user and proprietary use. Also covered were the required steps for users after submission of a scientific proposal and arrival on-site.

Ken Herwig of SNS Experimental Facilities summarized the requirements for the sample management program at SNS and the desire to track all samples and sample equipment through release or shipment. A centralized tracking system will monitor the status of all samples that enter SNS. Users will be required to describe their plans for sample disposition as part of the experiment approval process. With appropriate training, users are expected to be able to carry out the majority of sample changes at SNS.

Initial SNS Users

During the commissioning phase of SNS instruments, there will be opportunities for "initial users" to test the instruments with a first round of experiments. The first three completed SNS instruments (Backscattering Spectrometer, Magnetism Reflectometer, and Liquids Reflectometer) will enter this phase during the late summer to early fall of 2006. At this time, the accelerator, target, and target moderators will be operated at relatively low power levels. During 2007, power levels should consistently increase, providing opportunities for more demanding science applications. The first call for the formal user program will be in the second half of 2007, with experiments scheduled for early 2008.



From left: user meeting participants Michael Hu (ORNL) and Ping Wang (Vanderbilt University).

increasing, and extensive installation and construction activities will be ongoing.

How will proposals by initial users be selected?

Input will be provided by the appropriate instrument team on the feasibility of the experiment. The SNS Experiment Safety Committee will conduct a safety review.

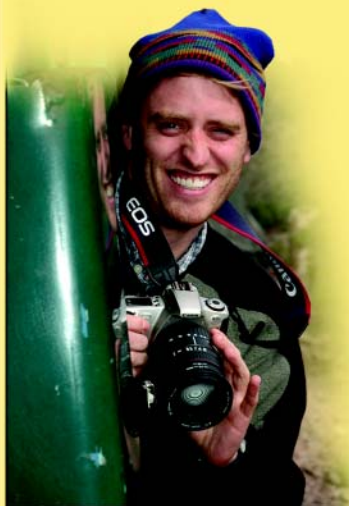
What will be the situation at SNS for initial users? Production of neutrons will be ramping up, as will beam time availability. Sample environment equipment will be

Proposals will be peer-reviewed by external panels, with recommendations based on scientific and technological impact and the experience of the experiment team. Panel members will be selected from the instrument advisory teams. Final approval of experiments will be made by the SNS Experimental Facilities director.

What is expected of initial users? Users will be expected to conduct experiments, produce good science, and keep smiling when things go wrong—an inevitability at startup of a complex facility. They will also be expected to use our proposal system and to assist in debugging all user activities, including the proposal system, site access, sample management, and training. They might also assist in instrument commissioning and development of initial data analysis tools. ✨

First Shull Fellowships Announced

The first ORNL Clifford G. Shull Fellowships were recently awarded. Sponsored by HFIR and SNS, appointments were presented to Andrew Christianson and Wei-Ren Chen. Both gentlemen will be joining ORNL in May of this year.



Andrew Christianson

Andrew Christianson received his Ph.D. in 2003 from Colorado State University, where he majored in physics. He also earned his M.S. from Colorado State University and his B.S. from the University of Northern Iowa. He is currently completing postdoctoral work with Professor Jon Lawrence at the University of California at Irvine and as a guest scientist at Los Alamos National Laboratory (LANL). Christianson will be assigned to HFIR.

Wei-Ren Chen received his Ph.D. in 2004 from the Massachusetts Institute of Technology (MIT), where he majored in nuclear science and engineering. He completed his M.S. at the National Taiwan University and his B.S. from the National Tsing Hua University. He is currently completing postdoctoral work with Professor Lee Magid at the University of Tennessee and is assigned to the Center for Neutron Research located at the National Institute of Standards and Technology (NIST). Chen will be assigned to SNS.



Wei-Ren Chen

ORNL established the Shull Fellowship to recognize Shull's pioneering work in neutron scattering. Corecipient of the 1994 Nobel Prize in Physics, Shull began his work in 1946 at what is now ORNL. The goal of this fellowship is to attract new scientific talent to ORNL for the development of its neutron science program. The selection committee looked for candidates with exceptional ability who were capable of developing innovative research programs and who showed the promise of outstanding leadership.

