Oak Ridge National Laboratory

MANAGED BY UT-BATTELLE FOR THE U.S. DEPARTMENT OF ENERGY

SNS

The NEUTRON PULSE

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Number 1
Spring 2003

Project Status

At the end of 2002, the SNS project was 56% complete and will be well over 60% complete by late spring. Adherence to the construction schedule allowed on-time, and in some cases early, occupancy of the Front-End, Linac, Klystron, and Central Helium Liquefier/Radio-Frequency (RF) buildings. By summer, the only two buildings that will still be under construction are the Target Building and the Central Laboratory and Office (CLO) Building.

The Tennessee Valley Authority's electrical transmission line to SNS was completed in January 2003. The line will be energized in late spring.

By the end of 2002, the Berkeley-designed front end (the ion source, low-energy beam transport, and medium-energy beam transport systems) was successfully installed, commissioned, and in operation—three months ahead of the milestone date. Beam current in excess of requirements was demonstrated in an extended commissioning run.

Installation of accelerator components is under way in a number of buildings, and installation of RF components for the coupled-cavity and superconducting sections of the linac has begun. Ring and target installation activities are also under way, and cryomodule installation is imminent. Target design will be complete by June, leaving instrument systems as the only remaining design activity.

(Top) Target Building with foundation for beam line 2 in the right forefront. Steel framing for the CLO can be seen behind the Target Building. (Right) Close-up of foundation for beam line 2.

In this Issue

Director's Comments

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New sign for the main SNS entrance.

The SNS project continues to be on schedule and within budget. Last fall, the project team agreed to include the option for a walkway from the Target Building as part of the CLO Building construction. This will facilitate the flow of people, equipment, and samples between the offices and specialized labs of the CLO, Center for Nanophase Materials Sciences (CNMS), and the experimental floor.

We now have 16 approved instruments. Discussions are under way on letters of intent for other instruments, and we continue to receive many communications about new instrument concepts.

The January 2003 meeting of the North American neutron facility directors was quite productive and will form the basis for future collaborations among the six facilities (see page 3). Although we've had informal discussions in the past, they have usually been on a one-on-one level. This meeting demonstrated that the facilities are committed to working together to enhance our mutual scientific productivity.

As construction continues at a progressive pace, I'm especially proud of our safety record. As of the end of April 2003, more than 1.8 million construction hours have been worked at the site without a lost workday incident—an outstanding record that exceeds U.S. Department of Energy (DOE) and industry averages. The entire Oak Ridge SNS staff, including project and construction staff, has worked more than 3.2 million hours without a lost workday case.

From the SHUG Chair

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The relationship between users and facility staff is often perceived to be like the customer-retailer relationship. Although there are certain aspects of this analogy that might be accurate, I believe that the ideal relationship should be one of collaboration, with the common goal of achieving scientific advances. Anytime a big group of highly energetic researchers comes together, there will be some friction. As I see it, part of the SNS-High Flux Isotope Reactor (HFIR) User Group (SHUG) role is to convert this friction into positive energy that can improve both facilities. I encourage you to help us fulfill that role by informing us of any issues that we can work on to make HFIR and SNS pleasant, productive havens for research.

On the news front, the HFIR users program was recently expanded, and Greg Smith was appointed group leader of the Neutron Scattering Users Program. The first call for user proposals went out last November. Numerous proposals were received and reviewed, and beam time was assigned in an amazingly short time. Although the success of the new user program is not yet known, the HFIR staff deserves special recognition for starting the program in time for resumption of reactor operation. A subgroup of the SHUG Executive Committee will soon conduct a survey of the effectiveness of the new users program. Please forward any comments to me or David Vaknin (vaknin@ameslab.gov), who is heading the subgroup.

SHUG Executive Committee Information

Member	Term Expiration
Paul Butler, Secretary	2003
Zema Chowdhuri	2003
Takeshi Egami, Chair	2004
Christina Hoffmann	2004
Joanna Krueger	2004
Scott Misture	2003
Nancy Ross	2004
Paul Sokol	2004
John Tranquada	2003
David Vaknin	2003
Angus Wilkinson	2003

For more detailed contact information, please see www.sns.gov/shug/comminfo.htm.

