OAK RIDGE NATIONAL LABORATORY

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The NEUTRON PULSE

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SNS Site Update

Linac commissioning began in August with successful acceleration of a 7.5-MeV beam through tank 1 of the drift-tube linac. Commissioning of the remaining tanks will start in early 2004. Cryogenic cooldown of the refrigerator for the superconducting linac will continue through Spring 2004, and installation of the ring and high-energy beam transport components is also well under way.

Target installation began in April, ahead of schedule. Installation of the core vessel began in October, and major hot-cell equipment installation will begin in Spring 2004. Design of the first five instruments is near completion, and instrument installation will begin in early 2004 with placement of components for the backscattering spectrometer.

CNMS Breaks Ground

SNS's sister facility on Chestnut Ridge, the Center for Nanophase Materials Sciences (CNMS), is officially under way. In July, Secretary of Energy Spencer Abraham, together with U.S. Senator Lamar Alexander and a host of other dignitaries, held a groundbreaking ceremony for CNMS. This 80,000-ft^2, \$65M facility will be the first of five nanoscale science research centers being built by the U.S. Department of Energy (DOE) Office of Basic Energy Sciences (BES). Developed in partnership with the user community, CNMS will provide a thriving, multidisciplinary environment for scientists, engineers, students, and postdoctoral scholars engaged in nanoscale research. The research will integrate nanoscale science with neutron science, synthesis science, and theory/modeling/simulation.

"CNMS will assist scientists in reaching new frontiers in the study of nanoscale research and its practical application," said Secretary Abraham. "It represents a beginning of a revolution in science, opening up a broad array of innovation in materials science, biology, medicine, technologies for environmental research, and national security." He added, "Oak Ridge is blessed with tremendous research resources from the computational science center to the CNMS and the Spallation Neutron Source."

The first call for proposals for the interim CNMS user program was announced, and more than 70 proposals have been received and reviewed. The initial user program will be based on existing ORNL facilities and expertise and is expected to get the user program off and running so that full operations can occur when the new CNMS facility is completed in FY 2006. More information is available at www.cnms.ornl.gov.

In this Issue

Director's Comments

Thom Mason
Associate Lab Director
masont@sns.gov

Anyone visiting the SNS overlook six months ago and then again today would be amazed at the progress. Not so readily apparent is the rapid progress also being made in the linac tunnel, target building, and other areas hidden by steel, concrete, and earth. By the end of 2003, the project will be more than 75% complete, with more than $1B having been spent.

Safety is still an important focus on the project. After completing more than 2 million construction hours without a lost-workday case, Knight/Jacobs Joint Venture, our architect engineer and construction manager, hosted a barbecue luncheon celebration for the construction workforce. This safety record is highly regarded throughout DOE and is a tribute to continued emphasis on safety by all SNS staff and contractors.

In June, permanent electrical power was established on site with the energization and dedication of the Tennessee Valley Authority (TVA) electrical transmission line. DOE, TVA, and UT-Battelle staff used an innovative approach to the design, construction, and operation of the line that saved the project millions of dollars.

We anticipate approval of our FY 2004 budget request of $143M, which was submitted to Congress as part of the president's budget. In preparation for the change from a construction project to an operating facility in 2006, we updated our operations plan for the first year of operation in 2007.

Of the 16 instruments approved by the Experimental Facilities Advisory Committee (EFAC), 5 are being funded as part of the construction project and 2 by DOE grants to universities. One instrument has received some conceptual design funding from the DOE Office of Nuclear Physics, and another has received funding from McMaster University. DOE has initiated funding for the design efforts for five more instruments that were recently approved by the EFAC.

One goal of SNS is to use innovative software analysis and data management techniques. I believe this effort, as described elsewhere in this issue, will revolutionize the utility of SNS.

SNS is on the path to completion on schedule and within budget. Thanks to all of you for your continuing support.

IConUSAS Workshop, Oak Ridge

Michael Agamalian
magamalian@sns.gov

A workshop of the International Consortium on Ultrasmall-Angle Scattering (IConUSAS) was held at Oak Ridge in July. The meeting was organized by SNS and the University of Tennessee (UT)/Oak Ridge National Laboratory (ORNL) Joint Institute for Neutron Sciences (JINS). Sponsors included SNS, the ORNL Condensed Matter Sciences Division, JINS, DuPont Central Research and Development Station, and the National Institute of Standards and Technology (NIST). Attendees totaled 45 participants from 8 countries.

The main goal of the workshop was to create an international collaboration of scientific groups working on the development of contemporary X-ray and neutron double-crystal, ultrasmall-angle diffractometers, which are becoming more applicable to studies of the microstructure of condensed matter. The X-ray and neutron USAS instruments are complementary not only because their designs are based on the same Bonse-Hart technique but also because of the opportunity to vary the contrast by changing the type of radiation.

Special attention has been paid to discussion of newly built instruments and new projects related to the next generation of X-ray and neutron sources. Dramatic progress in the development of spallation neutron sources gave rise to a new generation of Bonse-Hart ultrasmall-angle neutron-scattering (USANS) instruments based on time-of-flight techniques (TOF-USANS). The development of these multiwavelength diffractometers will extend the USANS range by an additional order of magnitude, allowing study of enormously large (up to several hundred microns) inhomogenieties in condensed matter. The two TOF-USANS projects being developed in the United States (SNS) and Japan (JAERI) were discussed, followed by creation of the SNS TOF-USANS Instrument Development Team (IDT).

