



An Assessment of the National Institute of Standards and Technology Center for Neutron Research: Fiscal Year 2010

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**AN ASSESSMENT OF THE
NATIONAL INSTITUTE OF STANDARDS
AND TECHNOLOGY
CENTER FOR NEUTRON RESEARCH**

FISCAL YEAR 2010

Panel on Neutron Research

Laboratory Assessments Board

Division on Engineering and Physical Sciences

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PANEL ON NEUTRON RESEARCH

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This report has been reviewed in draft form by individuals chosen for their diverse perspectives and technical expertise, in accordance with procedures approved by the National Research Council's Report Review Committee. The purpose of this independent review is to provide candid and critical comments that will assist the institution in making its published report as sound as possible and to ensure that the report meets institutional standards for objectivity, evidence, and responsiveness to the study charge. The review comments and draft manuscript remain confidential to protect the integrity of the deliberative process. We wish to thank the following individuals for their review of this report:

Ian Anderson, Oak Ridge National Laboratory,
Susan Coppersmith, University of Wisconsin,
Peter Moore, Yale University,
R.G. Hamish Robertson, University of Washington, and
Alton Romig, Jr., Sandia National Laboratories.

Although the reviewers listed above have provided many constructive comments and suggestions, they were not asked to endorse the conclusions or recommendations, nor did they see the final draft of the report before its release. The review of this report was overseen by Alton D. Slay, Warrenton, Virginia. Appointed by the National Research Council, he was responsible for making certain that an independent examination of this report was carried out in accordance with institutional procedures and that all review comments were carefully considered. Responsibility for the final content of this report rests entirely with the authoring panel and the institution.

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Summary

The NIST Center for Neutron Research (NCNR) is a national user facility whose mission is to ensure the availability of neutron-measurement capabilities to meet the needs of U.S. researchers from industry, universities and other academic institutions, and other government agencies. The NCNR continues to provide reliably a high flux of neutrons to an evolving suite of high-quality instruments and sample environments. The array of thermal and cold neutron instruments available at the NCNR enables measurements over a wide range of time, energy, and length scales.

These capabilities of the NCNR play a critical role in advancing science and developing new technologies in the United States, and they enable the National Institute of Standards and Technology (NIST) to fulfill its role of promoting science, standards, and technology. The new instruments and upgrades associated with the planned facility expansion over the next few years will ensure that the NCNR continues to provide users with access to internationally competitive instruments.

As requested by the Director of NIST, the scope of the assessment of the NCNR by the National Research Council's (NRC's) Panel on Neutron Research included the following criteria: (1) the technical merit of the current laboratory programs relative to current state-of-the-art programs worldwide; (2) the adequacy of the laboratory budget, facilities, equipment, and human resources, as they affect the quality of the laboratory's technical programs; and (3) the degree to which the laboratory programs in measurement science, standards, and services achieve their stated objectives and desired impact.

RECOMMENDATIONS

The panel makes the following recommendations with respect to enhancing the effectiveness of the NCNR in the pursuit of its goals.

1. Collaborative partnerships of the NCNR with the Center for Nanoscale Science and Technology (CNST) and the Chemical Science and Technology Laboratory (CSTL) should be further developed to enhance the scientific impact of NCNR activities in the areas of nanotechnology and biological sciences. A joint, senior hire in membrane protein biophysics with CSTL's Biochemical Science Division should be a high priority.
2. As new facilities come online and improvements are made to the existing facilities worldwide, it is imperative that the NCNR carry out continual instrumentation renewal so as to maintain state-of-the-art instruments and neutron-measurement capabilities for U.S. researchers.
3. Along with the new instruments that will become available through the NCNR Expansion Project, the importance of sample environments (rheometry, magnetic fields, humidity, and other variables of importance to an experiment) should not be overlooked. The NCNR should continue its tradition of maintaining an aggressive program for their development.
4. The NCNR, CSTL's Biochemical Science Division, and NIST users—especially in biological sciences—will benefit greatly if a deuteration and

- isotope-labeling facility becomes available. NIST should aggressively pursue this objective.
5. The continued development of robust and user-friendly data-analysis tools will broadly benefit the neutron scattering community and will aid in the growth of this community by enabling non-expert users to utilize neutron scattering techniques. The SASSIE software package, if fully realized, could have an impact similar to that of the small-angle neutron scattering (SANS) analysis program based on the IGOR software tool, developed earlier at the NCNR.
 6. As highlighted by the research productivity and impact of the hard condensed-matter group in high-critical-temperature (T_c) superconductors, the close synergy between theory and experiment can lead to major breakthroughs. Such relationships should continue to be pursued across the NIST organizational units so as to broaden the modeling and theory capabilities accessible to NCNR scientists and users.
 7. With the planned transition from highly enriched uranium (HEU) to low enriched uranium (LEU) fuel, a new deuterium cold source would be beneficial for maintaining the flux at the NCNR to specific instruments. The use of focused beams may also provide an opportunity to broaden the range of experimental capabilities at the NCNR. One potential concern in the future will be the availability of helium-3 (^3He) for detectors and cryogenics.
 8. The NCNR should regularly inform users regarding the Expansion Project. Changes in schedule, planned instruments and modifications, the expected time line for utilization of instruments, and coordination with other facilities will enable users to better mitigate the effects of the facility's shutdown and subsequently enable them to exploit the new capabilities at the NCNR in a timely fashion.
 9. The NCNR has established a system that seems to preserve all safety requirements while keeping the openness and accessibility needed for a user facility. Continuing to maintain a rational security program within the constraints of increasing security demands is critical in order to allow efficient use of the facility, especially as the number of users increases with the Expansion Project.