Neutron Facility Managers Meet at Los Alamos

In January 2003, the inaugural meeting of the Neutron Facilities Roundtable was held at Los Alamos National Laboratory (LANL). Represented were HFIR and SNS at Oak Ridge National Laboratory (ORNL), the Intense Pulsed Neutron Source (IPNS) at Argonne National Laboratory (ANL), the Center for Neutron Research at the National Institute of Standards and Technology (NIST), the Neutron Program for Materials Research of the National Research Council Canada (NRC-CNRC), and the Los Alamos Neutron Science Center (LANSCE) at LANL. To avoid duplicated efforts and maximize effective use of research funds, periodic meetings of the neutron facilities were recommended by the Interagency Working Group of the White House's Office of Science and Technology Policy. The group's recommendation appeared in their June 2002 report *Status and Needs of Major Neutron Scattering Facilities in the United States* (www.ostp.gov/html/neutron.pdf). Similar recommendations had been made at recent conferences. A primary goal of such meetings is to share neutron techniques in basic and applied research and development (R&D). Current collaborative R&D programs were identified, along with the potential for future efforts. Examples include the joint detector development activities under way involving many institutions and a February 2003 pulsed polarized neutron workshop sponsored by DOE and the National Science Foundation (NSF) (see page 6).

Back row: Pat Gallagher, NIST; Paul Lisowski, LANSCE, Jim Richardson, IPNS; Thom Mason, SNS; Greg Smith, HFIR; Steve Nagler, HFIR. Front row: Audrey Archuleta, LANSCE; Alan Hurd, LANSCE, Mike Rowe, NIST; Zin Tun, NRC-CNRC; Ray Teller, IPNS; Al Ekkebus, SNS.

Several first steps were taken at the January meeting. LANL will determine whether a common radiation training course could be made available for users at all or many DOE facilities that currently have different training requirements. To improve facility access and communication, HFIR and SNS agreed to explore a common data format for sharing lists of users.

In addition, results of software development at the California Institute of Technology (CalTech) were reported. CalTech has received funding from DOE's Office of Basic Energy Sciences for software development as part of the ARCS chopper spectrometer at SNS and has made great strides in its efforts. A future opportunity presented itself in the form of software collaboration, which could include areas such as data analysis evaluation (instrument control) and simulation. CalTech hosted an exploratory meeting of this multifacility team on March 15.

New metrics were proposed that would allow us to better understand how our facilities are used, for example: counting and binning users by subject; number of refereed publications, patents, etc.; identifying participants; number of experiment visits; experiments; and the number of first-time users. This will be discussed more at future meetings after facilities have experience using these statistics.

Another discussion topic involved recognition (or lack thereof) of contributions by facility scientists in publications. The SNS policy on authorship endorses guidelines on authorship by organizations like the American Physical Society. To avoid misunderstandings, it is appropriate that the experiment proposer and colleagues at the host facility discuss recognition as coauthor, or other acknowledgment, before beginning an experiment.

Continued meetings will be the basis for effective, high-level interaction and coordination among the neutron user facilities in the United States and Canada. Through formal meetings like this one and informal communications, the facility managers believe they can maximize the scientific return of their facilities while optimizing their use. Sharing information is important, such as coordinating dates of summer schools or other educational programs or timing of facility events. The next meeting will be in Chicago in January 2004.