The existing reactor-based USANS instruments have been upgraded at several major neutron-scattering facilities and are state of the art in performance. The highest neutron flux at the sample position reached at the Institut Laue-Langevin (ILL) was at the level of ~6000 n/cm^2/s. The USANS instrument at NIST is equipped by the two-dimensional focusing pre-monochromator, which generates significant intensity gain.

A new Bonse-Hart ultrasmall-angle X-ray-scattering (USAXS) instrument was built and is now operational at the Advanced

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Tallahassee Workshops Plan for the Future

Al Ekkebus
ekkebusae@sns.gov

The U.S. neutron users' community is eagerly awaiting operation of SNS. In recent conferences coordinated by JINS, many research opportunities and corresponding equipment and facility needs were identified. To address some of these needs, the Neutron Scattering for Chemistry and the Chemistry/Biology Interface (NSFChemBio) and the Sample Environments for Neutron Scattering (SENSE) conferences were held at the Florida State University Conference Center in Tallahassee, Florida, on September 23-26.

The NSFChemBio Conference focused on the scientific challenges and the role of neutrons in areas such as catalysis, materials for energy production and storage, and structure and dynamics in liquids, glasses, and complex fluids. Also covered were compounds with exotic magnetic and electronic properties and complex self-assembled materials of molecular and macromolecular components, studied at multiple-length scales. During breakout sessions, ideas were solicited about the needs for instrumentation, detector development, time-resolved neutron scattering, and labeling of both low- and high-molecular weight compounds. Also included were ideas on data analysis suites that integrate modeling and simulation and educational efforts in designing, executing, and analyzing scattering experiments.

A growing number of scientists are using neutron-scattering techniques, with their research increasingly calling for advanced sample environments (temperature, pressure, magnetic field, pressure, chemical environment, etc.). The SENSE conference was devoted to exploring the scientific needs that are driving sample environment issues and to developing a plan for addressing these needs.

In his remarks outlining the goals for the SENSE Workshop, SNS Experimental Facilities Division Director Ian Anderson stressed the importance of sample environments at SNS. When operating, SNS plans to have about six research support staff per neutron-scattering instrument; this is comparable with other high throughput user facilities, including support for instruments, detectors, and sample environments. The initial suite of three SNS instruments will grow by one to two per year after construction is completed in 2006. SNS anticipates a two-year period during which facility reliability and power levels will develop to design levels. SNS will have a significant inventory of sample environments and will use the input from this meeting and other discussions to determine that inventory.

Important elements of the conferences were presentations describing funding opportunities with DOE, the National Science Foundation (NSF), and the National Institutes of Health. A tour of the National High Magnetic Field Laboratory provided a venue for the poster session on research on hard and soft materials and related neutron-scattering instruments.

Reports on the workshops will outline paths toward reaching the aforementioned goals and the formation of concept teams to develop proposals for instrumentation, sample environments, and supporting lab facilities. Corresponding educational programs for new users will also be identified.

Workshop sponsors included NSF, JINS, Florida State University, SNS, CNMS, and Oak Ridge Associated Universities. For more information, see the conference web site at www.sns.gov/jins/tallahassee_workshops_2003/workshops.htm.

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Photon Source (Argonne National Laboratory). A Bonse-Hart USAXS apparatus also operates at the European Synchrotron Radiation Facility in Grenoble, France. Both instruments have high levels of performance and strong user programs.

IConUSAS Workshop participants.

An important part of the workshop was discussion of application of the existing USANS instruments in various fields. In several talks, it was demonstrated that the Q-range of contemporary reactor-based USANS cameras is not sufficient to study the largest diffraction distances in polymer and rock samples under study. Therefore, it became clear that the proposed TOF-USANS technique, which is capable of extending the low limit of neutron-scattering vectors by an additional order of magnitude, solves this problem and opens new opportunities.

Several non-Bonse-Hart USANS techniques developed in Europe were also discussed, in particular, a variant of the so-called spin-echo USANS apparatus that is operational at the Delft University of Technology Research Reactor (Netherlands). This instrument is capable of measuring SANS scattering in real space and thus looks promising for correlation measurements.

Data Analysis at SNS

Kent Crawford
crawfordrk@sns.gov

SNS will be one of the premier user facilities for condensed matter research, but to maximize its potential scientific impact it is essential that the facility also provide its users with state-of-the-art software for analyzing their data. SNS will have a broad spectrum of users, ranging from professional users who are essentially full-time neutron scatterers to casual users who use neutron scattering only occasionally as just one of many tools to try to answer important research questions. SNS must be able to provide data analysis software that is appropriate for everyone.

Professional users typically want highly sophisticated analysis capabilities so that they can push the techniques to the limits and glean every bit of information from the data. These capabilities include correcting for a variety of sources of error and following the data-reduction process and visualizing the intermediate results at various steps along the way. Such users may also want the ability to fit various models to the data or to apply Monte Carlo, reverse Monte Carlo, or molecular dynamics in modeling the data. They may also want to use similar techniques to plan their experiments. All of these capabilities should be available in a user-friendly, easily maintainable form.

