

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

FISCAL YEAR 2011

Panel on Neutron Research

Laboratory Assessments Board

Division on Engineering and Physical Sciences

NATIONAL RESEARCH COUNCIL
OF THE NATIONAL ACADEMIES

THE NATIONAL ACADEMIES PRESS
Washington, D.C.
www.nap.edu

THE NATIONAL ACADEMIES PRESS 500 Fifth Street, N.W. Washington, DC 20001

NOTICE: The project that is the subject of this report was approved by the Governing Board of the National Research Council, whose members are drawn from the councils of the National Academy of Sciences, the National Academy of Engineering, and the Institute of Medicine. The members of the panel responsible for the report were chosen for their special competences and with regard for appropriate balance.

This study was supported by Contract No. SB134106Z0011, TO #10, between the National Academy of Sciences and the National Institute of Standards and Technology, an agency of the U.S. Department of Commerce. Any opinions, findings, conclusions, or recommendations expressed in this publication are those of the authors and do not necessarily reflect the views of the agency that provided support for the project.

International Standard Book Number-13: 978-0-309-22012-5

International Standard Book Number-10: 0-309-22012-2

Copies of this report are available from

Laboratory Assessments Board
Division on Engineering and Physical Sciences
National Research Council
500 Fifth Street, N.W.
Washington, DC 20001

Additional copies of this report are available from the National Academies Press, 500 Fifth Street, N.W., Lockbox 285, Washington, DC 20055; (800) 624-6242 or (202) 334-3313 (in the Washington metropolitan area); Internet, <http://www.nap.edu>.

Copyright 2011 by the National Academy of Sciences. All rights reserved.

Printed in the United States of America

THE NATIONAL ACADEMIES

Advisers to the Nation on Science, Engineering, and Medicine

The **National Academy of Sciences** is a private, nonprofit, self-perpetuating society of distinguished scholars engaged in scientific and engineering research, dedicated to the furtherance of science and technology and to their use for the general welfare. Upon the authority of the charter granted to it by the Congress in 1863, the Academy has a mandate that requires it to advise the federal government on scientific and technical matters. Dr. Ralph J. Cicerone is president of the National Academy of Sciences.

The **National Academy of Engineering** was established in 1964, under the charter of the National Academy of Sciences, as a parallel organization of outstanding engineers. It is autonomous in its administration and in the selection of its members, sharing with the National Academy of Sciences the responsibility for advising the federal government. The National Academy of Engineering also sponsors engineering programs aimed at meeting national needs, encourages education and research, and recognizes the superior achievements of engineers. Dr. Charles M. Vest is president of the National Academy of Engineering.

The **Institute of Medicine** was established in 1970 by the National Academy of Sciences to secure the services of eminent members of appropriate professions in the examination of policy matters pertaining to the health of the public. The Institute acts under the responsibility given to the National Academy of Sciences by its congressional charter to be an adviser to the federal government and, upon its own initiative, to identify issues of medical care, research, and education. Dr. Harvey V. Fineberg is president of the Institute of Medicine.

The **National Research Council** was organized by the National Academy of Sciences in 1916 to associate the broad community of science and technology with the Academy's purposes of furthering knowledge and advising the federal government. Functioning in accordance with general policies determined by the Academy, the Council has become the principal operating agency of both the National Academy of Sciences and the National Academy of Engineering in providing services to the government, the public, and the scientific and engineering communities. The Council is administered jointly by both Academies and the Institute of Medicine. Dr. Ralph J. Cicerone and Dr. Charles M. Vest are chair and vice chair, respectively, of the National Research Council.

www.national-academies.org

PANEL ON NEUTRON RESEARCH

TONYA L. KUHL, University of California, Davis, *Chair*
MEIGAN ARONSON, Stony Brook University and Brookhaven National Laboratory
FRANK S. BATES, University of Minnesota, Minneapolis
DONALD M. ENGELMAN, Yale University
PAUL A. FLEURY, Yale University
CHRISTOPHER R. GOULD, North Carolina State University
PETER F. GREEN, University of Michigan
ALAN J. HURD, Los Alamos National Laboratory
JAMES R. LEE, Sandia National Laboratories
JOHN B. PARISE, Stony Brook University and Brookhaven National Laboratory
SUNIL K. SINHA, University of California, San Diego