From top: user meeting participants Mohana Yethiraj (ORNL) and Jerel Zarestky (ORNL).



SNS-HFIR User Meeting Technique Sessions

Diffraction Methods

Angus Wilkinson

angus.wilkinson@chemistry.gatech.edu

This session covered both applications and the development of new data analysis strategies. Hanno zur Loye (University of South Carolina) discussed crystal growth and structural studies for $(\text{Ln}_2\text{Na})\text{NaPtO}_6$ ($\text{Ln} = \text{La}, \text{Nd}$), $(\text{Ln}_{2.5}\text{Na}_{0.5})\text{NaRhO}_6$ ($\text{Ln} = \text{La}, \text{Pr}, \text{Nd}$), LnNaIrO_4 ($\text{Ln} = \text{Gd} - \text{Er}, \text{Y}$), and $\text{Ln}_{14}\text{Na}_3\text{Ru}_6\text{O}_{36}$ ($\text{Ln} = \text{Pr}, \text{Nd}$). These materials were prepared using molten hydroxide fluxes, and all have sodium cations in trigonal prismatic environments, which is uncommon for oxide materials. Sossina Haile (California Institute of Technology) presented some of her work on proton-conducting inorganic electrolytes. Materials of this type are alternatives to polymeric proton conductors. Their proton transport mechanisms are related to both local and global structural features associated with hydrogen bond formation, making them good candidates for study

using neutrons. Experiments on $\text{Cs}_2\text{Na}(\text{HSO}_4)_3$, $\text{Cs}_3\text{Li}(\text{DSO}_4)_4$, and $\beta\text{-Cs}_3(\text{HSO}_4)_2[\text{H}_{2-x}(\text{P}_{1-x}\text{S}_x)\text{O}_4]$ help explain the absence of a so-called superprotonic transition in the first compound, provide an important correction for the reported structure and stoichiometry of the second compound, and enable an accurate assessment of the configurational entropy in the third compound. Such insights guide the search for optimal proton conductors.

John Evans (University of Durham) illustrated some areas that the SNS Powder Diffractometer (POWGEN3) will further open up when it becomes operational in 2007. He described the technique of “surface Rietveld refinement,” in which an ensemble of diffraction patterns (e.g., 50 or more individual profiles collected as a function of temperature) is fitted to a single evolving structural model. This allows the extraction of “noncrystallographic” information. For example, by using internal standards, the true sample temperature can be determined along with the crystallographic parameters. The method can also be used to obtain “good information” from statistically “bad data.” In the second half of his talk, he looked at several apparently simple stoichiometric metal oxides with remarkably complex structures, including ZrP_2O_7 (136 unique atoms) and $\text{Mo}_2\text{P}_4\text{O}_{15}$ (441 unique atoms). The development of new instruments at SNS will lead to the characterization of more materials with great complexity.

Engineering Materials Behavior

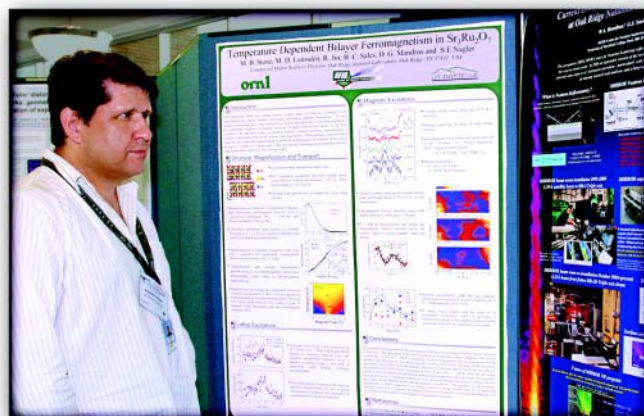
Camden Hubbard
Hubbardcr@ornl.gov

This session included a presentation on the status of NRSF2, the second-genera-

tion neutron residual stress mapping facility at HFIR, and the construction status of VULCAN, the engineering instrument at SNS. NRSF2 commissioning is well along, and initial results are indicative of its impressive capabilities. (Results from eight research studies using NRSF2 were illustrated via posters later in the day.) The highlights and status of VULCAN’s design and construction promise significant future contributions from this instrument to studies of materials behavior when it comes online in summer 2008.