1

The Charge to the Panel and the Assessment Process

At the request of the National Institute of Standards and Technology, the National Research Council has, since 1959, annually assembled panels of experts from academia, industry, medicine, and other scientific and engineering environments to assess the quality and effectiveness of the NIST measurements and standards laboratories, of which there are now nine,¹ as well as the adequacy of the laboratories' resources. In 2010, NIST requested that five of its laboratories be assessed: the Building and Fire Research Laboratory, the Manufacturing Engineering Laboratory, the Materials Science and Engineering Laboratory, the NIST Center for Neutron Research, and the Physics Laboratory. Each of these was assessed by a separate panel of experts; the findings of the respective panels are summarized in separate reports. This report summarizes the findings of the Panel on Neutron Research.

For the fiscal year (FY) 2010 assessment, NIST requested that the panel consider the following criteria as part of its assessment:

1. The technical merit of the current laboratory programs relative to current state-of-the-art programs worldwide;
2. The adequacy of the laboratory budget, facilities, equipment, and human resources, as they affect the quality of the laboratory's technical programs; and
3. The degree to which laboratory programs in measurement science, standards, and services achieve their stated objectives and desired impact.

The context of this technical assessment is the mission of NIST, which is to promote U.S. innovation and industrial competitiveness by advancing measurement science, standards, and technology in ways that enhance economic security and improve the quality of life. The NIST laboratories conduct research to anticipate future metrology and standards needs, to enable new scientific and technological advances, and to improve and refine existing measurement methods and services.

In order to accomplish the assessment, the NRC assembled a panel of 12 volunteers, whose expertise matches that of the work performed by the NCNR staff.² The panel members visited the NCNR facility at Gaithersburg, Maryland, for 2 days, during which time they attended presentations, tours, demonstrations, and interactive sessions with NCNR staff. The panel members also conducted interactive sessions with NCNR managers and with leaders of NCNR user groups and met in a closed session to deliberate on the panel's findings and to define the contents of this assessment report.

¹ The nine NIST laboratories are the Building and Fire Research Laboratory, the Center for Nanoscale Science and Technology, the Chemical Science and Technology Laboratory, the Electronics and Electrical Engineering Laboratory, the Information Technology Laboratory, the Manufacturing Engineering Laboratory, the Materials Science and Engineering Laboratory, the NIST Center for Neutron Research, and the Physics Laboratory.

² See <http://www.ncnr.nist.gov/> for more information on NCNR programs. Accessed May 1, 2010.

The approach of the panel to the assessment relied on the experience, technical knowledge, and expertise of its members, whose backgrounds were carefully matched to the technical areas of NCNR activities. The panel reviewed selected examples of the technological research covered by the NCNR; because of time constraints, it was not possible to review the NCNR programs and projects exhaustively. The examples reviewed by the panel were selected by the NCNR. The panel's goal was to identify and report salient examples of accomplishments and opportunities for further improvement with respect to the following: the technical merit of the NCNR work, its perceived relevance to NIST's own definition of its mission in support of national priorities, and specific elements of the NCNR's resource infrastructure that are intended to support the technical work. These examples are intended collectively to portray an overall impression of the laboratory, while preserving useful suggestions specific to projects and programs that the panel examined. The assessment is currently scheduled to be repeated annually, which will allow, over time, exposure to the broad spectrum of NCNR activity. The panel applied a largely qualitative rather than a quantitative approach to the assessment, although it is possible that future assessments will be informed by further consideration of various analytical methods that can be applied.

The comments in this report are not intended to address each program within the NCNR exhaustively. Instead, this report identifies key issues. Given the necessarily nonexhaustive nature of the review process, the omission of any particular NCNR program or project should not be interpreted as a negative reflection on the omitted program or project.

2

General Assessment of the NIST Center for Neutron Research

The execution of the overall NIST mission—to promote U.S. innovation and industrial competitiveness by advancing measurement science, standards, and technology in ways that enhance economic security and improve our quality of life—is enabled in important ways by the unique capabilities and facilities of the NIST Center for Neutron Research.

