# Serving the Science and Technology Community

## NCNR Partnership Celebration

This year marks the tenth anniversary of the start of user experiments in the NCNR guide hall. The NCNR has maintained working partnerships with a number of government agencies, industrial laboratories, and academic institutions since it was commissioned over 30 years ago. Several key partnerships are highlighted in this section. A special event celebrating NCNR partnerships and a decade of success was held on August 5, 2002, with a number of distinguished visitors in attendance. The inside cover of this report identifies persons addressing the audience at this celebration. The speakers noted the key role of partnerships in the growth and success of the NCNR and their impact on U.S. neutron science. Many of their comments referred to a recent report from the Office of Science and Technology Policy on the "Status and Needs of Major Neutron Scattering Facilities and Instruments in the United States." This report encourages the formation of partnerships such as those at the NCNR, especially between federal agencies, to promote effective stewardship of large federal research resources. The speeches and a guided tour of the facility for the visitors provided a satisfying perspective on the development of the NCNR into one of the world's leading and most productive neutron scattering facilities.

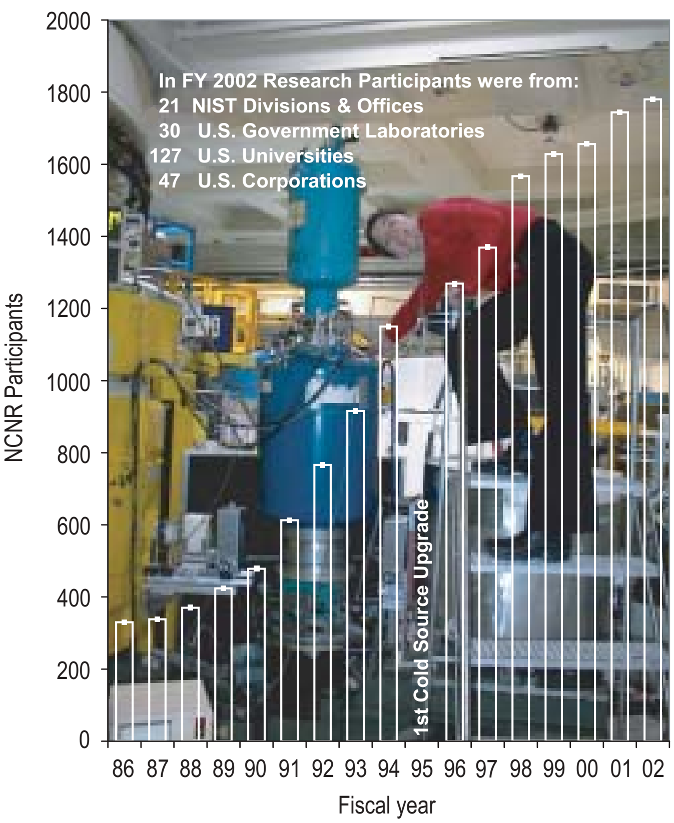


**Fig. 1. Numbers of NCNR Research Participants over time.**

The number of NCNR research participants has more than doubled over the last decade (Fig. 1) and has continued to increase, despite an extended shutdown for the installation of the advanced cold source and new cooling towers. As detailed in the recent OSTP report, the NCNR now accommodates more than half of all neutron users in the US.

## The NCNR User Program

During the past year, we have made a significant shift toward entirely Internet-based proposal submission and review. Users have been sending proposals to us on our Web-page form for more than six years, but now it has become the exclusive method for standard submission of beam time proposals. Local beam time requests from NIST staff are managed through the same system. Peer reviews of proposals are also communicated to us electronically through a Web form, resulting in faster and more efficient decisions on instrument time, to the benefit of users and their research programs.

Two calls for proposals were made in the past year, and more than 390 proposals were received in response. The proposed experiments show increasing activity in research on soft condensed matter and bioscience, although more mature areas such as magnetism and polymer research have held their own. Proposals are now nearly equally divided between those for structural investigations, mainly SANS and reflectometry, and studies of dynamics, requesting one of the newer high-resolution spectrometers in the guide hall.

After a thorough review process by external referees and by the NCNR Program Advisory Committee (PAC), approved proposals were allocated beam time. The PAC is a panel of accomplished scientists with expertise across a broad range of neutron methods and scientific disciplines. It is the body primarily responsible for proposal review and recommending user policies for the NCNR, working closely with the Center's Director and staff. Its current membership includes Sanat Kumar (Rensselaer Polytechnic Institute, chair), Robert M. Briber (University of Maryland), Michael K. Crawford (DuPont), Yumi Ijiri (Oberlin College), Dieter K. Schneider (Brookhaven National Laboratory), Kenneth Herwig (Oak Ridge National Laboratory), Michael Kent (Sandia National Laboratory), Robert Leheny (Johns Hopkins University), John Tranquada (Brookhaven National Laboratory), and Sossina Haile (California Institute of Technology).

