SPALLATION NEUTRON SOURCE
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SNS
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Thom Mason Named to Lead SNS Project

On February 22, Oak Ridge National Laboratory (ORNL) Director Bill Madia named Dr. Thom Mason to lead the SNS, effective March 1, 2001. Mason had been serving as director of the Experimental Facilities Division. His new title is Associate Laboratory Director for the Spallation Neutron Source. Madia commented "Over the last eight weeks, I have conducted an extensive international search and interviewed numerous highly qualified candidates to lead the SNS project. Among these candidates, Thom brings an unparalleled combination of scientific skills and direct project experience. In addition to scientific awards and honors too numerous to list here, Thom also enjoys the respect of the scientific community, the SNS staff, and our sponsors at the Department of Energy."

Since joining the SNS project in 1998, Mason has been responsible for the technical, cost, and schedule performance of the target and instruments components of the SNS. These systems represent more than $250M of the technical components, research and development, and preoperational portions of the SNS, as well as planning and requirements for $150M for the project's conventional facilities.

Mason is the coauthor of more than 85 publications. He earned a bachelor of science degree in physics in 1986 from Dalhousie University in Halifax, Nova Scotia, and a doctorate in condensed matter physics in 1990 from McMaster University in Hamilton, Ontario.

Jim Decker, DOE's acting director of the Office of Science, said "Thom is a superb choice to lead the SNS. His management skills combine with his focus on the facility's scientific output to ensure strong and continued support by the international scientific community."

Madia also noted that over the coming months the project will be working to ensure a smooth leadership transition. Madia expressed confidence that the SNS project will continue on the path to delivering the world's most impor-

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Director's Comments

Thom Mason
Associate Lab Director

I am honored to have been selected to lead the SNS, which I believe will become the world's leading facility for neutron studies of the structure and dynamics of materials.

The partnership among the six national labs is strong, and we are working more closely together than ever before. The teamwork and commitments from the lab directors and their staffs give me confidence that the project will be completed on time and on budget.

Our FY 2002 budget request to DOE is $291.4M, up about $13M from the FY 2001 level. This is the largest annual sum the project will request. In the past, the project has been fortunate to receive budgetary support from DOE and from the congressional appropriations process. Although changing budgetary priorities are expected with a new administration, I anticipate continued strong support for the SNS.

As my title indicates, SNS is beginning integration into ORNL. I will be working closely with colleagues at ORNL to focus initially on encouraging ORNL staff to examine research opportunities at SNS. The SNS will continue to function with the full authority needed to execute a construction project of this magnitude.

The SNS and High Flux Isotope Reactor (HFIR) User Group are providing valuable input on the policies and practices being developed for the user program. I look forward to receiving their ideas on how to enhance the productivity of both SNS and HFIR users.

Later this year, progress on the SNS will be much more visible as concrete and steel will begin to rise on the top of Chestnut Ridge. We hope to have a web camera installed soon for you to follow the progress. We're also receiving requests to approve instrument development teams. As the teams are approved, we will provide additional information in *The Neutron Pulse* and on the SNS web site.

This project is being built for you, the users of the instruments. I hope you can help increase the potential users of the SNS by assisting students and colleagues in learning more about the capabilities of the SNS. The neutron-scattering community will benefit from the exchange of ideas and development of new concepts for experiments.

The valuable contributions of David Moncton and Ed Temple have set the course toward project completion. The outline of their efforts is carved today on Chestnut Ridge. I will do everything I can to fill in the outline by 2006.