Through its suite of instruments—among the best in the world—for neutron scattering and fundamental neutron science, coupled with a strong staff of scientists and technicians who lead their own research programs and support those of hundreds of users both within and outside of NIST each year, the NCNR has a firm place in advancing the NIST mission. The NCNR continues to succeed admirably in this regard. There are, however, both unprecedented challenges and opportunities currently facing the center.

First, the Expansion Project promises to advance the center’s capabilities significantly in both the quantity and the quality of its instrumentation and in the size and scope of the user community to be served. The project has been carefully planned, and its management appears to be in good hands and on track. However, the timing of its implementation was recently delayed by about a year, owing to a procurement failure. The potentially serious negative impact that might have ensued can become a positive impact: the timely development of a new instrument (the Multi-axis Crystal Spectrometer), which advances the state of the art significantly for inelastic scattering, will have time to “mine” substantial new science before the new, April 2011 start date for the shutdown. There remain challenges associated with the shutdown that would occur regardless of its timing, but these will be easier to address given the additional time resulting from the delay. These challenges include coordinating with other neutron facilities to provide access to current NIST users, thoughtful and careful use of staff resources during the outage, and the building of stronger interactions within NIST and with the soft-matter and biological communities outside of NIST. The NCNR should use the additional time to pursue these opportunities.

Second, an opportunity lies in better utilization of existing expertise and capabilities at NIST to enhance the research productivity and impact of the NCNR, particularly through increased collaborations with NIST’s Center for Nanoscale Science and Technology and Chemical Science and Technology Laboratory. As these centers focus on the nanoscale and the chemical-biological arenas, respectively, they could and should provide additional interfaces for the NCNR to enhance its impact both inside and outside NIST. Similar opportunities might materialize for software and theory more generally.

On the national neutron landscape of today and in the near future, the NCNR is the leading U.S. facility. The Spallation Neutron Source (SNS) and the High Flux Isotope Reactor (HFIR) at the Oak Ridge National Laboratory (ORNL) will begin to compete for this leadership role in 2 to 3 years. However, by 2015 (after the new instruments in the Guide Hall extension will have been commissioned, the spin echo spectrometer will have been upgraded and relocated to the Guide Hall extension, and

other instruments currently under development will have been installed in the original Guide Hall), the NCNR will gain an additional cushion until the SNS Second Target Station instruments come online in 2018. The future enhancements of the Lujan Neutron Scattering Center at the Los Alamos Neutron Science Center (LANSCE), adding roughly two times the capacity and new capability, should be viewed as complementing NCNR's instrumentation strategy. To take one example, the Chromatic Analysis Neutron Diffractometer or Reflectometer (CANDoR) at the NCNR will provide crucial experience with multiwavelength reflectometry below reflectivities of 10^{-8} to complement the inherently multiwavelength time-of-flight instruments at the SNS and LANSCE. The United States will have then a healthy mix (though too few) of horizontal and vertical neutron reflectometers for meeting the needs in biophysics, soft condensed matter, and energy research.

On the international landscape, the general consensus of the panel is that the Institut Laue Langevin (ILL) in France is the leading facility. After the NCNR expansion, if the ILL were to do nothing further to enhance its position, the NCNR could challenge and even overtake the ILL in importance by 2015. The ISIS Spallation Neutron Source in England, with its new second target, will similarly raise the bar, and any further delay in NCNR expansion could shift leadership. However, on present trajectories, the ILL-NCNR-ISIS hierarchy is stable until the SNS and the Japan Proton Accelerator Research Complex are mature in 10 years or so. The Paul Scherrer Institute in Switzerland, Forschungsreaktor München II research reactor in Germany, the Australian Nuclear Science and Technology Organisation (ANSTO), HFIR, the Laboratoire Léon Brillouin (LLB) in France, LANSCE, and others will provide pressure from the next tier, and the NCNR must continually work to maintain its position. In particular, the ANSTO aspires to be number three among reactor sources, and its aggressive operating schedule of 340 days per year, if achieved, will be hard to match. The fact that NCNR management anticipates that the scientific and technical research services funds for the Expansion Project will continue beyond the time line of the project and be used for continual instrumentation renewal is welcome in this regard. In addition, the NCNR should target areas of strength in which it can have leadership despite the existence of higher-flux facilities that exist now or will be coming online in the future.

These impressions of NCNR's position are based on user metrics (numbers of users and user hours per year), number and quality of publications, and innovative instrumentation science, but the facilities comparison is not precise. In carefully considering the first element of its charge, the panel determined that the level of comparison that it used (as described) is sufficient for providing a good indication of the NCNR's position in the broader community. The panel did not think that it should perform an assessment of the capabilities of other facilities, or that a more detailed and exhaustive comparison of additional metrics was necessary. Although a precise comparison of U.S. facilities is challenging, the NCNR is currently in a strong position to carry the North American flag with respect to numbers of users and publications, whereas instrumentation innovation has been pushed mainly by European facilities. This playing field will tilt even more as the European Spallation Source project flourishes over the next 5 years. The U.S. neutron community including the NCNR must invest increasingly more resources in cutting-edge instrumentation to stay even.