Casual users, on the other hand, are usually not interested in any of the intermediate steps in data reduction or analysis. Ideally, the data would be turned into an answer to the problem of interest in a way that is transparent to the user. Classic examples of this approach pushed to the extreme are the various medical imaging technologies such as PET, CAT, and MRI scans. In these cases, the end user sees the image of interest, typically presented in the form of slices through the biological system, without ever having to know or even be aware of the underlying physical processes and computations that generated the images. SNS should be able to provide analogues of this extreme approach to casual users in a variety of fields.

For intermediate users, intermediate approaches will be needed. These needs must also be considered as part of any comprehensive approach to data analysis.

Up to now, SNS neutron-scattering software efforts have focused on the data acquisition and control system, along with data storage and some visualization. These efforts have been proceeding quite well, and we expect to have a prototype system operating this fall that demonstrates the full hardware capabilities and core software capabilities. We are now starting to focus on what will be needed for data analysis software. A major software development effort taking a number of years will be required and will require significant input from the user community to ensure that this software ultimately meets the needs of the entire community. A first step in this direction is a workshop that was held October 13-15, 2003. This workshop brought together professional developers of software systems and representatives from the user community, with the goal of defining the requirements for SNS software. Later issues of *The Neutron Pulse* will report on the status of the data analysis activities as this work progresses.