David Moncton and Ed Temple – Thanks for two years of dedicated support to SNS

Macromolecular Single-Crystal Diffraction Workshop

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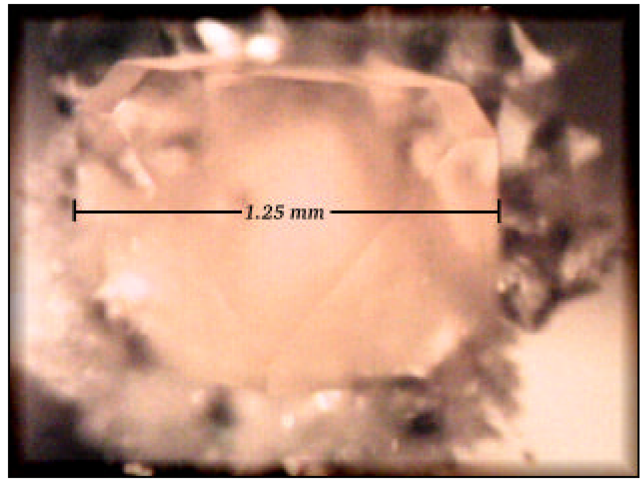
On December 18-19, 2000, a workshop cosponsored by SNS and NASA was held in Knoxville, Tennessee, to discuss single-crystal neutron diffraction studies and the potential role of the SNS in such studies. Presenters and participants included structural biologists, instrumentation specialists, and microgravity-crystal growth experts from local, national, and international locales. First-day presentations included scientific advances with macromolecular neutron diffraction, developments of neutron sources, detectors and beam lines worldwide, and the role microgravity is playing in the growth of crystals suitable for neutron diffraction experiments.

The scientific case for neutron diffraction was presented by keynote speaker John Helliwell, University of Manchester, whose research into the basis of sugar recognition by concanavalin A (con A) has encompassed extensive synchrotron X-ray and neutron data collection. The traditional basis for neutron diffraction is the ease with which accurate positions of hydrogens/deuterons can be determined in crystals of macromolecules. Both deuterium and oxygen scatter similarly in neutron diffraction experiments, and solvent position and proton exchange can be readily identified from neutron diffraction data. A more recent rationale for neutron diffraction can be seen in the comparative diffraction data for con A between an ultrahigh resolution X-ray cryostructure and a medium-resolution neutron room-temperature structure. Data were collected in 10 days and were 89% complete to 2.4 Å. The neutron structure provided six times the number of well-determined waters (position and orientation) compared with the ultrahigh resolution X-ray data (0.9 Å). Additional features seen in medium-resolution neutron structures are the differences in the bond lengths (short vs long) of acidic side chains, which cannot be interpreted from X-ray data at resolutions less than 1.2 Å. Thus, neutron diffraction data could have a preeminent role in assisting future modeling studies by providing a structural database for understanding the role of solvent in ligand interaction and by providing further needed information to determine interaction thermodynamics from structural data.



This crystal of glucose isomerase is about as deep as the average cross section seen in the photograph and is suitable for neutron diffraction studies. The out-of-focus areas contain many small crystals. The growth of this crystal was an offshoot of research sponsored by NASA in Bunick's laboratory.

Peter Timmins of the Institut Laue-Langevin reported that unique information on the location of hydrogen atoms and water has been obtained by neutron fiber diffraction of biological polymers, including cellulose, hyaluronic acid, filamentous viruses, and DNA. Other significant diffraction information can be obtained at low resolution, including the localization of surfactants added to proteins. The detergent structure in integral membrane proteins has not been possible to determine in X-ray diffraction studies because of the disorder of the surfactants in the unit cell.

Improvements in neutron sources, detector design, and interpretation of multiwavelength diffraction have improved the speed with which data can be collected. Detector improvements include the neutron image plate, which is currently in use in both Japan and Europe, a neutron area detector with 1-mm-pixel size being developed at Oak Ridge, and detector research at Brookhaven National Laboratory for the SNS project. Nobuo Niimura of the Japan Atomic Energy Research Institute presented rubredoxin data collected with a neutron image plate in 11 hours. The resolution of the data is 1.5 Å, and refinement of the hydrogen positions at 1.5 Å is currently under way.

As a result of microgravity studies supported by both NASA and the European Space Agency, production of crystals sufficiently large for neutron diffraction studies could become commonplace. Dan Carter reported reliable growth of crystals with the

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1-mm^3 volume needed for current neutron diffraction experiments for such problematic proteins as bacteriorhodopsin. With the commissioning of the International Space Station, a permanent venue now exists that should be available to crystallographers interested in using microgravity for crystal growth.

One significant application for protein structures determined by neutron diffraction will come in the area of rational drug design. Chris Dealwis of the University of Tennessee pointed out the practicality of this approach, discussing the problems associated with finding an agonist of angiotensin to bind with rennin and how this study carried over to drug discovery of anti-HIV proteases.