Operational reliability is outstanding at the NCNR. On a per flux basis, the NCNR is competitive with the best neutron facilities in the world, considering

publications and “high-impact journal” results. Given the wide scientific footprint of the NCNR, a broadening of the definition for “high-impact journals” would be appropriate, and this could help quantify metrics more precisely. Competitor sources in the Department of Energy broadly acknowledge NCNR’s lead in user numbers, and European Union sources graciously salute NCNR’s high-impact publications. Demographically, the NCNR—like all scattering facilities—exhibits a regional impact distribution and, given the intellectual richness of the eastern seaboard, this regionality is a considerable strength.

The NCNR instrument suite is well matched to future needs in materials and low-energy nuclear research. In particular, the facility management is anticipating a shift toward energy materials research; the NCNR should monitor national directions in this area, including materials for nuclear power, to ensure that the suite of instruments continues to evolve to meet national needs.

3

Science and Technology at the Center

Cutting-edge scientific research is conducted at the NCNR in diverse areas of condensed-matter science: hard and soft condensed-matter physics, including biological physics, chemistry, and biology. The number of participants continues to increase, representing 142 universities, 32 government organizations and national laboratories, and 46 U.S. corporations; national laboratory and university researchers comprise 80 percent of the participants. The proposal pressure continues to be high, as does the quality as well as the number and impact of the publications. Overall, the metrics of assessment in the areas of research conducted during the past year, publication quality, and impact continue to be impressive.

Continuous improvements in the resolution and sensitivity of measurement techniques—combined with increasingly effective integration of theoretical analysis of data—and the availability of functional sample environments (rheometry, magnetic fields, humidity) are essential for state-of-the-art studies of the structure and properties of condensed matter. The problems investigated by NCNR researchers during the past year are diverse, covering both fundamental and applied topics. They include the following: materials for batteries, solar cells, fuel cells, hydrogen storage, magnetocaloric materials, polymer nanocomposites, drug delivery, properties of magnetic nanoparticles, structure and dynamics of lipid bilayers, superconductors, metals, and electronic ceramics. Publications resulting from research performed at the NCNR appear most frequently in four journals, *Physical Review B*, *Physical Review Letters*, *Macromolecules*, and *Langmuir*, covering hard and soft condensed matter. It is anticipated that, with the increasing emphasis on biology, the publications in more biologically relevant journals will reflect this new trend.

The research described in the oral and poster presentations for the panel is at the forefront, reflecting the output of highly competent researchers. The following sections discuss the assessment of the research reviewed in these areas: (1) soft matter—synthetic polymer systems and biological systems; (2) hard matter (energy, magnetic properties); (3) engineering (structural materials); (4) chemical physics; (5) earth science; and (6) fundamental physics.

SOFT MATTER

Synthetic Polymers

The soft-matter research conducted at the NCNR in the area of polymers is at the leading edge, covering diverse areas of structure, dynamics, and functionality, particularly in the area of energy, including research on fuel cells and solar cells. NCNR researchers effectively exploited the strengths of the facilities by carefully identifying and investigating problems for which the use of neutrons was necessary and critical. In some cases, neutron scattering provided information that was otherwise difficult, or impossible, to ascertain. In other cases, the information gained using neutrons provided

complementary information, thereby providing important new insight into the properties of complex systems.

In an example involving a commonly studied organic solar cell, a thin-film blend of poly(3-hexylthiophene) (P3HT) and phenyl-C61-butyric acid methyl ester (PCBM), neutron reflectometry was used to determine the distribution of PCBM in the film, thereby providing insight into the efficiency of these materials. The depth distribution of PCBM had not been determined before these studies were conducted. With regard to polymer thin films, neutrons are uniquely suited for understanding the interactions between chains grafted to a substrate and free chains in a melt, or solution. The role of molecular weight and the degree of interpenetration between the brush layer and free chains, and the connection to dynamics illustrated by these studies are new and previously not predicted or anticipated. An understanding of these so-called brush-brush interactions is central to the understanding of interactions in a range of systems, including colloidal suspensions and brush coated nanoparticles in polymer nanocomposites. Information gained from the neutron measurements of the structure of hydrogels, formed using triblock copolymers, combined with information from other structural probes, provided important new insight into the structure of these complex nanostructured, technologically important materials. Neutron scattering thus far has proven to be one of the single most important probes toward understanding the structure and dynamics of polymer nanocomposites (PNCs). The uses of PNCs range from structural, to biomedical, to sensors and organic electronics. The primary challenges are associated with understanding and controlling the structure of these materials. Combinations of SANS, ultra-small angle neutron scattering (USANS), and inelastic neutron scattering (INS)/quasielastic neutron scattering (QENS) are able to discern much of the short-range and long-range structure and relaxations of these technologically important materials. This was illustrated rather well by the work conducted by the NCNR over the past year and by high-quality publications from the facility in this area.