SEQUOIA

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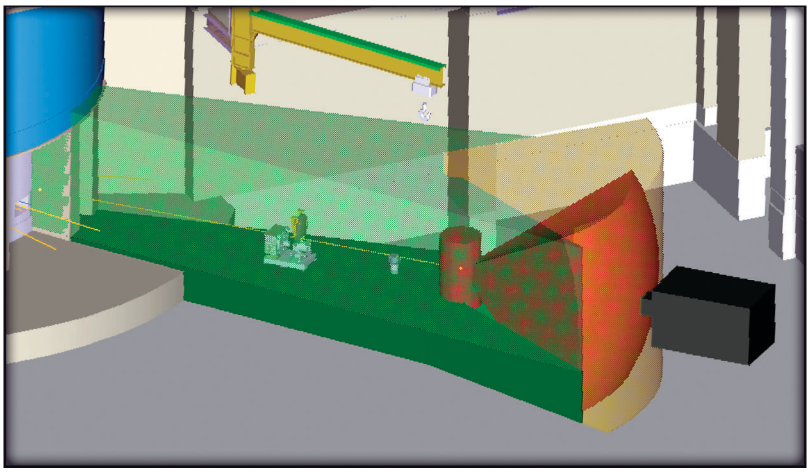
SEQUOIA is a next-generation, direct geometry time-of-flight chopper spectrometer with fine energy transfer and wave-vector resolution and high incident fluxes of 10 meV to 1 eV neutrons. Excellent resolution is achieved using a Fermi chopper, suitable flight paths, and a large, solid-angle detector bank, pixelated in ~0.3° increments covering scattering angles from -30° to 60° in the horizontal and ±30° in the vertical. With these design features, SEQUOIA will enable unprecedented high-resolution, inelastic neutron-scattering studies of magnetic excitations and fluctuations and lattice vibrations over a broad range of energy scales.



SEQUOIA schematic.

SEQUOIA will contribute to a wide cross section of important research areas in condensed matter and materials science. Today, these would include strongly correlated electron systems; high-temperature superconductors; colossal magnetoresistive materials; quantum and molecular magnets, itinerant magnets, and multilayers; alloys; ferroelectric, piezoelectric, and thermoelectric materials; and soft condensed matter. Furthermore, SEQUOIA will be an outstanding tool for investigations of novel systems and materials that are unknown today. The SEQUOIA instrument development team (IDT), led by Steve Nagler of ORNL, is composed of scientists from diverse institutions and includes partners from several universities.

HYSPEC

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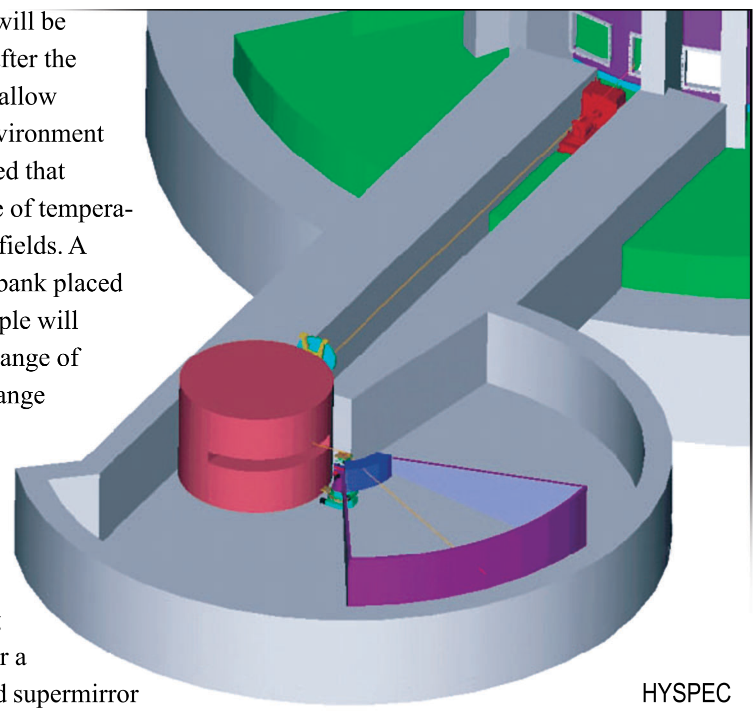
The crystal time-of-flight hybrid spectrometer (HYSPEC) is a unique direct geometry inelastic scattering instrument that has been approved for SNS. It combines time-of-flight spectroscopy with focusing Bragg optics to enhance the flux on small single-crystal samples. It will be located on a beam line looking at a coupled H_2 moderator and will use a 20- to 25-m supermirror guide to transport the neutron beam. A counter-rotating chopper pair will monochromate the beam and determine the neutron burst width. A short distance from the chopper pair, a vertical focusing crystal will be placed in a drum shield that will reduce the beam size of 15(h) × 4 (w) cm^2 to a size of 2(h) × 4(w) cm^2, maximizing the flux at the sample position. Collimators and beam definers will be placed before and after the sample, which will allow standard sample environment equipment to be used that covers a wide range of temperatures and magnetic fields. A moveable detector bank placed 4.5 m from the sample will cover a horizontal range of 60° and a vertical range of ±7.5°. HSYPEC can easily be converted to a polarized beam instrument by using a Heusler crystal for a monochromator and supermirror benders for polarization analysis of the scattered beam. HYSPEC is a moderate resolution instrument optimized for an incident energy range of 5<E_I<60 meV.