## The Center for High Resolution Neutron Scattering

One of the most important partnerships between the NCNR and another agency is with the National Science Foundation (NSF) through its support of the Center for High Resolution Neutron Scattering (CHRNS). Five instruments in the NCNR guide hall, and one in the thermal instrument area, are operated by CHRNS, comprising a crucial component of the user program. The instruments include a 30 m SANS instrument, the SPINS triple-axis spectrometer, the neutron spin-echo spectrometer, the high-flux backscattering spectrometer, the disk-chopper time-of-flight spectrometer, and the ultra-small angle scattering diffractometer. Most of the instrument time allocated by the PAC now goes to experiments carried out on CHRNS instruments. An additional SANS diffractometer on neutron guide NG-1, which up to now has been used primarily for NIST programmatic research, is being upgraded to a more powerful 10 m instrument with a new detector, and will be made available to CHRNS users. In aggregate, the CHRNS instruments provide structural information on a length scale from 1 nm to ≈ 10 µm, and dynamical information on energy scales from ≈ 30 neV to ≈ 100 meV. These are the widest ranges accessible at any neutron research center in North America.

## Collaborations

Direct collaborations on specific experiments remain a common way for users to pursue their ideas using NCNR facilities, accounting for approximately half of the number of instrument-days. The thermal-neutron triple-axis spectrometers are mainly scheduled in this way. Most of the time reserved for NIST on these and all other NCNR instruments is devoted to experiments that are collaborations with non-NIST users. Collaborative research involving external users and NIST scientists often produces results that could be not obtained otherwise.

**Fig. 2. Sanat Kumar, Dieter Schneider, and Rob Briber of the PAC consider proposals for beam time.**

Another mode of access to the NCNR is through more formal research consortia. Groups of researchers from various institutions join forces to build and operate an instrument. Typically, a substantial fraction of the time on the instrument is then reserved for the consortium members, and the remaining time is allocated to general user proposals. For example, a group including ExxonMobil, the University of Minnesota, and NIST cooperates on the NG-7 30 m SANS instrument. Similar arrangements involving other consortia apply for the horizontal-sample reflectometer, the high-resolution powder diffractometer, the filter-analyzer spectrometer, and the neutron spin-echo spectrometer.

## Cold Neutrons for Biology and Technology

An important new partnership with five universities, NIST and the National Institutes of Health is now proceeding with the design and construction of a new reflectometer dedicated to bioscience and biotechnology. The University of California at Irvine leads the consortium whose purpose is to provide a new national resource for investigations in structural biology. Research leaders from Penn State, Rice, Carnegie Mellon, Duke, and the Los Alamos National Laboratory are included in the consortium.

## Independent Programs

There are a number of long standing programs located at the NCNR that involve other parts of NIST, universities, industrial laboratories, or other government agencies.

The **Nuclear Methods Group** (Analytical Chemistry Division, Chemical Science and Technology Laboratory) has as its principal goals the development and application of nuclear analytical techniques for the determination of elemental compositions with greater accuracy, higher sensitivity and better selectivity. A high level of competence has been developed in both instrumental and radiochemical neutron activation analysis (INAA and RNAA). In addition, the group has pioneered the use of cold neutron beams as analytical probes with both prompt gamma activation analysis (PGAA) and neutron depth profiling (NDP). PGAA measures the total amount of a particular analyte present throughout a sample by the analysis of the prompt gamma-rays emitted upon neutron capture. NDP, on the other hand, determines concentrations of several important elements (isotopes) as a function of depth within the first few micrometers of a surface by energy analysis of the prompt charged-particles emitted during neutron bombardment. These techniques (INAA, RNAA, PGAA, and NDP) provide a powerful combination of complementary tools to address a wide variety of analytical problems of great importance in science and technology, and are used to help certify a large number of NIST Standard Reference Materials.

A large part of the group's efforts is directed towards the exploitation of the analytical applications of the guided cold-neutron beams available at the NCNR. The Group's involvement has been to design and construct state-of-the-art cold neutron instruments for both PGAA and NDP and provide facilities and measurements for outside users, while retaining and utilizing our existing expertise in INAA and RNAA.

**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 scientific instrument calibration, electric power production, radiation protection, defense nuclear energy systems, radiation therapy, neutron radiography, 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, 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 utilizing both thermal and fast neutron fields for materials dosimetry in nuclear reactor applications 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 neutron cross section standards, as well as evaluation, compilation and dissemination of these standards.

