Serving the Science and Technology Community

The past year has been perhaps the best ever for users at the NCNR, in terms of numbers of participants, and the diversity and quality of their research activities at our facility. Nearly all of the originally envisioned instruments have been operational for several years, and forefront science, as represented by the highlight articles in this report, is being produced at a steady rate. Although it is fair to say that the NCNR has reached a mature state of development, new instruments are still being developed and brought on line. The CNBT reflectometer (AND/R) is being completed during the summer of 2003, and the MACS cold-neutron triple-axis and an upgraded 10 m SANS diffractometer will be made available in the near future.

The User Program

Making the NCNR accessible to a diverse community from academia, government and industry requires continual effort. Efficient proposal handling, fair and thorough review, and timely allocation of instrument time are essential to our user community. For the past year, our proposal process, including proposal review as well as submission, has been entirely Internet-based, resulting in a significant shortening in the time between proposal deadline and beamtime allocation. Despite increased security, physical access to our facility has been significantly delayed in only a handful of cases. User demand has remained very strong, with research participation (see Fig. 1) and the number and quality of proposals at an all-time high.

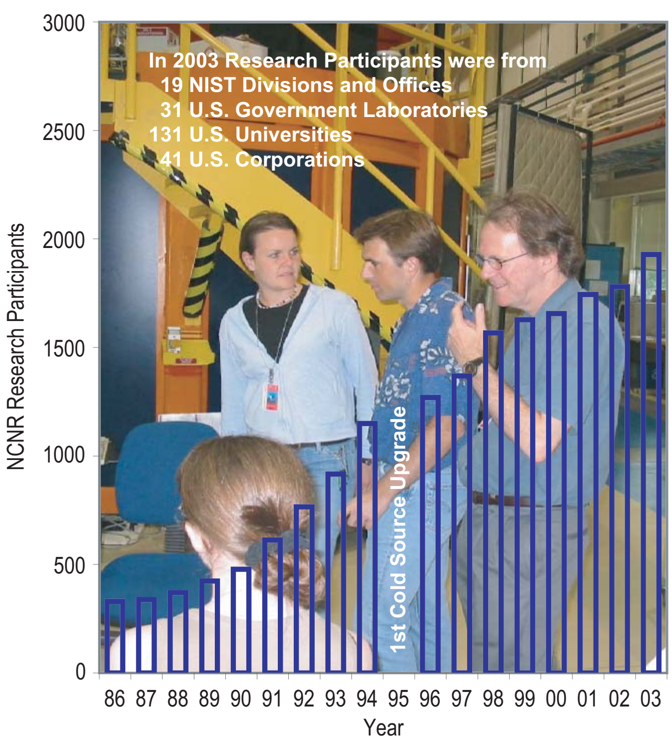

Fig.1. Numbers of NCNR Research Participants over time.

While there are several ways in which users access NCNR instrumentation, the most important is through our formal proposal process. At approximately six-month intervals, users may submit proposals for beam time. After each proposal has received written reviews from external referees, our Program Advisory Committee (PAC) allocates beam time to the best proposals, based on the reviews, their own judgment, and technical input from NCNR staff. Current PAC members include Andrew Allen (NIST Ceramics Division), Robert Briber (Maryland), Michael Crawford (DuPont), Sossina Haile (Cal Tech), Kenneth Herwig (Oak Ridge), Yumi Ijiri (Oberlin), Michael Kent (Sandia), Sanat Kumar (Rensselaer), Robert Leheny (Johns Hopkins), Dieter Schneider (Brookhaven), and John Tranquada (Brookhaven). Over the course of a year, the PAC allocated more than 1100 instrument-days to more than 290 experiments. In doing so, it had to make some difficult choices, since a total of more than 2400 days were requested in more than 380 proposals. The proposal system applies to only about half the instruments at the NCNR, but these are our most advanced ones, supported at a high level by NCNR staff and all our available resources. Although the other instruments are not offered through proposals, most of the time on the latter is also allocated to users through direct collaborations with local staff, or through more formal collaborative research consortia, as detailed below. For example, short- and long-term collaborations account for most of the beam time scheduled on the thermal triple-axis spectrometers.