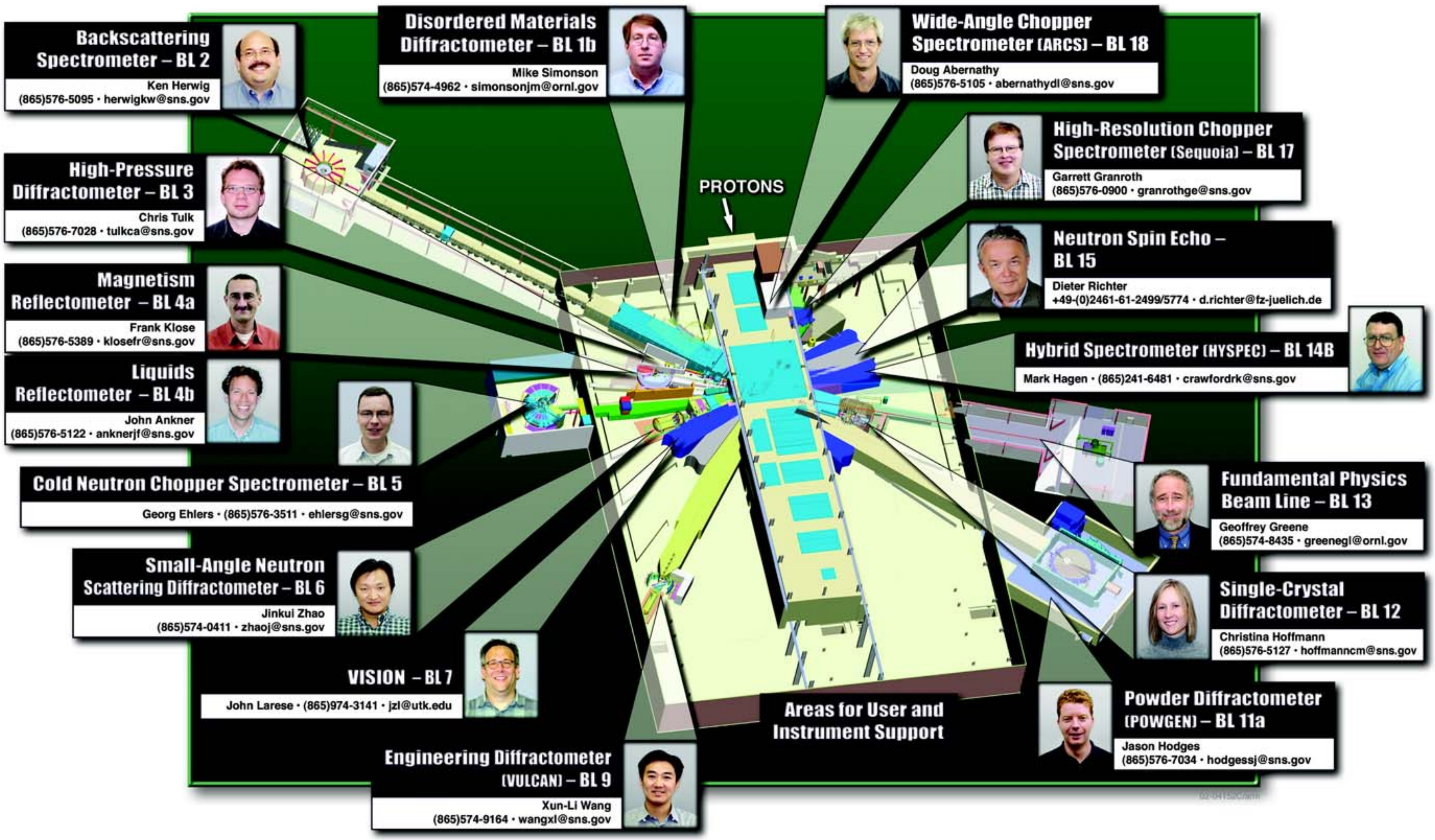
SHUG Update

Joanna Krueger
JKKruege@email.uncc.edu

The SNS-High Flux Reactor (HFIR) User Group (SHUG) Executive Committee is meeting about every other month. Users are invited to visit our web site (www.sns.gov/shug/) to read announcements and minutes from these meetings. Current hot topics include monitoring and assessing the newly restarted user program at HFIR, developing a fast access policy, viable methods of attracting new users to the neutron community, providing input to management on lodging and access issues, and staying abreast of instrumentation development for SNS and HFIR.

This summer, members of the Executive Committee met to discuss instrumentation status, sample environment issues, software for data acquisition and analysis, and other infrastructure issues with the scientists and management for both HFIR and SNS. We were delighted to see HFIR operational and the triple-axis spectrometers collecting data for users. Recently, the HFIR subgroup of the Executive Committee sent out a survey that will be used to test the effectiveness of the user program. Because SNS will use experience with HFIR policies to develop the SNS program, we strongly encourage you to report your experiences and share your ideas with us. This is a particularly important time for user input as decisions are being made that will affect us all for years to come.

This fall, SHUG will conduct its annual elections via e-mail, in accordance with the SHUG by-laws. There are six outgoing members, five of which had two-year terms and one of which is a one-year term for a postdoctoral or graduate student. Another mechanism for adding your voice to the user community is to support the activities of the Executive Committee by providing membership nominations and voting in the upcoming election. Please see the SHUG web site for more information.