Biological Systems

Previous NRC assessment reports have encouraged the NCNR to place a greater emphasis on addressing questions of interest in contemporary biological science. Recommendations have included the employment of direct hires to enhance the NCNR staff, the development of new partnerships—for example, a joint hire with NIST's Chemical Science and Technology Laboratory (now CSTL's Biochemical Science Division [BSD])—and better utilization of the large research enterprise of the National Institutes of Health, located near the NCNR facility.

The NCNR has demonstrated a significant increase in efforts over those of previous years to address questions of biological significance. For example, the chief of the BSD discussed the application of SANS and neutron-reflectivity measurements and NCNR expertise in these areas in tackling biological problems of relevance to the BSD and its mission of the advancement of measurement science in biomolecular structure. In addition, a joint proposal by the NCNR and the BSD to support a deuteration and isotope-labeling facility was submitted. Although the proposal is not yet funded, the impact of such a facility for biological studies would greatly benefit not only BSD and NCNR scientists but the broad array of potential NCNR researchers who could better utilize

neutron scattering techniques given this capability—especially to investigate biomolecular structure and dynamics.

Such collaborative projects between the NCNR and the BSD are expected to be facilitated by a joint position focused on membrane protein biophysics (a focus area for the advancement of measurement science in biomolecular structure) that is currently being advertised. The expectation is that the primary focus of the person hired would be neutron scattering. A strong candidate has been identified, but a firm hire has not been made. As this joint hire has been “on the books” for more than 2 years, the renewed vigor in the pursuit of a mid- to senior-career research leader for the position is encouraging.

Finally, complementary techniques available at the BSD and the Center for Advanced Research in Biotechnology—for example, nuclear magnetic resonance, x-ray crystallography, and synthesis capabilities—could also be better leveraged to advance biological research at the NCNR by staff and external users.

The soft-matter group is to be commended for a number of developments over the past year. First, the SASSIE software package has the potential to greatly facilitate the analysis of SANS (as well as small-angle x-ray scattering [SAXS], reflectometry, and electron microscopy) measurements of protein structure. The arduous tasks of data analysis and the determination of a physically realistic structure have stymied such measurements previously. A user-friendly and robust analysis package, if fully realized, will have a significant, broad impact and likely lead to a much more vigorous utilization of SANS by the biological community.

Second, NCNR scientists have developed a routine method for fabricating cushioned biological membranes. Indeed, the NCNR reported that this new platform can be viewed as a readily available sample environment for any user of the facility. Again, such enabling capabilities are a necessity for meeting the needs of nontraditional neutron scattering users and for demonstrating the greater emphasis that the NCNR is making to reach out to the broad biological research community.

HARD MATTER

The hard-matter group has established important leadership in studies of high- T_c superconductors. Here the close synergy between theory and experiment has led to major breakthroughs during the past year, in particular in the advances made in the pnictide superconductors. The calculations show that the magnetism of iron is key to understanding the superconductivity in these new materials. The work has included important high-pressure studies in which transitions were found experimentally (i.e., within the range of techniques available at the NCNR) and in excellent agreement with theory. These studies show the importance of maintaining a strong program of sample environments in hard-matter experiments. Recent papers, with their extraordinary number of citations, represent one of the great success stories of the past year. The close interactions between theory and experiment demonstrated by this group serve as a model for other groups and programs within the NCNR.

Hard-matter studies also include high-quality measurements on ferroelectrics. Like the oxide superconductor studies, these experiments take advantage of the important role of neutrons for diffraction studies of oxides, particularly as a function of temperature, in which cases detailed studies of ferroelectric transitions can be carried out.

Recent measurements on single crystals are providing important new insight into the origin of the very high dielectric response of lead zirconate titanate (PZT). The work is important for the NIST mission and could lead to the development and application of new classes of transducer materials for data memory, medical devices, sonar, and energy storage.

Another strength of the NCNR has been in neutron scattering investigations of the structures and dynamics of hydrogen-rich materials. The hard-matter group has exploited this strength over the years to explore the incorporation of hydrogen in various solids, most recently in the development of new hydrogen-storage materials, as a function of pressure and temperature. This work has also benefited strongly from a close association between theory and experiment, most recently for graphene-based materials.

ENGINEERING (STRUCTURAL MATERIALS)

The study of texture development in metals is a good example of the use of NCNR capabilities for tackling industrial challenges important for the NIST mission, in this case for the automobile industry's need for light, high-strength vehicles. The work involves the development of new approaches for inverting stresses from strains in polycrystalline metals. The effort could take advantage of important advances that have been made for texture development with submicron and nanoscale diffraction x-ray imaging techniques.