Hahn Choo (University of Tennessee) presented “In Situ Neutron Diffraction Studies of Mesoscopic Deformation Behavior of Structural Alloys,” which highlighted the rich and unique understanding of materials deformation that can be obtained using neutron and in situ load frames with furnaces. Suresh Babu (Edison Welding Institute) summarized prior studies of materials following and during thermomechanical processing via neutron scattering. He ended his presentation with a vision of future studies that the new facilities at ORNL should enable.

Les Butler (Louisiana State University) closed the session by addressing the opportunities and unique data that can be obtained if a world-class tomography and radiography facility were to be developed at SNS. The changes in image contrast as a function of neutron energy caused by the Bragg edges of crystalline phases was



Edward Kintzel (ORNL) at a user meeting poster session.

shown to be a valuable tool for imaging with neutrons at pulsed sources.

Inelastic Neutron Scattering

Steve Shapiro, Shapiro@bnl.gov

This session included three talks focused on the science obtained with inelastic neutron scattering and one talk on the instrumentation available at HFIR and soon to be available at SNS. Garrett Ganroth (ORNL) discussed inelastic capabilities at HFIR and SNS, reviewing the triple-axis instruments at HFIR and the time-of-flight instruments being built at SNS.

The science talks included one by Young Lee (MIT), who spoke on “Magnetism in Frustrated Systems.” He used the triple-axis instruments at HFIR and NIST to study a novel system and stressed the importance of having high-quality single crystals. Andrew Christianson (University of California at Irvine, and ORNL Shull Fellow) described recent experiments on heavy fermions in his talk “Magnetic Excitations in YbAl_3 .” He and his colleagues observed two excitations believed to be gap excitations. He compared results taken on the MAPS spectrometer at ISIS and triple-axis work measured at HFIR. The presentations concluded with remarks by Dimitry Sokolov (University of Michigan), who described his inelastic neutron studies in a talk entitled “Quantum Criticality in Itinerant Antiferromagnet Cr(V) .”

Quasi-Elastic Neutron Scattering

Despina Louca, louca@virginia.edu

The quasi-elastic neutron scattering (QENS) session covered a wide range of science, from the physics of well-defined problems involving the fragile to strong transitions in supercooled water, to vibrational motions of water in zeolite cages, to the more contemporary biological

From left: user meeting participants Aravinda Raghavan (ORNL), Sow-Hsin Chen (MIT), and Pappannan Thiyagarajan (ANL).



issues involving dynamics in phospholipids. These areas reflect the increasingly broad application of quasi-elastic scattering to dynamical problems in materials science, biology, and polymers.

Technically, the QENS method is becoming very advanced; invited speakers for this session showed high-quality data from both spallation and reactor sources. Speakers showed how it is possible to use a backscattering technique to probe more than one length scale at a time. They also demonstrated how, when combined with high resolution, different time scales of motion for one kind of ion can be resolved easily. The scientific community is well aware of the capabilities of QENS, and one can only imagine the vastness of information that will be obtained at SNS.

Reflectivity

Paul Butler, butler@nist.gov

Chuck Majkrzak (NIST) started off the session by introducing the basics of reflectivity and providing an overview of how the neutron’s magnetic moment can be used to advantage to study the detailed magnetic structure in thin films, such as those used in the recording industry. He gave examples of recent work on the noncollinear spiral structures that form between hard and soft magnetism. Tonya Kuhl (University of California at Davis) then discussed some exciting recent work she has been doing with

polymer brushes under confinement. She showed that as two adsorbed polymer brushes are brought into contact, the typical parabolic profile of polymer density gets replaced with an increased density at the walls, as well as in the very middle where the brushes meet. She also shared some promising work on attempting to shear these thin film systems.