HYSPEC schematic.

The HYSPEC IDT is led by Steve Shapiro of Brookhaven National Laboratory.

NOMAD

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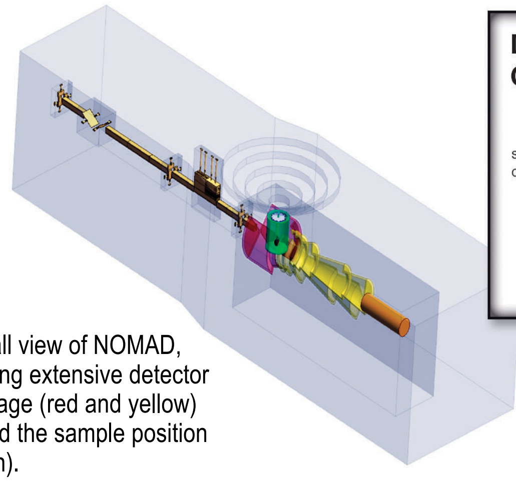
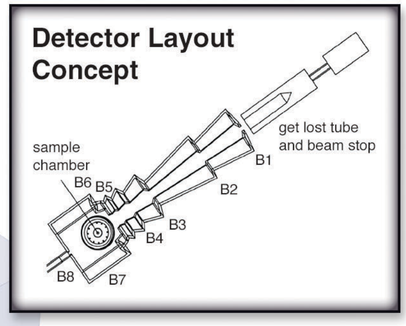
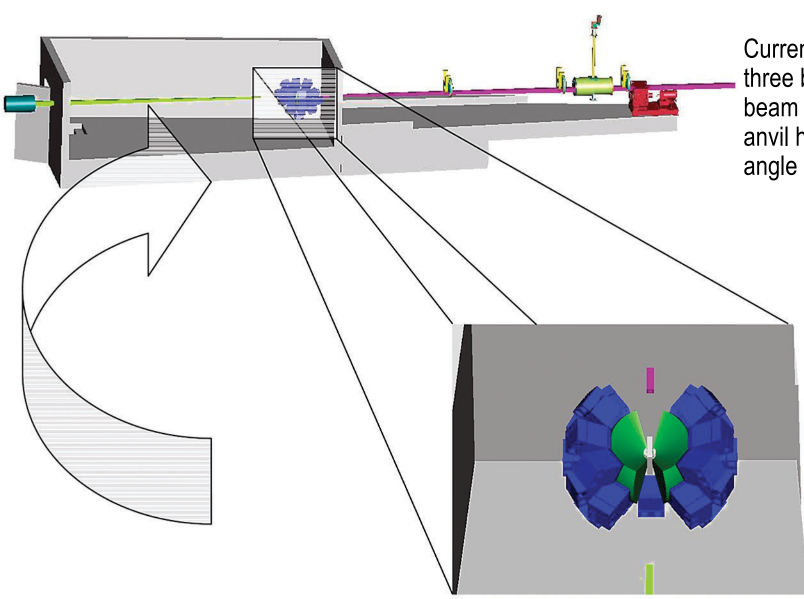
NOMAD is SNS's nanoscale-ordered materials diffractometer. This instrument was conceived to effectively use the world-leading flux of SNS, providing atomic-level structural details for the next generations of soft, crystalline, and hybrid materials. The IDT is led by ORNL's Mike Simonson.