SNS Instrument Scientists

Ian Anderson
Experimental Facilities
Division Director

Ann Jordan
Experimental Facilities
Division Secretary

Rick Riedel
Data Acquisition
Team Leader

SNS Experimental Facilities Division

Kent Crawford
Instrument Systems
Senior Team Leader

Caroline Zimmer
(not pictured)
Instrument Systems Group
Secretary

Al Ekkebus
User Administration
Manager

Peggy Anderson
User Administration
Training Coordinator

Selected

André Parizzi
Instrument Systems
Electrical Engineer

Wai-Tung Hal Lee
Neutron Polarization
Scientist

Michael Agamalian
Optical Components
Research & Development Lead

Gayle Greene
Data Acquisition
Software Developer

Peter Peterson
Data Acquisition
Software Developer

Steve Hicks
Data Acquisition
Electrical Engineer

Carol Tang
Data Acquisition
Software Developer

Lou Santodonato
Sample Environment
Team Leader

Bryan Coulter
Experimental Facilities
Division Finance Officer

Lee Magid
Joint Institute for Neutron
Sciences Acting Director

Annetta Hendricks
(not pictured)
Joint Institute for Neutron
Sciences Secretary

Science, Administration, and Support Groups

Chuck Roberts
Data Acquisition and
Detectors

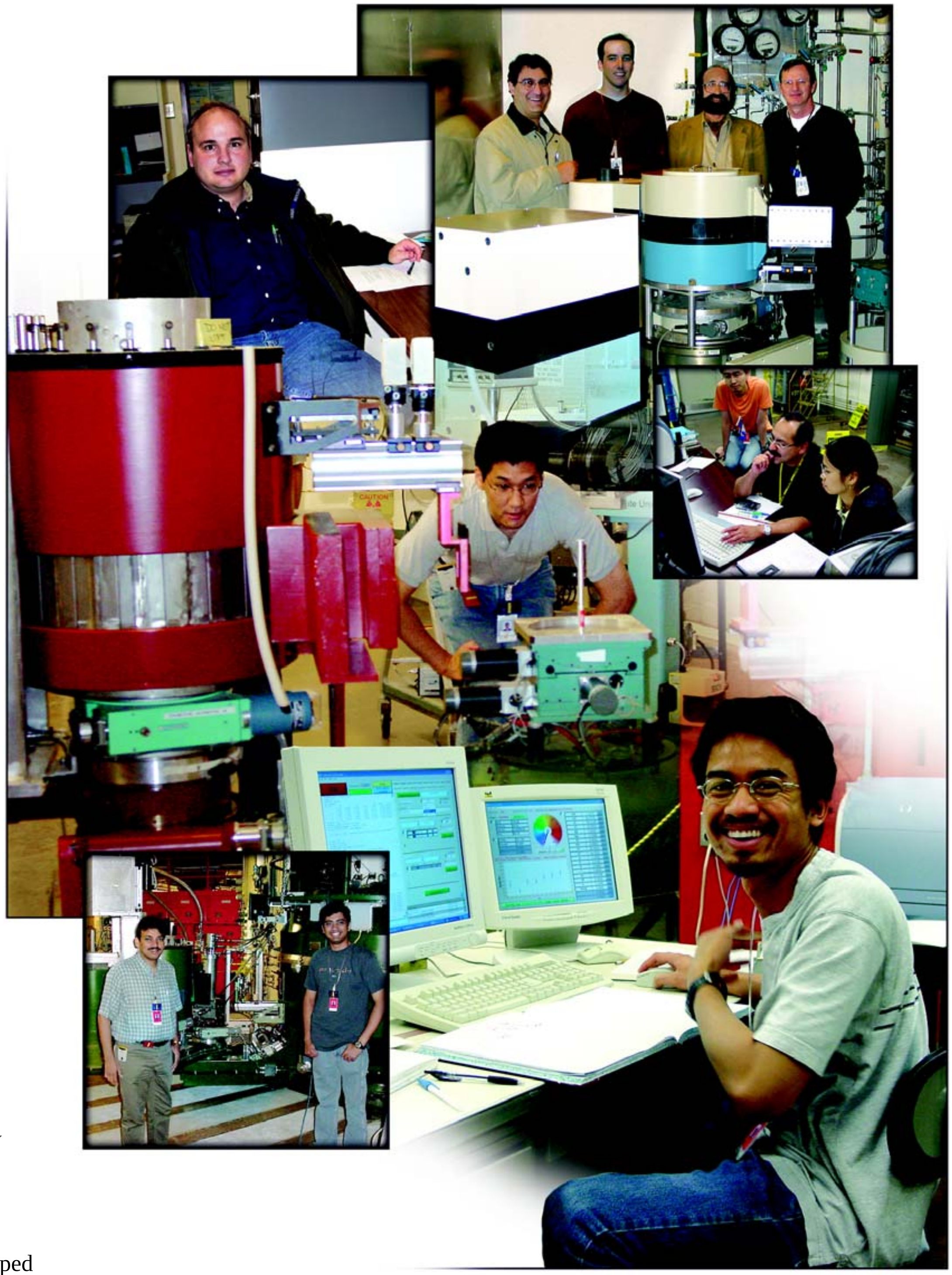
Ron Cooper
Detector Team Leader

Lowell Crow
Detector Physicist

HFIR CNS Begins Formal User Program

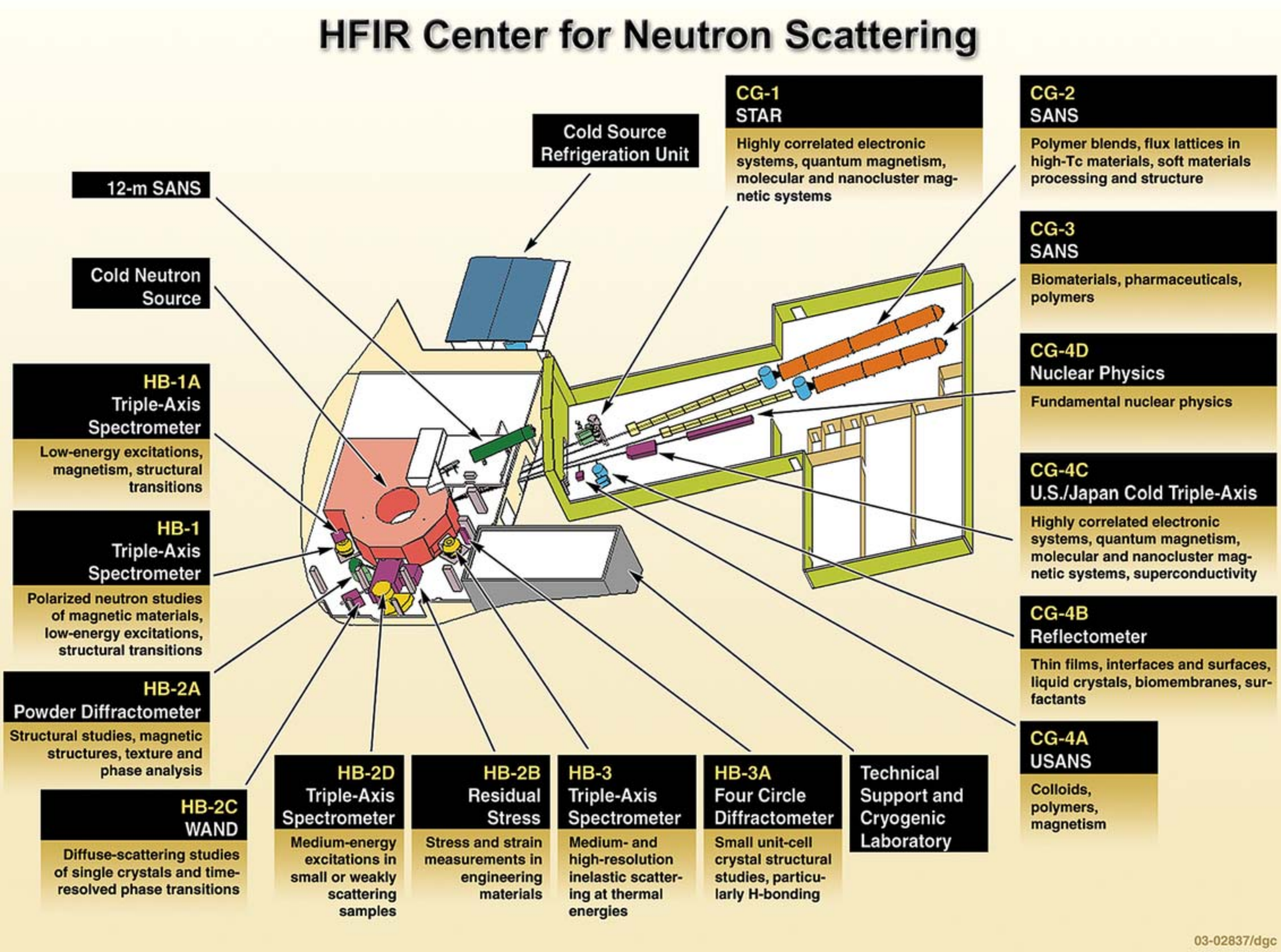
Greg Smith
smithgs1@ornl.gov

The HFIR Center for Neutron Scattering (CNS) is undergoing a major upgrade with the installation of both new and upgraded instruments and a high-performance cold neutron source. When completed, three of the four larger beam tubes will be used to provide thermal neutrons to eight essentially new instruments, each of which is state of the art in capability. Currently, two triple-axis spectrometers are operational at the HB-1 beam port and a third at the HB-3 port. Installation of four instruments is in progress at the HB-2 port. The new triple-axis spectrometers have on average about three times more neutron intensity than the old ones—making them equal to the best available. The cold source on the fourth large beam tube will illuminate four neutron guides to bring beams to seven instruments in a recently constructed cold guide hall. The cold neutron beams will be equaled only by those at the ILL in Grenoble, France.