Michael Kent (Sandia National Laboratories) discussed how reflectivity, coupled with grazing incidence techniques, can be used to understand how proteins and peptides bind to a lipid layer and how they affect the structure of the layer to which they bind. He showed an interesting example of how the existence of multiple binding sites can cause a protein to unfold using reflectometry. Finally, Mathias Lösche (Carnegie Mellon University and NIST) discussed current issues with substrate-supported biomembranes. Using the unique neutron tool of magnetic contrast variation to investigate minute structural details without risk of slight morphic variations caused by isotopic effects, he showed how the system can be tuned by studying the effects of grafting density, electric fields, solvent backfilling, etc.

The session was concluded by John Ankner (ORNL), who spoke for all three reflectometers at ORNL: his own Liquids Reflectometer at SNS; Frank Klose's Magnetism Reflectometer, also at SNS; and Bill Hamilton's HB-2D Reflectometer at HFIR. Both Hamilton's and Klose's reflectometers have a vertical sample geometry, while Ankner's is a horizontal geometry appropriate for liquid/gas interfaces. Ankner pointed out that while the Magnetism Reflectometer would be particularly suited to magnetism studies, it would also be useful for almost any other problem that does not have a solution gas interface. All three instruments will be world-class. Hamilton's reflectometer is running in a temporary location at HFIR and will be moved in late 2006 to the new guide hall. Ankner's and Klose's instruments will be two of the first three instruments coming online at SNS in fall 2006. With these instruments so close to being commissioned, this session was particularly timely. Users were able to get a feel for how their research would benefit from the reflectometry technique and learned when they might expect to start using the instruments themselves.

Small-Angle Neutron Scattering

Megan Ruegg, mruegg@berkeley.edu

This session included talks on SANS experiments in biology and polymer science, as well as a discussion of the new SNS and HFIR instruments. The first presentation was by Joe Zaccai (Institut Laue-Langevin), who discussed the importance of SANS experiments in understanding biological systems. In particular, he detailed the powerful technique of using the contrast between hydrogen and deuterium to decouple different aspects of a complex sample's structure. By changing the level of deuteration in the solvent, different

components of the sample will be probed, and it is possible to characterize a complex structure, such as in a virus. The next speaker was George Wignall (ORNL), who spoke about SANS on polymer systems. He discussed a variety of applications: understanding the morphology of blends of CO₂ and CO₂-phobic materials solubilized by poly(styrene-block-fluoro-octyl acrylate), characterizing the Flory-Huggins interaction parameter in polymer blends, determining the void fraction in carbon-filled polyethylene, and analyzing the shear alignment of cylindrical block copolymer phases.

The final two speakers were Jinkui Zhao (ORNL) and Gary Lynn (ORNL), who discussed future possibilities for SANS at SNS and HFIR. The new instruments at these facilities will have complementary capabilities. SNS will have an extended Q-range SANS instrument in which the Q-range will be 0.004 to 10 Å⁻¹. HFIR will have two new cold source SANS instruments with a Q-range of < 0.001 to 1 Å⁻¹ (with lenses, Q < 0.0005 Å⁻¹ could be achieved). Both speakers detailed various aspects of beam line design, such as shielding, detector design, improved resolution and intensity, sample environment, data acquisition, and other support areas such as wet labs, sample preparation, and computational tools. ✨

ARCS Fermi choppers and translation table under testing at the chopper manufacturer.