Overall view of NOMAD, showing extensive detector coverage (red and yellow) around the sample position (green).



Knowledge of atomic-level structure in condensed phases provides a window to understanding the atomic and molecular interactions of its components and a sound basis for advancing predictive theoretical descriptions of complex materials. For many soft materials and liquids, structures arising from interatomic and intermolecular interactions can be probed only through detailed investigation of short-range order. Many of these samples have inherently low contrast, placing a premium on high flux, extensive detector coverage, and system stability. Liquid samples can be created at extreme temperatures by laser heating of levitated droplets, and structural studies of these small samples depend on high flux and optimized detector geometry. In glasses, both short-range order and the growth of crystallite phases can be examined with scattering techniques, and observing crystallite growth in real time will be possible. For crystalline materials, combining results over a wide range of scattering vector with pair distribution function analysis gives insight into the local disorder that leads to unique properties in nanoparticles.



Current SNAP components, including the incident flight path of 15 m, three bandwidth choppers, a T_0 chopper, focusing guide system, and beam collimation. The inset shows the integration of the panoramic gem anvil high-pressure cell with the detector array (scattered neutron solid-angle coverage in green).

SNAP

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SNS's ultrahigh pressure neutron diffractometer is known as SNAP (spallation neutrons and pressure) and will allow studies of a variety of powdered and single-crystal samples under extreme conditions of pressure and temperature. The increased neutron flux and timing resolution from the poisoned, decoupled hydrogen moderator, along with the development of large-volume pressure cells using large, synthetic opposed gem anvils, will allow significant advances in the pressure range accessible to high-resolution neutron diffraction. The pressure goal is in the range of 50 to 100 GPa on an ~1-mm^3 sample on a routine basis. In addition, recent advances in next-generation microdetectors (arranged from ~35 to 142° in 2θ and ±34° out of the scattering plane) will allow the incident beam focusing optics, high-pressure device, and detector array to be highly integrated, thus providing a highly flexible facility for materials studies under extreme conditions.

The SNAP IDT is led by John Parise, State University of New York at Stony Brook, and Rus Hemley, Carnegie Institution of Washington (Washington, D.C.).

Neutron Pulse Single-Crystal Diffractometer

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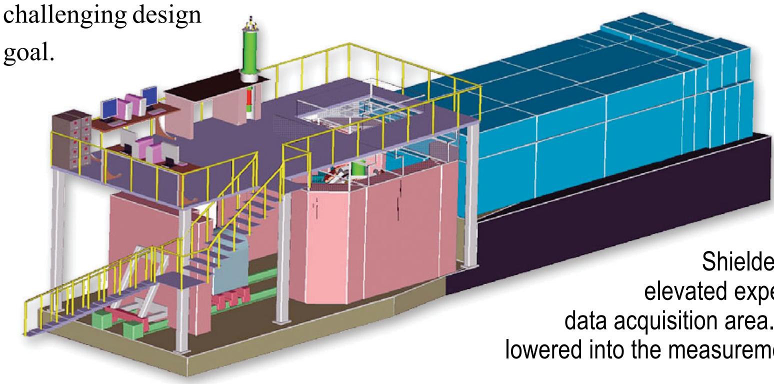
The SNS single-crystal diffractometer (SCD) will be optimized for the rapid measurement of Bragg intensities on materials with moderate-sized unit cells (up to ~50-Å cell repeats). A major goal for the SCD is to be able to study 0.1-mm^3 samples, approaching the size that is routinely used for single-crystal X-ray studies. By greatly expanding the range of materials that can be explored, the SCD will revolutionize single-crystal neutron diffraction as we know it, especially from the viewpoint of the synthetic chemist. To maximize its scientific impact, the instrument design also includes provision for magnetic scattering, using polarized neutron beams, and for diffuse scattering. In addition to the core SCD applications in chemistry, this flexible design should allow for major advantages in studying critical structural problems in biology, earth science, materials science and engineering, and solid-state physics.