A New Voice for Users

A separate advisory committee has recently been formed to represent our user community. At monthly conference call meetings, members of the NCNR Users' Committee discuss users issues, sometimes with the participation of NCNR staff and management. The current membership includes Nitash Balsara (UC Berkeley, chair), Collin Broholm (Johns Hopkins), Paul Butler (Oak Ridge), Tonya Kuhl (UC Davis), Robert Leheny (Johns Hopkins) (liaison to the PAC), and Paul Sokol (Penn State). Among recent topics of discussion were software for data analysis, sample environments, the proposal process, and obtaining feedback from users. The committee welcomes comments from users at any time. Please see http://www.ncnr.nist.gov/NCNR_Users_Commitee.html for the members' email addresses.

Center for High Resolution Neutron Scattering

The Center (CHRNS) is a most important component of user participation at our facility. Funded by the National Science Foundation (NSF) and NIST, it offers a suite of instruments unmatched in North America for the investigation of the structure and dynamics of solids by neutron scattering, probing length scales from 1 nm to ≈ 10 µm and energies from ≈ 30 neV to ≈ 100 meV. Most of the proposals we receive ask for time on one of the CHRNS instruments, which include two 30 m SANS diffractometers, a high-resolution USANS diffractometer, a backscattering spectrometer, a neutron spin echo spectrometer, and a cold-neutron triple-axis spectrometer. An upgraded 10 m SANS diffractometer will be included among the CHRNS instruments in the near future.

Cold Neutrons for Biology and Technology

A new instrument for structural biology, the Advanced Neutron Diffractometer/Reflectometer, AND/R, has recently been completed. (See highlight on page 6 of this report.) This instrument and other facilities dedicated to studies of biological membrane systems are part of the Cold Neutrons for Biology and Technology (CNBT) program, funded by the National Institutes of Health (NIH), with contributions from NIST, the University of California at Irvine and the University of Pennsylvania. In addition to the above-mentioned institutions, the CNBT partnership consists of investigators from Johns Hopkins University, Rice, Carnegie Mellon, and Duke University. Other collaborators are from UC San Diego, the Los Alamos National Laboratory, and NIH. Other facilities at NCNR dedicated to CNBT include 10 % of the time on the NG-7 30 m SANS diffractometer, a fully equipped biology laboratory, and a state of the art computer facility for molecular dynamics computations. The combination provides a powerful set of capabilities for U.S. researchers interested in structural biology investigations by neutron scattering.

NOBUGS 2002

A conference on scientific computing at user facilities was hosted by NIST on November 4–6, 2002, addressing both software and hardware issues at neutron and synchrotron x-ray user facilities. The 77 participants represented nearly all the world's major scattering laboratories. The 2002 conference, organized by NCNR staff, was the fourth in the biennial NOBUGS series, providing an opportunity for those involved to compare notes, discuss techniques and results, and establish collaborations in the area of computing and data acquisition infrastructure for research, a field not normally covered by traditional scientific conferences. Among the topics highlighted at NOBUGS 2002 were Data Acquisition and Instrument Control Methods, Data Formats, Data Reduction, Visualization and Analysis, Collaborative Initiatives and Distributed Computing, and Computer Security at User Facilities.

Ninth Annual Summer School

More than 30 students from 23 different institutions traveled to the Gaithersburg, MD campus of the National Institute of Standards and Technology to attend the ninth annual summer school on neutron scattering during the week of June 9–13, 2003. The school was organized by the NCNR and CHRNS with support from the National Science Foundation, and involved students from 18 states and Canada with diverse backgrounds ranging from chemistry, physics, and materials science, to polymer science, nuclear engineering, and biophysics. The summer school alternates every year between the two central themes of diffraction and spectroscopy. This year's school focused on four different dynamical studies using the NCNR's Disk Chopper Spectrometer (DCS), High-Flux Backscattering Spectrometer (HFBS), Neutron Spin Echo (NSE) spectrometer, and Spin Polarized Inelastic Neutron Scattering (SPINS) spectrometer. Most of the students' efforts were directed to hands-on experiments, a direction that we have followed for several years. Course materials about the experiments and underlying principles were made available through our website prior to the school. Small groups of students rotated among the instruments, performing illustrative experiments, and analyzing their data with the aid of our software and the advice of our staff. Among the experiments was the study of the diffusion of surfactant micelles and shape fluctuations of microemulsions using the NSE spectrometer, and quantum rotations in methyl iodide using the HFBS. On the final day, each of the student groups presented the results of their studies to the rest of the school. According to evaluations, the school was highly effective in introducing the students to the various methods and applications of neutron spectroscopy.