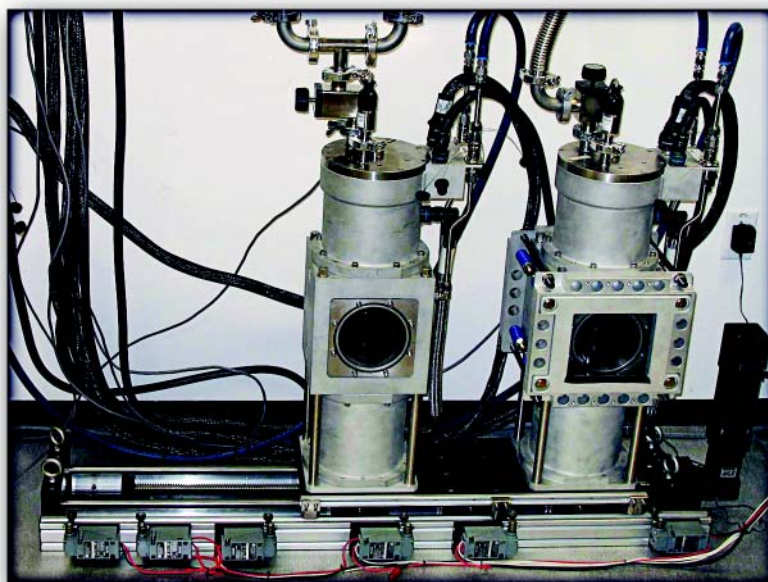
User Meeting Instrument Sessions

Angular-Range Chopper Spectrometer

**Doug Abernathy, abernathydl@sns.gov
Brent Fultz, btfc@caltech.edu**

This meeting began with an update on the hardware construction of the Angular-Range Chopper Spectrometer (ARCS). Considerable progress has been made in installation and procurement for this instrument. The T₀ chopper is still in a preliminary design stage, and a new concept for the vertical axis design using a quill shaft was shown. The sample area radiation shielding is also under active consideration, and the hardware project appears to be on time and within budget.

An update on software efforts was also presented. An alpha release of the software development has been made for limited evaluation and discussion. The project has concentrated less on user interfaces and more on the structure and module development to provide the software framework needed. The neutron instrument package



has been incorporated into the framework, allowing for a flexible environment for connecting Monte Carlo simulations to experimental work. Calculations using the current framework show that the momentum transfer information available with ARCS may be a powerful addition to the study of powder samples.

Although specific initial experiments were not discussed, there was a lively discussion on work with three-dimensional single crystals on chopper spectrometers, a topic that holds much promise but requires much development.

Backscattering Spectrometer

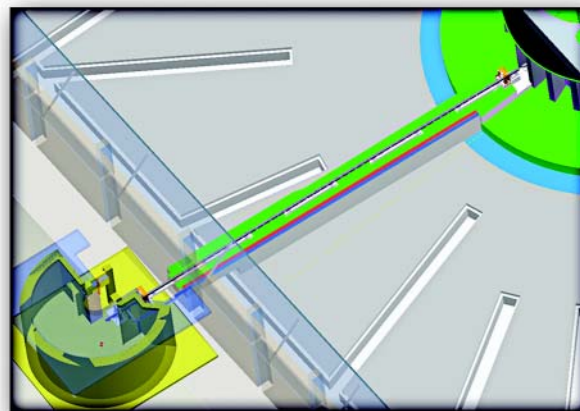
Ken Herwig, herwigkw@sns.gov

The team meeting for the SNS Backscattering Spectrometer was well attended, with participants from several universities and national laboratories. The original instrument advisory team was also well represented.

The session began with a description of the capabilities of the spectrometer and an update of its status. There was considerable discussion of three possible upgrade possibilities: (1) complete the full complement of Si (111) analyzers, doubling the count rate of the baseline instrument; (2) extend the Q-range of the instrument at lower energy resolution by adding the planned complement of Si (311) analyzers; and (3) implement a mica analyzer bank that would give a lower Q-range than the baseline instrument but that would improve the energy resolution by an order of magnitude. Attendees were supportive of all these proposals but were most enthusiastic of the last.

The session continued with a discussion of initial experiments and of available and desired sample environment equipment. A description of the planned power levels

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



and instrument capabilities was presented, along with the plan for scientific peer review for initial experiments during the 2007 time frame, before start of the formal user program. Several members of the group volunteered to participate in the science peer review of these initial experiments. There was strong support for low-temperature capabilities (<3 K), modest gas pressure cells capable of low-temperature operation, and—for routine operation—a top-loading, closed-cycle refrigerator system with a high-temperature option.