The SCD will be located on beam line 12, which views a decoupled, poisoned hydrogen moderator. The instrument will have a relatively short flight path for maximum intensity. A portion of the beam guide assembly upstream, 1 to 2 m from the sample, will be removable for convenient insertion of focusing optics to optimize performance for small crystals. Provision will be made for insertion of a ^{3}He polarizer and a spin flipper in the incident beam. Detector coverage will exceed 50%, on a sphere of 1-m radius, with an opening at the top for insertion of cryostats, furnaces, magnets, etc. The detector spatial resolution should approach 1 mm. A major development effort will be undertaken to identify the most suitable detector technology that will meet this challenging design goal.

In March 2002, a workshop was held at ANL to bring together a broad cross section of the interested single-crystal user community and to assemble the scientific case for the SCD. An IDT was formed, chaired by Robert Bau (University of Southern California). The ranks of IDT members now include more than 50 investigators from around the globe who have expressed interest in new developments in single-crystal diffraction.

In October 2002, the SNS Experimental Facilities Advisory Committee reviewed the scientific case for the SCD and recommended its approval to SNS management. The DOE Office of Science is currently considering the IDT's proposal to fund construction of the instrument.



Shielded SCD showing the elevated experiment staging and data acquisition area. The sample will be lowered into the measurement chamber below.

Pulsed Polarized Neutrons Workshop

A workshop on pulsed polarized neutrons was held in Gaithersburg, Maryland, on February 10, 2003. During two and a half days, 60 attendees from the United States, Europe, and Japan discussed the various technologies and methods that use polarized neutrons. Special focus was placed on those methods that need to be developed to take full advantage of polarized neutrons at an advanced pulsed neutron source such as SNS. The list of discussion topics included neutron polarizers, neutron spin manipulation devices, experimental methods that use the interaction of the neutron spin with a sample of interest, and methods that use the neutron spin to achieve some other goal, such as good energy or angular resolution. Summaries of science that requires polarized neutrons were also presented.

The workshop, sponsored by DOE and the NSF, identified enabling technologies along with concepts for new instruments. Important to developing this technique at neutron facilities in the United States is bringing U.S. researchers up to speed with techniques used overseas. Workshops, short courses, summer schools, overseas postdoctoral and other appointments, and other training mechanisms need to be considered and developed.

At the conclusion of the workshop, assignments were made to help construct a consensus road map for U.S. R&D on polarized neutron methods. The road map will include clearly defined priorities and deliverables, a coherent strategy for achieving R&D goals, a list of researchers who intend to collaborate to achieve the goals, and an analysis that shows how work in the United States will be coordinated with similar efforts in Europe and Japan. The road map is intended to form the basis of a proposal to fund an R&D network that will achieve the goals described in the road map. For additional information on this topic, contact Ian Anderson (andersonian@sns.gov).

Structural Biology Task Force

At the April 2002 Joint Institute for Neutron Science (JINS) workshop on "Using Neutrons to Probe Structure and Dynamics in Biological Systems," Oak Ridge Associated Universities (ORAU) agreed to fund follow-on studies for determining facility needs to enhance understanding of biological materials. A Structural Biology Task Force was formed and met at ANL on October 24, 2002, with three goals. First, advise both SNS and the ORNL Center for Structural Molecular Biology (CSMB) on the scope of equipment needs for support labs and sample preparation areas for biological neutron scattering and the need for specialized sample environments. Second, advise SNS on optimization of funded SNS instruments for biology users. Third, identify potential additional SNS instruments of interest for biological neutron scattering. Chaired by Kent Blasie and Steve White, the task force produced a summary report that forms the basis for future actions.