Theory, Modeling, and Neutron Scattering

Modern materials research relies heavily on developing models that explain and predict behavior under a variety of conditions. Because of the relatively simple nature of the interaction between neutrons and materials and the wide dynamical and spatial ranges that can be probed, neutron scattering is an important method for testing the validity of these theoretical models. To promote a fruitful exchange between theory and experiment, NCNR's Taner Yildirim, Seung-Hun Lee and Dan Neumann organized a workshop entitled Theory, Modeling and Neutron Scattering co-sponsored by the NCNR and NIST Center for Theoretical and Computational Materials Science. This workshop brought experts from around the world on both theoretical and modeling methods and neutron scattering measurements to the NCNR for a three-day meeting in August 2003. Invited presentations covering a wide range of materials from proteins to nanotubes to magnetic perovskites sparked an intense discussion among the more than 50 attendees on how combining these techniques offers key insights into a remarkable variety of phenomena in materials.

Independent Programs

The Neutron Interactions and Dosimetry Group (Physics Laboratory) provides measurement services, standards, and fundamental research in support of NIST's mission as it relates to neutron technology and neutron physics. The national and industrial interests served include homeland defense, neutron imaging, scientific instrument calibration, nuclear-electric power production, radiation protection, defense nuclear energy systems, radiation therapy, and magnetic resonance imaging. The group's research may be represented as three major activities. The first is Fundamental Neutron Physics including magnetic trapping of ultracold neutrons, operation of a neutron interferometry and optics facility, development of neutron spin filters based on laser polarization of ^{3}He, measurement of the beta decay lifetime of the neutron,

Fig. 2. Daniel Phelan, Souleymane Omar Diallo, Hui Wu and Seth Jonas analyze results of a backscattering spectrometry experiment at the ninth annual Summer School on Neutron Scattering.

and investigations of other coupling constants and symmetries of the weak interaction. This project involves a large number of collaborators from universities and national laboratories. The second is Standard Neutron Fields and Applications using both thermal and fast neutron fields for materials dosimetry in nuclear reactor applications, neutron spectrometry development, and for personnel dosimetry in radiation protection. These neutron fields include thermal neutron beams, "white" and monochromatic cold neutron beams, a thermal-neutron-induced ^{235}U fission neutron field, and ^{252}Cf fission neutron fields, both moderated and unmoderated. The third is Neutron Cross Section Standards, including experimental advancement of the accuracy of such standards, as well as their evaluation, compilation and dissemination.

The **Smithsonian Center for Materials Research and Education's (SCMRE) Nuclear Laboratory for Archeological Research** has chemically analyzed over 26,600 artifacts by INAA at the NCNR over the last 26 years. SCMRE's research programs draw extensively upon the collections of the Smithsonian, as well as those of national and international institutions. The chemical analyses provide a means of linking these diverse collections together to study continuity and change involved in the production of ceramic objects. INAA data are used to determine if groups of ceramics have been made from the same or different raw materials. The ceramics can then be attributed to geographic regions, specific sources, workshops and even individual artists. The ability to use chemical composition to link specific pottery groups to specific production locations through the analysis of less portable fired tiles and bricks has shown that nearly all individual California missions were producing earthenware ceramics for their own use soon after their founding. Moreover, potters at five missions had mastered the technologically demanding process of glazing and were also producing Pb glazed pottery previously thought to have all been imported from Mexico.