CHEMICAL PHYSICS

A number of important problems of technological importance were studied under the topic of chemical physics. The research spanned areas of ion transport and mobility in materials for energy storage, water dynamics under hydrophobic confinement, and hydrogen storage. Achieving an understanding the interaction of hydrogen with different chemical entities poses major scientific and technological challenges. The research on hydrogen interactions with coordinated metals (specifically, metal-organic frameworks) combines first-principles calculations with inelastic scattering to learn about the short-range structure and dynamics. These studies take advantage of the unique strengths of inelastic neutron scattering. The work on ion transport in polyelectrolytes was interesting; the information gleaned from neutrons provided information about the short-range structure and dynamics, which was essential and could not have been otherwise obtained.

EARTH SCIENCE

Earth and environmental science applications of NCNR capabilities include a study of the interface between bedrock and soils using SANS and USANS. This study made good use of NCNR capability for addressing nanoscale heterogeneity in complex materials, in this case for understanding the transitional regime between soils and bedrock. The use of focusing optics described below (see the section entitled "Other Comments and Broader Issues") would open up capabilities for a broader range of earth science problems (such as measurements on earth materials at high pressures and temperatures, and examination of polyphase assemblages—that is, rocks and geological

fluids). Only one earth science article was published in the 2009 NCNR annual report,³ which describes accomplishments for 2009. Applications in earth, environmental, and planetary science could be a growth area for the future.

FUNDAMENTAL PHYSICS

NCNR's continuing support of basic physics experiments is laudable. The aCORN—"a CORelation in Neutron decay"—experiment to measure the electron-antineutrino correlation in neutron beta decay probes the nature of the electroweak force at the most elementary level. This is a compelling example of using the unique capabilities of the NCNR to make a significant improvement in a fundamental measurement. This work also complements experiments done at other facilities to test the limits of the Standard Model of fundamental particles and interactions. The NCNR is encouraged to support this and other similar experiments.

OTHER COMMENTS AND BROADER ISSUES

The large beam and low flux relative to spallation neutron sources preclude certain types of measurements at the NCNR. Fiber focusing methods are being used to focus beams to increase flux on samples. This approach is being used, for example, on the prompt-gamma neutron activation analysis (PGNAA) experiments. There have also been important developments in other neutron focusing methods. For example, Kirkpatrick-Baez mirrors that can focus beams to below 100 microns have been developed at the ORNL. These could be built and used at the NCNR, opening up a broad range of new experimental capabilities for measurements on small length scales—for example, for heterogeneous materials, and properties of samples that are necessarily small, as well as samples in extreme environments of pressure, temperature, and magnetic or electric fields. Other important developments in techniques allow larger samples to be studied under extreme environments, thereby increasing the range of opportunities for scattering studies using the flux available at the NCNR. The NCNR should remain aware of these methods and remain positioned to serve a growing user community in extreme environments.

Neutron and x-ray scattering are complementary techniques. Thus, having an x-ray program in-house based on conventional x-ray (for example, rotating anodes) forms an essential component of the support laboratory for sample characterization at the NCNR. NIST scientists in general and NCNR scientists in particular could benefit from greater involvement in advanced synchrotron sources. In fact, competing facilities in Europe benefit from having both neutron and synchrotron sources on the same site (the ISIS Spallation Neutron Source and Diamond Light Source in England, the ILL and the European Synchrotron Radiation Facility in France), whereas the United States no longer has this capability. However, new opportunities are becoming available in the United States with the creation of new x-ray sources, most notably the future National Synchrotron Light Source (NSLS-II) at the Brookhaven National Laboratory. NIST could

³ National Institute of Standards and Technology, *2009 NIST Center for Neutron Research Accomplishments and Opportunities*, NIST Special Publication 1105, December 2009. Available at <http://www.ncnr.nist.gov/AnnualReport/>. Accessed August 2010.

take advantage of these developments by being a part of, or in fact by leading, the construction of NIST-managed beam lines (e.g., for biology, hard matter, imaging, etc.).

The recent report on crystal growth from the National Research Council made strong recommendations for investments in single-crystal growth in this country because of its importance for technological advances.⁴ The United States was once a leader in this area but now lags behind numerous other countries (notably in Asia). NIST could be an ideal place to develop this effort. If the effort were embraced as a part of the NIST mission, the NCNR would be very well positioned to take advantage of such renewed focus by providing a crucial tool for the characterization of new single-crystal materials, as demonstrated by the recent work on PZT.

Finally, the plans of the NCNR for the development of new techniques, improvements in resolution, and data collection will place the NCNR in a highly competitive position worldwide. Future instruments to be added include very small angle neutron scattering (vSANS), the new CANDoR, and the Materials Diffractometer. With the addition of new instruments and improved capabilities, the number of users will undoubtedly increase. Moreover, the scope, diversity, and intellectual depth of problems that users can examine within the broad and diverse field of condensed-matter science will improve considerably.

⁴ National Research Council, *Frontiers in Crystalline Matter: From Discovery to Technology*, Washington, D.C.: The National Academies Press, 2009.