ORAU is now funding a postdoctoral position to develop the preliminary conceptual design and beam line optimization for a protein crystallography instrument at SNS. A subcommittee of the task force (headed by Joanna Krueger of the University of North Carolina, Charlotte), also funded by ORAU, will specify the lab equipment and sample environment needs in greater detail after identifying the equipment to be available in the CNMS. After these two elements are completed, a decision will be made on how to vest pursue funding.

The task force is a joint venture of ORAU, JINS, SNS, and CSMB. For more information on the task force, contact Kent Blasie (jkblasie@sas.upenn.edu). For information on these workshops, please see www.sns.gov/jins/jins.htm.

Geographical Diversity of Neutron-Scattering Authorship

Each year, neutron-scattering articles are published by authors from many countries. The Institute for Scientific Information (ISI) Web of Science was used to examine the country and U.S. state affiliations of the authors of neutron-scattering articles for 2001-2002. For this two-year period, about 5000 articles were identified that deal with neutron scattering, neutron diffraction, neutron spectroscopy, or neutron reflection. The following lists reflect those countries and U.S. states with more than 100 articles in the past two years. For multiple authors, each country of origin is counted. Almost 60% of the published articles came from one or more of eight European countries, and one or more of the top ten countries were included in 86% of the total articles. A two-year period is used to even out the potential distortions of a one-year period.

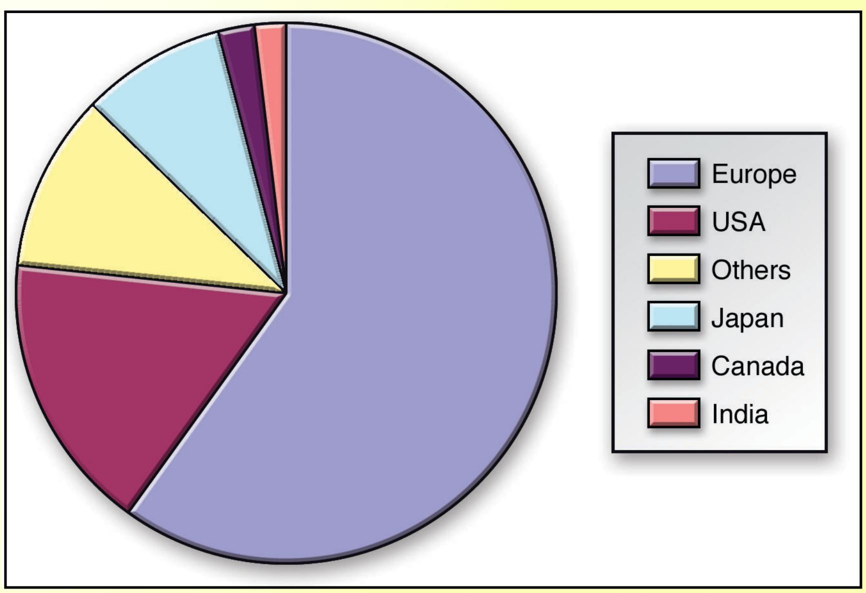
Top Author Affiliations of Neutron-Scattering Articles for 2001-2002

Top Countries

1.	United States	1278
2.	France	1122
3.	Germany	916
4.	Japan	674
5.	England	668
6.	Russia	390
7.	Italy	258
8.	Spain	204
9.	Switzerland	181
10.	Poland	162
11.	Canada	157
12-13.	India & The Netherlands	152
14.	Sweden	132
15-16.	China & Australia	111

Top U.S. States

1.	Maryland	230
2.	Illinois	202
3.	California	191
4.	New York	157
5.	New Mexico	113
6.	Tennessee	112
7.	New Jersey	104



Survey of neutron-scattering publications, 2001-2002.

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Aerial view of the SNS site, April 14, 2003.

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