The **Nuclear Methods Group** (Analytical Chemistry Division, Chemical Sciences and Technology Laboratory) develops and applies nuclear analytical techniques for the determination of elemental compositions, striving for improvements in accuracy, sensitivity, and selectivity. The group has pioneered the use of cold neutrons as analytical probes in two methods, prompt-gamma activation analysis (PGAA) and neutron depth profiling (NDP). In PGAA, the amount of a particular analyte is measured by detecting characteristic gamma-rays emitted by the sample while it is being irradiated in an intense cold-neutron beam. NDP is another in-beam method that can characterize the concentration of several elements as a function of depth in the first few microns below a surface. It accomplishes this by energy analysis of the charged particles emitted promptly during neutron bombardment. In addition to NDP and PGAA, the group has a high level of capability in two more conventional methods, instrumental and radiochemical neutron activation analysis (INAA and RNAA). In aggregate, the techniques used by the group are a powerful set of complementary tools for addressing analytical problems for both in-house and user programs, and are used to help certify a large number of NIST Standard Reference Materials.

The **Center for Food Safety and Applied Nutrition**, U.S. Food and Drug Administration (FDA), directs and maintains a neutron activation analysis (NAA) facility at the NCNR. This facility provides agency-wide analytical support for special investigations and applications research, complementing other analytical techniques used at FDA with instrumental, neutron-capture prompt-gamma, and radiochemical NAA procedures, radioisotope x-ray fluorescence spectrometry (RXRFS), and low-level gamma-ray detection. This combination of analytical techniques enables diverse multi-element and radiological information to be obtained for foods and related materials. The NAA facility supports agency quality assurance programs by developing in-house reference materials, by characterizing food-related reference materials with NIST and other agencies, and by verifying analyses for FDA's Total Diet Study Program. Other studies include the development of RXRFS methods for screening food ware for the presence of Pb, Cd and other potentially toxic elements, use of instrumental NAA to investigate bromate residues in bread products, use of prompt-gamma NAA to investigate boron nutrition and its relation to bone strength, and the determination of the elemental compositions of dietary supplements.

The **ExxonMobil Research and Engineering Company** is a member of the Participating Research Team (PRT) that operates, maintains, and conducts research at the NG-7 30 m SANS instrument and the NG-5 Neutron Spin Echo Spectrometer. Their mission is to use those instruments, as well as other neutron scattering techniques available to them at NCNR, in activities that complement research at ExxonMobil's main laboratories as well as at its affiliates' laboratories around the world. The aim of these activities is to deepen understanding of the nature of ExxonMobil's products and processes, so as to improve customer service and to improve the return on shareholders' investment. Accordingly, and taking full advantage of the unique properties of neutrons, most of the experiments use SANS or other neutron techniques to study the structure and dynamics of hydrocarbon materials, especially in the fields of polymers, complex fluids, and petroleum mixtures. ExxonMobil regards its participation in the NCNR and collaborations with NIST and other PRT members not only as an excellent investment for the company, but also as a good way to contribute to the scientific health of the nation.

The NCNR provides its resources to a large number of researchers from US universities and colleges, and the latter in turn have provided substantial aid to the construction of NCNR instruments and participation in collaborative research programs. For example, **the Johns Hopkins University** has taken a leading role in the development of the MACS spectrometer, and conducts extensive studies of magnetism and soft condensed matter, involving several faculty members, as well as engineering staff. The **University of Maryland** is likewise heavily involved at the NCNR, maintaining several researchers at our facility. Other institutions that have noteworthy long-term commitments at the NCNR are the **University of Minnesota** (member of the participating research teams, or PRTs, for the NG7 SANS instrument and the NG7 reflectometer). **UC Irvine**, **Johns Hopkins, Penn**, **Rice**, **Duke**, and **Carnegie-Mellon University** are all members of the CNBT collaboration. The **University of Pennsylvania** is also a member of the PRT for the FANS spectrometer.

The **U.S. Army Research Laboratory** has sponsored a scientific program based at the NCNR for three decades. Among its accomplishments are investigations of materials at high pressure, determinations of crystal structure of molecular solids, and the initiation of residual stress measurements at the NCNR.