4

Facilities and Resources

The NIST Center for Neutron Research continues to operate its facilities effectively in the service of the research community. The Reactor Operations and Engineering Group has achieved an exemplary performance reliability factor of greater than 98 percent on days scheduled for operation. The NCNR's number of instrument operating days (3,741) in 2009 led the neutron facilities in the United States by a wide margin while supporting the research of more than 2,250 NCNR participants.

The NCNR is to be congratulated for receiving a new operating license from the Nuclear Regulatory Commission. There were no reportable occurrences in 2009. Continued diligence to ensure safe, reliable operations is essential to supporting the research community. Updating the NCNR Final Safety Analysis Report annually is a commendable best practice. Regular external safety assessments by the NCNR Safety Assessment Committee (SAC) are important, and the NCNR should carefully consider SAC recommendations.

At the NCNR, total staffing is 209 (not including about 50 staff from Physics, Chemistry, and Health Physics), broken down among three groups—in Reactor Operations and Engineering there are 46 staff members; in Research Facility Operations, 54; and in Neutron Condensed Matter Science, 85—and the NCNR Center Office, which has 24 staff members. Additional postdoctoral appointments were made over the past year, allowing the science group staffing to grow from 79 to 85. The reactor now has a full complement of 20 operators, whose presence and services will be required even during the shutdown. In contrast to earlier years, operations and facilities staffing levels are viewed by management as being satisfactory and also well aligned with the needs of the Expansion Project. Three new instrument scientists and 6 mechanical engineers have been hired in the past year. To oversee the work during the expansion, a project management office has been established with 2 new hires who have expertise in civil construction and instrument development. The Expansion Project schedule is very intense and can be expected to take all the time of the operations and facilities staff during the shutdown period. The year's delay referred to above will provide additional time for a well-coordinated effort during the aforementioned shutdown. The management is encouraged to maintain scientific productivity during the shutdown by not calling more than necessary on the science staff, particularly the postdoctoral members and earlier-career personnel.

The total NCNR budget for FY 2009 was \$42.7 million, and the budget for FY 2010 is estimated to be \$39.8 million. The NCNR budget appears to be adequate. The NCNR is aggressively taking advantage of funding from the American Recovery and Reinvestment Act of 2009 (ARRA; Public Law 111-5) and the America COMPETES Act of 2007⁵ to upgrade its infrastructure and improve the scientific capabilities of its instruments. These changes should resolve two areas of concern for facility maintenance: repairing the thermal shield and replacing the safety shim arms. The new instruments

⁵ The America Creating Opportunities to Meaningfully Promote Excellence in Technology, Education, and Science Act of 2007 (Public Law 110-69).

should expand the cold neutron measurement capacity of the NCNR by 30 percent while significantly advancing the research potential of the facility.

The long shutdown for the Expansion Project beginning in April 2011 must be planned for very carefully. Several separate installations must be staged during this shutdown. The delay caused by the procurement of the Secondary Cooling Pump Building is an example of what can go wrong in a complex project. There is a significant opportunity cost to having a major research facility suspend operations for an extended period. It is important to the user community that something unexpected does not prolong the shutdown beyond what is scheduled, and the NCNR staff should make every effort to minimize this possibility. The strategy of having all procured equipment in hand prior to beginning the shutdown seems prudent. It is important to keep the user community informed of the status of the Expansion Project as the plans evolve. Information flow has been limited.

The future availability of ^3He is uncertain. This issue is not unique to the NCNR; it is a concern of the whole neutron community. Potentially, it could severely compromise important areas of research, especially quantum fluids and cryogenics. In neutron detection where there are alternative choices, NCNR's strategy to partner is appropriate. To mitigate risk to future instruments, the NCNR should consider expanding its program to develop alternative detector techniques.

Planning is ongoing to convert the reactor from highly enriched uranium fuel to low enriched uranium fuel when a fuel has been developed and approved by the Nuclear Regulatory Commission for operation. The Department of Energy projects that fuel will be available in time for the conversion of reactors regulated by the Nuclear Regulatory Commission starting in 2015. It appears that this can be accomplished without disrupting operations or degrading the performance of the NCNR facility. Users should be informed in a timely fashion if there are changes in operation and performance. With the transition from HEU to LEU fuel, a new deuterium cold source would be beneficial for maintaining the flux at the NCNR to specific instruments. The use of focused beams may also provide an opportunity to broaden the range of experimental capabilities at the NCNR.

5

The Center as a User Facility

The NIST Center for Neutron Research is a national facility whose mission is to ensure the availability of neutron-measurement capabilities to meet the needs of U.S. researchers from industry, university, and other government agencies. By providing a wide array of thermal and cold neutron instruments, as well as a broad range of sample environments and complementary analytical instruments, the NCNR enables measurements that help advance science and develop new technologies in the United States. Thus, the NCNR plays a key role in NIST's mission to promote science, standards, and technology. New instruments and the planned upgrades to instruments that are part of the facility expansion will ensure that the NCNR remains competitive on the international stage.