Recent HFIR Users. From the top left are Thomas Enck (UT); David Vaknin, Rob McQueeney, Costa Stassis, and Jerel Zarestky (AMES Laboratory); Takashi Nagata (Ochanomizu University), Jaime Fernandez-Baca (ORNL), and Hazuki Furukawa (Ochanomizu University); Young Lee (MIT); Kittiwit Matan (MIT); and Krishnamurthy Vemuru and Prakash Mani (University of Alabama-Tuscaloosa).

Following the program plan developed jointly between HFIR and SNS, a formal CNS user program began in March 2003, making the facilities available to the scientific community. Scientists from academia, industry, and other government laboratories are performing research at the center based on peer review of proposals. An external proposal review committee assigns beam time for roughly six-month periods on the basis of scientific merit. Although a limited number of instruments (HB-1, HB-1A, and HB-3 triple-axis spectrometers) were available for the first proposal round (March–September 2003), 94 proposals were received. A total of 58 experiments were completed, with excellent results.



The HFIR CNS will have 15 state-of-the-art neutron-scattering instruments that will be among the world's best. Full descriptions of these instruments are available at neutrons.ornl.gov.

HFIR Instrument Contacts

HB-1 Triple Axis:
Andrey Zheludev (zheludevai@ornl.gov)
Stephen Nagler (naglerse@ornl.gov)

HB-1A Triple Axis:
Jerel Zarestky (zarestkyjl@ornl.gov)

HB-2A Powder Diffractometer:
Bryan Chakoumakos
(chakoumakobc@ornl.gov)

HB-2B Residual Stress:
Steve Spooner (spooners@ornl.gov)
Cam Hubbard (hubbardcr@ornl.gov)

HB-2C Wide-Angle Neutron Diffractometer:
Jaime Fernandez-Baca
(fernandezbja@ornl.gov)

HB-2D Triple Axis:
Lee Robertson (robertsonjl@ornl.gov)

HB-3 Triple Axis:
Mark Lumsden (lumsdenmd@ornl.gov)
Mohana Yethiraj (yethirajm@ornl.gov)

HB-3A Single-Crystal Diffractometer:
Bryan Chakoumakos
(chakoumakobc@ornl.gov)

CG-1 Cold Triple Axis:
Steve Nagler (naglerse@ornl.gov)

CG-2 SANS:
George Wignall (wignallgd@ornl.gov)
Paul Butler (butlerpd@ornl.gov)
Yuri Melnichenko (melnichenkoy@ornl.gov)

CG-3 SANS:
George Wignall (wignallgd@ornl.gov)
Volker Urban (urbanvs@ornl.gov)
Dean Myles (mylesda@ornl.gov)

CG-4A Ultra SANS:
George Wignall (wignallgd@ornl.gov)

CG-4B Reflectometer:
Bill Hamilton (hamiltonwa@ornl.gov)

CG-4C Cold Triple Axis:
Barry Winn (winnbl@ornl.gov)

CG-4D Fundamental Nuclear Physics:
Geoff Greene (greenegl@ornl.gov)