The **Polymers Division** of the Materials Science and Engineering Laboratory has several program elements at the NCNR covering the technological areas of electronics, multiphase polymeric, and biological materials. The purpose of the electronics materials program is to help the U.S. microelectronics industry address their most pressing materials measurement and standards issues. The structure of nanoporous thin films, used in integrated circuits as low-dielectric-constant insulators, is characterized through a combination of small angle neutron scattering (SANS), x-ray reflectivity, and ion scattering measurements. Advances such as vapor contrast matching techniques provide unique information about critical parameters such as the porosity, average pore size, and wall mass density. In addition, several instruments at NCNR provide unique high-resolution measurements that guide the development and fundamental understanding of next-generation polymeric photoresist materials for sub-100 nm lithography. Measurements include the segmental dynamics of the polymers that govern the mobility of an acid catalyst, direct measurement of the deprotection reaction that leads to patterned areas, and the structural characterization of lithographically prepared structures.

In the multiphase polymeric materials program, the objective is to understand underlying principles of phase behavior, local structure, and flow that control morphology and structure during processing of multiphase materials such as polymer blends and nanocomposites (polymers filled with clay platelets, carbon nanotubes, or triblock copolymer micelles). SANS and reflectivity measurements in equilibrium, in transient conditions, and under external fields, provide essential information for general understanding as well as for specific application of polymer blend/alloy systems. For example, the structure induced by shear alignment of nanoparticle/polymer solutions has been elucidated with SANS, small angle light scattering, and rheological measurements. Customers include material producers and users, ranging from chemical, rubber, tire, and automotive companies, to small molding and compounding companies. The research focus on polymeric materials includes commodity, engineering and specialty plastic resins, elastomers, coatings, adhesives, films, foams, and fibers.

The biological materials initiative is committed to demonstrating the use of inelastic neutron scattering (INS) as a unique measurement tool for understanding the dynamics in several important biological systems. For example, INS has been used to elucidate changes in protein dynamics that occur in the final stages of protein folding. Likewise, INS and low frequency Raman scattering have been developed as measurement tools to identify the dynamical aspects of a good sugar or polyalcohol for protein stabilization and cryopreservation. Effective preservatives must suppress the high frequency motions that are precursors to protein unfolding and denaturation.

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 **U.S. Army Research Laboratory** is the current manager of a 30-year NCNR-Army partnership sponsoring a research team. This group performs materials research and engineering in support of Army needs and missions and works jointly with NIST/NCNR in developing and improving neutron methods and instrumentation. A key contribution of Army researchers at the NCNR is a highly successful neutron facility to map residual stress and texture within large components such as jet turbine blades and structural welds. This resource is critical to development and performance of industrial and transportation systems and military hardware.

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 foodware for the presence of Pb, Cd and other potentially toxic elements, use of instrumental NAA to investigate bromate residues in bread products, and use of prompt-gamma NAA to investigate boron nutrition and its relation to bone strength.

The **Smithsonian Center for Materials Research and Education Nuclear Laboratory for Archeological Research** (SCMRE) has chemically analyzed over 24 000 artifacts by INAA at the NCNR over the last 25 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 then can be attributed to geographic regions, specific sources, workshops and even individual artists. The ability to combine chemical data for semi-complete or whole vessels with that derived from the analysis of materials recovered from recent excavation programs provides many new opportunities for study. Museum vessels that are found to be similar and attributable to some geographic location provide a basis for exploring changing aspects of style, iconography, textual history and even ideology. In an integrative manner, the INAA program enhances the importance of collection materials for the study of the past.

A number of universities have also established long-term programs at the NCNR. The **University of Maryland** is heavily involved in the use of the NCNR, and maintains several researchers at the facility. **Johns Hopkins University** participates in research programs in magnetism, soft condensed-matter physics, bioscience, and in instrument development at the NCNR. The **University of Pennsylvania** is working to help develop biological applications of neutron scattering. It is also participating in the second stage construction of the filter analyzer neutron spectrometer, along with the **University of California at Santa Barbara, DuPont, Hughes, and Allied Signal**. **The University of Minnesota** participates in two PRTs, the NG-7 30 m SANS and the NG-7 reflectometer. The **University of Massachusetts** also participates in the latter PRT.

## Eighth Annual Summer School

With support from the National Science Foundation, NCNR and CHRNS held their annual Summer School on Neutron Scattering from June 3-7, 2002. The subject matter of the school alternates in successive years between techniques designed to investigate structure, and those devoted to spectroscopy and dynamics. The course this year focused on structural studies with SANS and neutron reflectometry (NR). Forty graduate students and postdoctoral fellows from institutions across the US attended the Summer School this year. The format of the meeting in recent years has emphasized hands-on experience with CHRNS instruments. For much of the week, students in small subgroups circulated among various instruments set up to perform illustrative experiments, and analyzed data using NCNR-supplied resources. Among the experiments was a characterization by SANS of the structure of clay platelets dispersed in water. The neutron reflectometry experiments comprised measurements on thin films and multilayer materials. On the final day, the subgroups made presentations on the results of their studies. According to student evaluations, the school was highly effective in introducing them to the principles and practice of structural studies with neutron instruments.

**Fig. 3. Eighth Annual Summer School on Neutron Scattering participants concentrate on neutron reflectometry results under the guiding hand of NCNR's Sushil Satija.**