Cold Neutron Chopper Spectrometer

Georg Ehlers, ehlersg@sns.gov

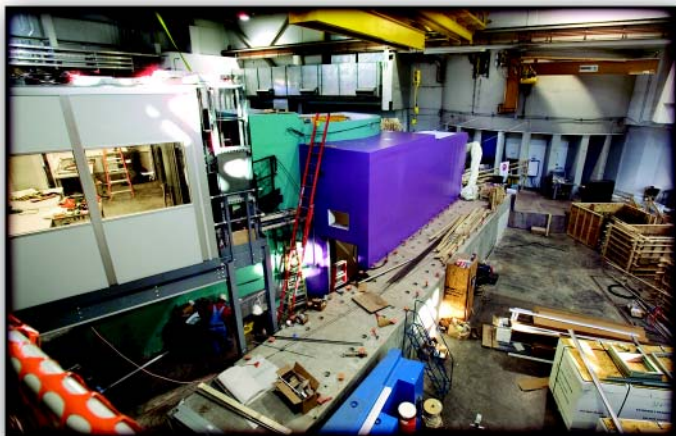
The Cold Neutron Chopper Spectrometer (CNCS) session included a presentation on current project status and schedule, as well as the scientific capabilities of the instrument. The discussion centered on the design details of the satellite building, operation of the instrument by users, and initial experiments during the rampup to full SNS design levels. Questions about support of visiting researchers were discussed, and the goals of data analysis software efforts were described. Ideas about sample environment equipment were discussed, and these discussions are expected to continue.

CNCS is a direct-geometry, inelastic neutron spectrometer that will be multipurpose, flexible, and versatile. Two high-speed choppers will deliver a short-pulsed monochromatic beam at the sample position. A detector coverage of (initially) 1.7-sr solid angle will ensure 1 to 2 orders of magnitude higher count rates, depending on incident neutron energy, than existing spectrometers of this class operating in other facilities. Potential applications of this instrument will be found in many different areas, such as condensed matter physics, materials science, chemistry, biology, and environmental sciences. The available ranges of energy resolution and momentum transfer for CNCS are complementary to the SNS backscattering spectrometer and ARCS instruments.

Liquids Reflectometer

John Ankner, anknerjf@sns.gov

This meeting included a presentation on the current design and status of construction and an open forum for questions. The instrument team in particular solicited and received input on outfitting the wet lab and on designing the Langmuir troughs. The framework was laid for consideration of early experiments during power rampup. Great interest was shown in data analysis software for this instrument in particular



SNS instrument construction. The green and purple structures in the center are part of beam lines 4a (Magnetism Reflectometer) and 4b (Liquids Reflectometer), respectively. The gray beam line in the forefront is beam line 5 (Cold Neutron Chopper Spectrometer).

combination of the high-power SNS neutron source and the use of advanced neutron optics will also allow off-specular diffraction studies of in-plane structures.

Powder Diffractometer

Jason Hodges, hodgesj@sns.gov

This meeting included a presentation outlining the instrument's capabilities, current status of construction, and detector fabrication. This presentation was followed by a discussion of SNS special sample environment projects. These included the closed-cycle refrigeration sample changer equipment and the 15-T self-shielded magnet and specifications for a high-temperature furnace. Discussion continued on the types of parametric neutron diffraction experiments that the instrument will be best suited for once it begins operation in 2007.

Extended Q-Range Small-Angle Diffractometer

Jinkui Zhao, zhaoj@sns.gov

This meeting included an update on the current status of the Extended Q-Range Small-Angle Diffractometer (EQ-SANS)

and for SNS in general. The need for cells for studying solid-liquid interfaces and for applying shear forces was discussed, and the determination was made to use cells similar to those used at HFIR.

The liquids reflectometer is designed to study the reflectivity of horizontal surfaces. This instrument will be useful for a wide range of science, including interfacial studies in polymers and surface chemistry involving thin layers of surfactants or other materials on the surfaces of liquids. Data rates and the 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 will include, for example, investigations of chemical kinetics, solid-state reactions, phase transitions, and chemical reactions.

Discussions identified some of the great science opportunities that will be available with the advanced sample environments planned for SNS, such as superconducting magnets up to and including 16 T in field strength. Ramping up to the planned intensities of SNS will provide time for detailed integration of all instrument components. These include the capability to change the beam intensity/instrument resolution ratio over a wide range. The goal is to have an instrument that will respond transparently to the scientific needs of users.