The second day of the workshop focused on macromolecular crystallography at SNS. Three primary conclusions were reached: (1) Single-crystal biological instrumentation must form an integral part of SNS future beam line planning. (2) Future planning at SNS should minimally encompass two protein crystal diffraction instruments: the High Power Target Station (HPTS) should have an instrument capable of collecting data from crystals with a maximum unit cell length of 100 Å, and the Long Wavelength Target Station should have a device capable of resolving atomic positions from crystals with unit cell axes of <250 Å. (3) A committee should be formed to submit a letter of intent for an HPTS beam line, with the identification of agencies for funding the instrument development team.

Workshop participants felt that educational and outreach activities should be undertaken to acquaint a new generation of crystallographers with the scientific merits of neutron diffraction and of the advances that have been made in recent years. Workshop participants will seek to make presentations at various national societies, including the American Crystallographic Association 2001 annual meeting, which includes a workshop on macromolecular neutron crystallography.

SHUG Update

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The SNS and HFIR User Group (SHUG) Executive Committee is monitoring the development of user policies that will be in place when HFIR comes back on-line after its upgrade. SNS user policies are also being developed with input from SHUG. Keeping in mind the intrinsic operating differences of the two facilities, it is the goal of SHUG and the management of both facilities to keep HFIR and SNS policies consistent. This, along with efforts to standardize computer interfaces and apparatus whenever possible, will facilitate the movement of users from one facility to the other to take advantage of the unique opportunities presented by each.

An important role of the Executive Committee is to be an advocate for the SHUG community. During the budgetary process last year, we expressed to Congressional committees the user community support for full funding of the SNS. We also wrote to ORNL Director Madia about our concerns regarding the resignation of SNS Executive Director Dr. David Moncton and the search for a replacement. After Dr. Thom Mason was appointed to head the SNS project, we invited him to join an Executive Committee phone conference. We were pleased by his willingness to work with us in promoting the interests of the user community.

The Executive Committee also plans SHUG general meetings. SHUG and the Neutron Scattering Society of America will coorganize a joint meeting with scientific and business meeting components for the summer of 2002, tentatively scheduled for Knoxville, Tennessee. This meeting will, among other things, highlight the newly upgraded HFIR facilities and the SNS facilities that will be taking physical shape by then.

The SHUG web site has been developed at by the Executive Committee members working with SNS Communications staff. The web site should facilitate communications between the committee and the SHUG membership. Users can sign up for SHUG membership, read announcements and minutes from previous committee meetings, and find contact information for the Executive Committee. Check it out at http://www.sns.gov/shug/.

Elections for new SHUG Executive Committee members are planned for fall 2001. Requests for nominations will be made soon.

SNS Educational Programs Participation

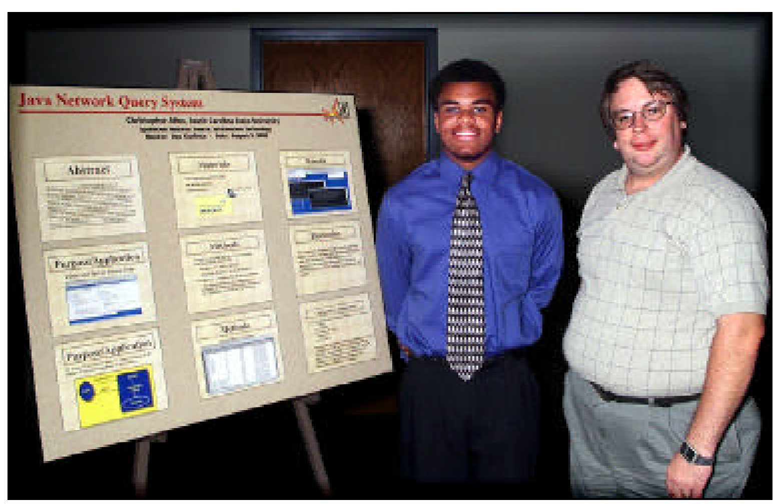
In 2000, SNS hosted eight undergraduate interns: three from South Carolina State University, two from Tennessee Technological University, and one each from Middle Tennessee State University, the Polytechnic University of Puerto Rico, and Montana Tech. All of the students had mentors throughout their research experience. The program included a poster session at SNS and at ORNL's Joint Institute for Heavy Ion Research describing the students' research activities. In addition to SNS funds, the summer students were also supported by the DOE Energy Research Undergraduate Laboratory Fellowships Program and the South Carolina Alliance for Minority Participation, a National Science Foundation program.