Ultrahigh-Resolution NSE Spectrometer

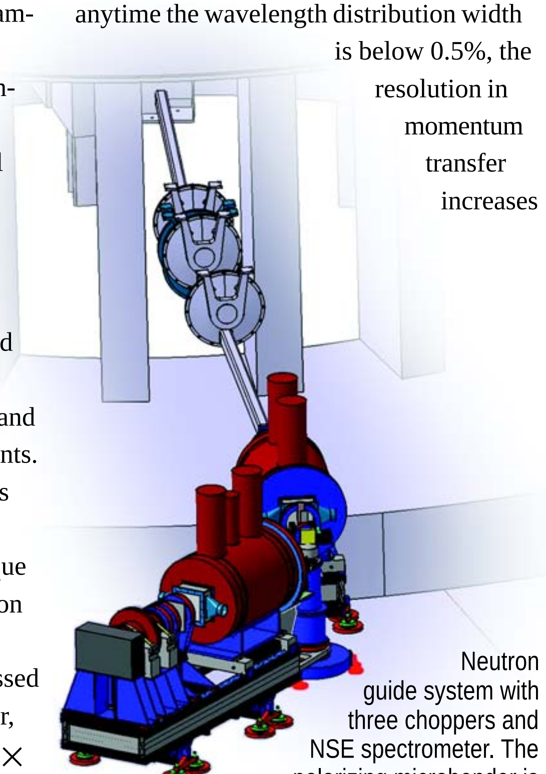
Michael Monkenbusch
m.monkenbusch@fz-juelich.de

The major role of the neutron spin-echo spectrometer (NSE) will be to analyze dynamics on mesoscopic scales and thereby unravel molecular motions and mobility at the nanoscopic level, which are of the utmost relevance for “soft matter” and biophysics problems. Of particular importance is the need for detailed comparisons with neutron-scattering results to validate rapidly improving molecular dynamics calculations that extend into the multi-nanosecond time domain.

NSE can contribute substantially to the study of glasses and the evolution of structural and molecular relaxation dynamics. The NSE’s unique combination of a huge dynamic range with a large momentum transfer (Q)-range is required in all studies of slow processes. The NSE will be ideal for investigating spin-glasses and ferromagnets, as well as new types of phase transitions.

The NSE’s unprecedented resolution and dynamic range will be achieved by exploiting superconducting technology and developing novel field correction elements. It will enable quasi-elastic investigations with a resolution of less than one nanoelectron volt. However, the technique yields the intermediate scattering function $S(Q,\tau)$ directly rather than $S(Q,\omega)$. The ultrahigh-resolution, therefore, is expressed in terms of the maximum time parameter, τ, which is determined by the product $J \times \lambda^3$. By combining design features that enable efficient use of long wavelengths up to λ = 1.8 nm and beyond with a high magnetic field integral of J > 1 Tm (IN15 at ILL: J = 0.27 Tm), the maximum time parameter will extend to τ =1 μs. The analysis is performed by consideration of individual neutron velocity changes that are measured by comparing the precession angles of the neutron spin in a magnetic field before and after the sample. The highest resolution requires use of long-wavelength neutrons. Using wavelength bands from 0.25 to 2 nm extends the dynamic range to more than six decades.

A system of three choppers in combination with a set of polarizing (micro)benders in a revolver mechanism will allow for the subsequent use of any wavelength band of $\Delta\lambda$ = 0.37 nm between 0.25 and ~2 nm. The time-averaged intensity on the sample will be comparable to the flux at the ILL reactor. Compared with single-detector NSE instruments, it will accept a significantly larger solid angle. Therefore, the effective data rate will gain an additional factor of 5. Additionally, because at anytime the wavelength distribution width is below 0.5%, the resolution in momentum transfer increases significantly compared with reactor instruments with 10% or more wavelength distribution width.



Neutron guide system with three choppers and NSE spectrometer. The polarizing microbender is located between the first and second chopper. The secondary instrument consists of two carriers with its two large magnets (indicated as red cylinders) on two arms connected by the sample stage. The scattering angle is changed by movement of the secondary arm.

The SNS EFAC has approved the NSE and has recommended a beam line assignment. The IDT for this instrument is a collaboration between two German groups from the Forschung-szentrum Jülich and the Hahn Meitner Institute.

Development of Novel Instrument Concepts

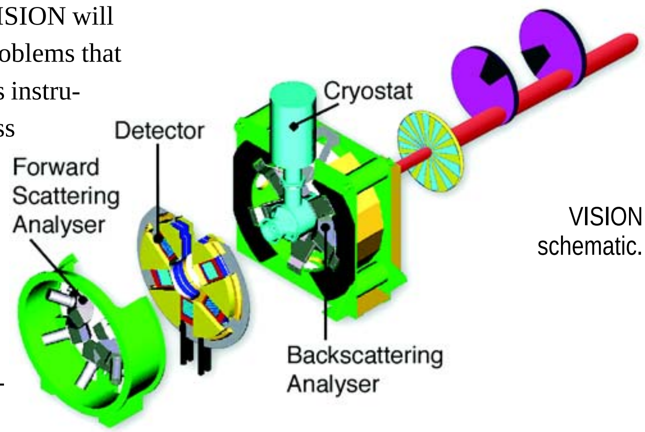
Ian Anderson
andersonian@sns.gov

Beam line positions at SNS are filling up rapidly. Currently, 16 instruments have been approved and allocated slots. Approval is being sought for several additional instruments, so beam lines for future instrumentation are quite limited. At this stage the project has decided to take an active role in creating an environment at SNS that fosters the development of new and unique instrumentation. The Novel Instrument Concepts (NIC) Program will enable a select team of well-known instrument developers to work together with SNS scientists, visiting fellows, and students in an environment conducive to unconventional approaches to instrumentation development. In June, a planning meeting was held in Chicago, under the chairmanship of Mike Rowe, to determine the best means of achieving the desired result. The NIC Program will most likely be the first component of the JINS activities as an intellectual center for neutron sciences. The program will run focused workshops on instrument techniques and an extended visitor program enabling researchers to spend time at the SNS-HFIR complex developing instrumentation. Operating the program within JINS allows a natural link between instrumentation and the science drivers developed through the JINS science programs.