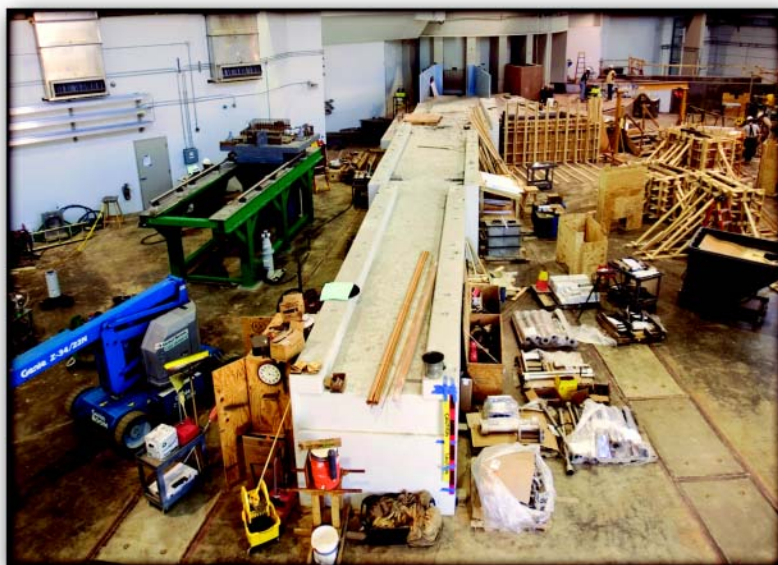
This instrument is designed mainly for polarized neutron reflectometry and high-angle diffraction studies of magnetic thin films, superlattices, and surfaces. The

Magnetism Reflectometer

Frank Klose, klosefr@sns.gov

The magnetism reflectometer session included a talk on the final design of the instrument components (guide, polarized neutron equipment, sample environment, shielding, user facilities, etc.) and the status of ongoing construction activities. Final guide and chopper installation occurred in late 2005 and early 2006, and shielding fabrication is under way for completion in April 2006.

Powder Diffractometer (POWGEN3) beam guide under construction.



instrument and its plan for completion. A range of topics were discussed, including better sample environments, beam collimation, transmission monitors, initial experiments, and software analysis tools.

Constructive comments were received on prioritizing future investments. The unique feature of this instrument will be its high wavelength resolution ($\Delta\lambda/\lambda = 0.5\text{-}1\%$) at the high flux level of SNS. This will enable new classes of experiments that require both higher wavelength resolutions and higher neutron fluxes, such as the study of membrane fusion with low-angle diffraction.

The construction of the EQ-SANS instrument is progressing according to schedule. The 2-m-long neutron bender section in the shutter has been installed and aligned. The first batch of the 8-mm ^3He tube detectors has been successfully tested to 5-mm longitudinal resolution. The remaining detector tubes are expected to arrive soon. One double-disk and two single disk bandwidth choppers have yet to be procured. The remaining major procurements, which include the scattering tank, mechanical support system for beam optics, secondary shutter (carousel), and shielding blocks, are on schedule. ✨

User Meeting Workshops

Nanoscience

Linda Horton, hortonll@ornl.gov

Nanoscience and technology was a hot topic at the user meeting. The information exchange began with an overview of CNMS, included a tour of the new facility, and culminated with a half-day user workshop on the last day of the meeting. Users expressed tremendous interest in CNMS, driven by the scientific overlap with SNS and HFIR. The CNMS User Program emphasizes synthesis; complementary characterization tools; and theory,

From left: user meeting participants Fei Tang (ORNL) and Wan Chuck Woo (University of Tennessee).



modeling, and simulation.

Almost 75 people attended the workshop, which focused on the scientific breadth of CNMS and discussions of collaborative opportunities. Presentations highlighted the opportunity for synergy between neutron characterization and nanoscience in polymers, new thick oxide hetero-structures (“superlattice crystals”), magnetic materials, catalysts, bulk nanomaterials, and theoretical studies, as well as the wide range of synthesis and characterization tools that will reside in CNMS.

In the future, all CNMS capabilities will be available to SNS and HFIR users through a single user proposal for all three facilities. CNMS is already open to user proposals; see our web site at www.cnms.ornl.gov to learn more.