Two interns, Brian Davis and Christopher Allen, won first and second place awards in computer science and math at the 6th Annual Science & Engineering Research Conference at the University of South Carolina. SNS supplied t-shirts and trophies for all student participants.

From left to right: (1) John Galambos, SNS accelerator physicist and mentor for Brian Davis, (2) Brian Davis, and (3) former Accelerator Systems Division Director Bob Kustom.

Thom Mason instructs a class at the National School on Neutron and X-Ray Scattering.

At the graduate student level, SNS and The University of Tennessee assisted 25 of the 60 students at the August 2000 National School on Neutron and X-Ray Scattering at Argonne National Laboratory. The 60 students were selected from 160 applications and had a wide distribution of academic backgrounds. The purpose of the national school is to educate students on the use of major neutron and X-ray facilities. During the first week, there were lectures on the principles of scattering theory and the characteristics of the sources. The second week was devoted to the application of scattering methods to condensed matter, including hands-on experiments of interest to materials science, solid-state physics, and soft matter. The experiments were held at the Intense Pulsed Neutron Source and the Advanced Photon Source and were designed to express the diverse properties of neutrons and X rays as evidenced in scattering experiments. Collaboration on assisting the students was accomplished through the National Science Foundation Long Wavelength Target System proposal, and the course was supported by the Office of Basic Energy Sciences in DOE's Office of Science.



Christopher Allen and his mentor, Dan Ciarlette, SNS Information Technology manager.

Neutron-Scattering Instrument Update

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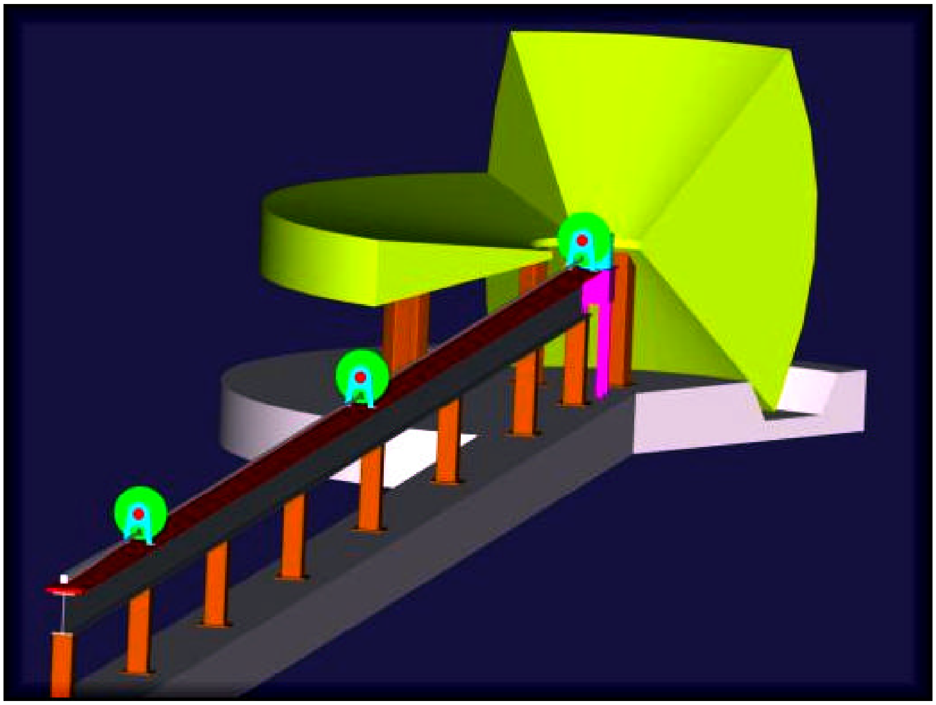
Argonne technicians Ray Ziegler and Lynette Jirik in the Argonne chopper lab carrying out acceptance testing for the E_0 chopper prototype.

A lot has been happening with the SNS neutron-scattering instruments in recent months. Between November 2000 and February 2001, the budget for construction of instruments was reduced from $93 to $60M. This $60M is still higher than the $45M that was available for instruments at the time the project first received construction funds, and it allows us to provide five instruments capable of world-class science. We will also provide the infrastructure for common components necessary for these and future instruments. It is likely that funding for additional instruments will become available as the project progresses, and we stand ready to help facilitate this process.