The NCNR user community continues to flourish. The most recent call for proposals resulted in more than 380 proposals, requesting 2,240 instrument days of beam time and corresponding to an average instrument oversubscription of 2.3. (The comparable numbers in 2008 were 321 proposals requesting 1,820 instruments days corresponding to an average oversubscription of 2.0.) In 2009, the number of distinct NCNR research participants was approximately 2,200, with about 800 users coming to the NCNR (comparable to 2008 levels). With an average of approximately 50 users per instrument, productivity at the facility continues to be on par with European sources. U.S.-based participants included 67 percent from universities, 13 percent from other national laboratories, 9 percent from NIST outside the NCNR—including scientists from the Physics Laboratory, the Chemical Science and Technology Laboratory, and CSTL's Polymers Division—and 5 percent from industry. With two-thirds of the beam time available for the user program and one-third reserved for internal use, the NCNR is meeting the needs of external users while continuing to attract and retain outstanding scientists. The flexibility inherent in unallocated time enhances the ability of NCNR scientists to bring in new users, provide rapid access for high-impact science, and work more effectively with industry by means of collaborative access. In addition to the peer-review process, industrial access is also fostered through participating research teams including, for example, the NCNR's neutron imaging facility that has led (through an ongoing partnership between NIST and General Motors) to a better understanding of water management in membrane-based fuel cells. Finally, progress is good on efforts to develop an industry-university-government consortium centered on the new 10-meter SANS instrument that will be part of the expanded instrument suite in the new Guide Hall. For visitors to the NCNR, the addition of the new office building in the summer of 2010 will significantly improve the availability of user office space as well as laboratory space for sample preparation and complementary analytical methods.

The NCNR User Group (NUG) acts as a conduit to management regarding user concerns, and executive committee members of the NUG hold bimonthly telephone meetings with NIST staff. One key function of the committee is to poll users regarding their satisfaction with respect to the NCNR. The most recent survey was conducted in 2007 and included responses from students and postdoctoral researchers, staff members,

and external principal investigators. In the 2007 survey, users rated the training, facilities, and instruments very highly and the performance of NCNR personnel as excellent. Users' concerns included the need for availability of specialized sample environments, easy access to data (on the Web, for example) after leaving the facility, the availability of software and associated tutorials for data analysis, and the compatibility of data formats among different facilities. The NUG is currently working to develop a questionnaire to poll users on their perceptions regarding the proposal review process. One concern expressed in advance of the new poll is the availability of an adequate number of informed reviewers as the number of proposals continues to rise—especially after the expansion is complete.

Despite the steady increase in proposal numbers, the beam-time allocation process at the NCNR is well run. Proposals are submitted on the Web and reviewed by from three to five external reviewers as well as by members of the appropriate Beam Time Allocation Committee (BTAC). Members of the BTAC, appointed by the NCNR, are all external to the NCNR and serve for nominal terms of 3 years. The regular rotation of BTAC members is encouraged so as to maintain fresh perspectives and to reduce the burden on individual scientists.

The National Science Foundation-supported Center for High Resolution Neutron Science program, renewed for an additional 5 years in the fall of 2009, continues to play a critical role in the success of the NCNR. This program provides direct support for instrument scientists associated with a subset of neutron scattering instruments. It also supports a wide variety of educational and outreach activities, including the summer schools on neutron scattering techniques, the Summer Undergraduate Research Fellowships program, and remote learning opportunities for SANS. The program is an outstanding example of collaborative activity among government agencies, and it contributes significantly to developing the next generation of scientists and engineers conversant in neutron scattering.

Although security is an ongoing issue, NIST and the NCNR are working hard to maintain an appropriate security program that preserves the efficient use of the facility. Access to the NCNR is facilitated by the Users' Office, with a staff of two. Foreign visitors must apply for access 35 days before arriving at the NCNR, which is on par with or better than the time requirements for visits to other national facilities. The system seems to preserve all safety requirements while keeping the spirit needed in a center of learning. Safety training at the NCNR remains thorough. The ability to train prior to arriving at the facility is helpful to streamlining the process.

6

Conclusions

The NIST Center for Neutron Research is a national user facility whose mission is to ensure the availability of neutron-measurement capabilities to meet the needs of U.S. researchers from industry, academia, and government agencies. Developing the next generation of neutron scattering scientists and engineers is also a vital part of the NCNR's program.

The NCNR continues to provide reliably a high flux of neutrons to an evolving suite of high-quality instruments and sample environments. The array of thermal and cold neutron instruments available at the NCNR enables measurements over a wide range of time, energy, and length scales.

These capabilities of the NCNR play a critical role in advancing science and developing new technologies in the United States and enable NIST to fulfill its role of promoting science, standards, and technology. The new instruments and upgrades associated with the planned facility expansion will ensure that the NCNR continues to provide users with access to internationally competitive instruments.