Reflectometry

John Ankner, anknerjf@sns.gov

The reflectometry workshop featured four talks, and the session began with an overall introduction to neutron reflectometry that focused on soft matter. Frank Klose (ORNL) then covered polarized-beam studies of magnetic materials. Jarek Majewski (LANL) considered the complementary qualities of X-ray and neutron measurements. Bill Hamilton (ORNL) closed the session with a clever derivation of the theory of near-surface, small-angle scattering and demonstrated its application to membrane studies.

Small-Angle Neutron Scattering

Volker Urban, urbanvs@ornl.gov

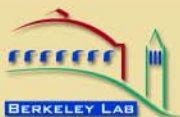
The SANS workshop began with an introduction for beginners, which explored the range of possible applications, the relation of SANS to microscopy and crystallography, and the basic concepts of the technique and data interpretation. ORNL experts from diverse scientific areas then illustrated the breadth of SANS applications in a series of presentations on exciting and novel topics, including fluid adsorption in nanopores, magnetic flux line lattices, time-resolved SANS of complex fluids, and modeling of bio-macromolecular complexes. The new Bio-Deuteration Lab at ORNL and materials research with ultra-SANS were also presented. The final discussion reemphasized infrastructure requirements, which had been determined at the 2003 NSFCHEMBIO and SENSE workshops (www.sns.gov/jins/Tallahassee_workshops_2003/workshops.htm). The workshop was well received and resulted in some good suggestions from the 50 or so participants, including scheduling the workshop for the first day of the user meeting to better prepare novice users for subsequent science sessions and hosting a hands-on tutorial. ✨

**SNS is funded by the
U.S. Department of Energy,
Office of Science,
Office of Basic Energy Sciences**

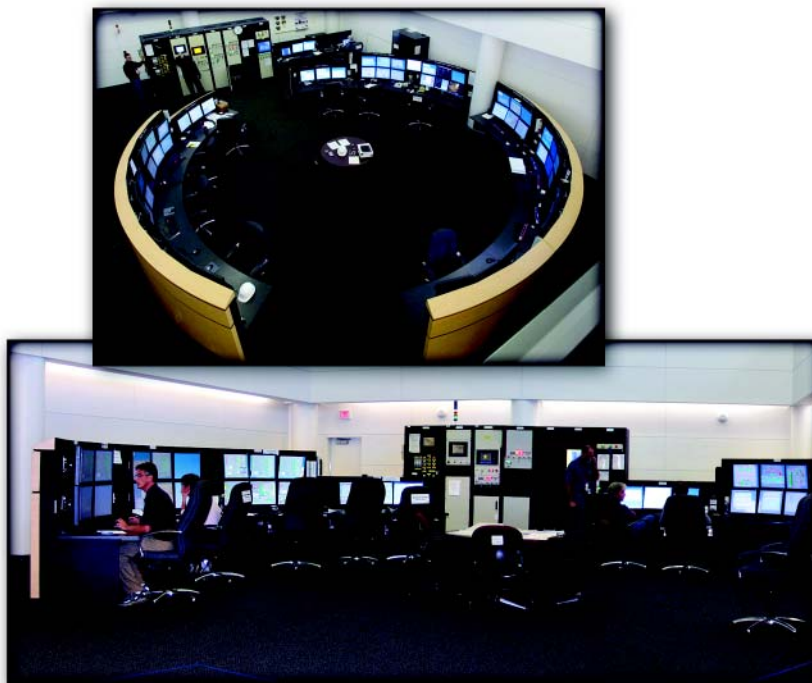
SNS User Administration Office
P.O. Box 2008
Oak Ridge, TN 37831-6474
E-mail: snsusers@sns.gov
Phone: 865-241-5644
Fax: 865-241-5177

The Neutron Pulse is published biannually by the
SNS Communications Office.
Editor: C. Horak (horakcm@sns.gov)

www.sns.gov



SNS is managed by UT-Battelle, LLC, under contract
DE-AC05-00OR22725 for the U.S. Department of Energy.



SNS Central Control Room.

**Spallation Neutron Source
User Administration Office
P.O. Box 2008
Oak Ridge, TN 37831-6474**

SNS 101040000-NL0002-R00

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