VISION

J. Z. Larese
jzl@utk.edu

The SNS VISION is designed to be a next-generation instrument for performing neutron vibrational spectroscopy (NVS). Broadly speaking, VISION is the neutron analogue of an infrared (IR)-Raman spectrometer. VISION is an indirect geometry instrument that is expected to incorporate a parametrically designed secondary spectrometer that matches the geometry of analyzer crystals with that of the detector banks. Improvements in the analyzer section of the instrument, along with the flux/moderator gains of SNS, indicate that VISION will exhibit at least two orders of magnitude gain in performance over current best-in-class instruments. Incorporation of a medium-resolution powder diffraction detector bank for simultaneous structural characterization ensures that users of VISION will be able to address scientific problems that are currently inaccessible. This instrument is ideally suited to address a wide range of scientific problems in fields such as biochemistry, catalysis, materials science, geology, polymers, and engineering.



VISION schematic.

Optical spectroscopy using IR-Raman spectrometers has demonstrated that the study of vibrational and torsional motions in a whole host of materials has been extremely useful for gaining direct insight into the potential energy surfaces, electronic structure, and nuclear dynamics that govern a vast number of molecular systems. VISION will provide information about these motions complementary to that obtained from optical spectroscopy because NVS is not restricted by the optical selection rules governing IR and Raman spectroscopy. Hence, VISION brings an entirely new segment of users and opportunities to the U.S. scientific community.

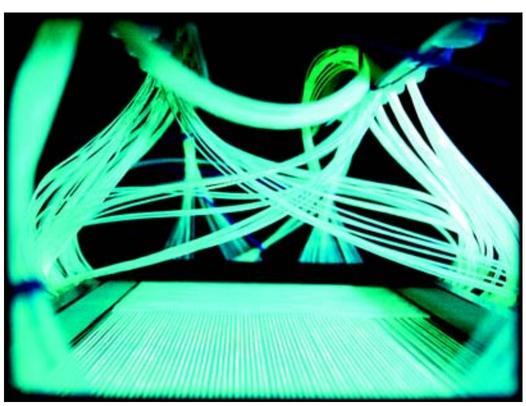
VISION has been approved by the EFAC, and the IDT is preparing a proposal to the NSF to request funding for the conceptual design. The VISION IDT is led by John Larese, a joint faculty member in the Chemistry Department at UT and member of the Chemical Sciences Division at ORNL.

Neutron Detector Workshop, Indiana University

Christina Hoffmann
hoffmanncm@sns.gov

Condensed matter physics, chemistry, metallurgy, and geo- and biosciences have benefited greatly from using neutrons to probe the structure, magnetism, and dynamics of materials. However, currently available neutron detectors are lacking the performance capabilities to fully exploit future neutron flux. With the completion of SNS in 2006, we are challenged to use this opportunity for sustained development of gas and scintillation detectors and for investigation of new scintillator materials, semiconductor detectors, new types of gas detectors, and low-efficiency neutron monitors.

In May 2003, a Neutron Detector Workshop was held at the Indiana University Cyclotron Facility (IUCF), supported by IUCF, SNS, DOE-BES, and the NSF. The workshop attracted 68 researchers from North America, Europe, Japan, and Australia. The purpose of the workshop was to encourage collaborative detector research among academia, national laboratories, and industry, with a strong emphasis on education. The meeting started with overview talks on emerging and developing technologies, followed by presentations on individual neutron detector development projects. Presentations and discussions focused on exchanging information on ongoing research and development (R&D) efforts at various places to find complementary projects.



The wavelength shifting fiber scintillation neutron detector prototype was assembled at SNS with DOE-BES support and is one candidate for collaborative R&D efforts with NSF-funded academia.

The workshop's agenda included research, overview, and educational presentations and posters, followed by discussion sessions divided according to major detector types: high-resolution, ^{3}He gas, and scintillator. Breakout sessions focused on bringing together groups to pool efforts on high-resolution, scintillation, and gas detector development. Participants worked

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SNS User Administration Office
701 Scarboro Road
Oak Ridge, TN 37830
E-mail: snsusers@sns.gov
Phone: 865-241-5644
Fax: 865-241-5177

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Aerial view of the SNS site, September 24, 2003.

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on ideas for new detector development proposals. The need for an internationally accessible news and exchange forum—besides regular meetings, conferences, workshops—was identified. In addition, SNS has agreed to host a web site centered on fast and interactive data exchange: www.sns.gov/detectors.

NSF provided information on funding opportunities for midsize projects, including new instrumentation and instrumentation support, which would widely include detectors. Options for overseas exchange programs for student, postdoctoral, and researcher appointments were also highlighted.

Spallation Neutron Source
User Administration Office
701 Scarboro Road
Oak Ridge, TN 37830

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