The funds removed from the instrument budget were placed in the project contingency fund. This was needed to raise the contingency to an acceptable amount in light of a higher than anticipated cost estimate for the conventional construction and recognition of the need for additional funds to support the buildup and training of SNS staff to operate the accelerator systems. As the project progresses, there will be fewer cost uncertainties and the need for contingency will diminish. Thus, it's possible that in the future additional funding for instruments will be made available from the contingency funds. For the time being, however, our scope is the construction of five instruments plus the development of the common-component infrastructure to support these and any other current or future instruments. This infrastructure includes designs for the data acquisition system and neutron choppers of various types, capabilities for installing beam line optics inside the target station, instrument simulation tools for instrument design, evaluation of various detector technologies and promotion of the development of new technologies, development of standards for sample environment equipment, and analysis of the requirements for neutron beam line shielding. It also includes beam line inserts and some shielding for the initially noninstrumented beam lines.

In the mean time, the development of concepts for additional instruments has proceeded. The process for instrument selection remains the same as before (*The Neutron Pulse*, Vol. 1, No. 1), with two differences. First, the Instrument Oversight Committee (IOC) has been replaced by the Experimental Facilities Advisory Committee as the group that makes recommendations on instrument selection. Second, the selection of an instrument as worthy of construction at the SNS does not necessarily mean that construction of that instrument will be funded within the SNS project. What it does mean is that an SNS beam line is tentatively allocated for that instrument and that the interested scientists have the go-ahead to pursue funding for the instrument, either internal or external to the SNS project.

So far, six instruments have been recommended for selection by the IOC. The first three of these, the backscattering spectrometer, the magnetism reflectometer, and the liquids reflectometer, are in the project baseline. Designs for these three instruments (*The Neutron Pulse*, Vol. 1, No. 1) are in the advanced stage, and procurements are beginning. These three instruments will definitely be funded



10-100 μeV multichopper spectrometer.

with SNS project funds, albeit with some of their planned scope deferred for now. The second three instruments recommended for selection by the IOC are a high-resolution Fermi chopper spectrometer, an extended-Q small-angle neutron-scattering instrument, and an engineering diffractometer (*The Neutron Pulse*, Vol. 1, No. 2). One or two of these may be funded from project funds, but that decision has not yet been made.

E_0 chopper phototype.

The Instrument Systems group is developing concepts for five additional instruments: (1) a high-resolution powder diffractometer, (2) a disordered materials diffractometer, (3) a high-pressure diffractometer, (4) a single-crystal diffractometer, and (5) a multichopper spectrometer with 10- to 100-meV resolution (see figure above). We also anticipate several additional letters of intent (LOIs). (*Requirements for LOIs can be found at www.sns.gov/users/loiguidelines.pdf.)*

On the technical front, designs for the first three instruments are proceeding rapidly. Design reviews for some components have been completed, and others will be held soon. Procurements will be initiated this year for several of the long-lead major components.

Work on the design of components common to many or all of the instruments is already well under way. We anticipate that a prototype data acquisition system will be operational by next fall. We have been operating prototype T_0 and Fermi (E_0) choppers for some time, and those will be installed on Intense Pulsed Neutron Source instruments at Argonne National Laboratory within the coming year to gain further experience. Extensive shielding analyses have been performed to help us optimize the types of materials and thicknesses to provide cost-effective beam line shielding that meets the facility shielding requirements. Benchmarking of these analysis tools against actual beam line measurements on operating facilities is under way. Procurement is under way for prototypes of the beam line inserts that provide for precise alignment of neutron optical components within the neutron shutters and inside the core vessel. Testing of these prototypes is planned for later this year in a design validation test stand that is a mockup of the SNS shutter and vessel arrangement. This testing will verify whether the current designs can in fact provide the required reproducibility of optical component alignment.

Instrument Systems has been ramping up its staffing and now has nearly all the staff necessary to support these activities. We have ten instrument scientists and technical team leaders for data acquisition, detectors, neutron choppers, sample environment, and optical components, along with several staff to support the technical teams and the instrument design.

Further information about SNS Instrument Systems activities can be found at www.sns.anl.gov.

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tant new scientific facility on budget and on schedule. This confidence comes in large measure from the two years of hard work and dedication of David Moncton and Ed Temple: “We thank them for their enormous contributions in moving the SNS project from an idea to a reality.”

Staging material for the target facility's mini-pile deep foundation.

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