Staff

JAMES P. MCGEE, Director
CY BUTNER, Senior Program Officer
LIZA HAMILTON, Administrative Coordinator
EVA LABRE, Program Associate

Acknowledgment of Reviewers

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 S. Anderson, Oak Ridge National Laboratory,
Susan N. Coppersmith, University of Wisconsin,
V. Adrian Parsegian, University of Massachusetts-Amherst,
R.G. Hamish Robertson, University of Washington, and
Alton D. Romig, Jr., Lockheed Martin Aeronautics Company.

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.

Contents

SUMMARY	1
1 THE CHARGE TO THE PANEL AND THE ASSESSMENT PROCESS	5
2 GENERAL ASSESSMENT OF THE NIST CENTER FOR NEUTRON RESEARCH	7
3 SCIENCE AND TECHNOLOGY AT THE CENTER	12
4 FACILITIES AND HUMAN RESOURCES	19
5 THE CENTER AS A USER FACILITY	21
6 CONCLUSIONS	24

Summary

The National Institute of Standards and Technology (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 safely and reliably to provide a high flux of neutrons to an evolving suite of high-quality instruments and sample environments. The current array of thermal- and cold-neutron instruments at the NCNR enables measurements over a wide range of timescales, energy scales, and length scales. Over the next few years, the cold-neutron capabilities at the NCNR will be increased by more than 25 percent through the center's Expansion Project. The enhancements associated with this project include the recent completion of a new building for technical services and administration, expansion of the guide hall, the installation of a new cold source, and the acquisition of new instruments, as well as improvements to some existing instruments.

The facilities and measurement capabilities at 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.

As requested by the Director of NIST, the scope of the assessment of the NCNR by the National Research Council's Panel on Neutron Research included the following: (1) the degree to which NCNR programs in measurement science, standards, and services achieve their stated objectives and fulfill the mission of the organizational unit (the NCNR); (2) the technical merits and scientific caliber of the current NCNR programs relative to comparable programs worldwide; and (3) the alignment between NCNR research and development efforts and those services and other mission-critical deliverables for which the NCNR is responsible. With the Expansion Project well underway, the report also contains the panel's more retrospective review of the NCNR in order to provide a benchmark for comparison as the facility goes through a major upgrade.

KEY FINDINGS AND RECOMMENDATIONS

The panel presents the following key findings and major recommendations from its 2011 assessment of the NCNR.

1. A signature feature of the NCNR is a culture and environment that promotes respect for science, user education and training, and internal leadership development.
2. The NCNR has been and continues to be a leading facility in cold-neutron research. The Expansion Project will significantly improve the capabilities of the facility. Continued support to upgrade instruments and develop the next generation of state-of-the-art instruments should enable the NCNR to remain among the best user facilities for neutron research in the world.

3. The NCNR has also developed and retained instrument scientists and research personnel with, in many cases, considerable scientific reputations. The continued scientific excellence of the NCNR scientific staff is critical for maintaining the quality and impact of neutron-scattering science by the facility and its users and for developing new measurement techniques and applications.

RECOMMENDATION 1: The NCNR management should continue to take care that the next generation of senior researchers continues to develop and remain excited about their research and that they are not overly burdened with administrative and other duties that are not characterized as research.

4. The NCNR has consistently operated safely, efficiently, and reliably. The NCNR has maintained a safe and secure facility while serving the needs of a robust neutron-scattering community through an open-call, merit-based proposal process.
5. Partnerships with universities and other agencies have strengthened the scientific impact and capabilities of the NCNR. For example, the Center for High Resolution Neutron Scattering (CHRNS) represents a long-standing partnership between the NCNR and the National Science Foundation. It provides funds for scientific staff to support users on the CHRNS instruments; instrument development such as the multi-angle crystal spectrometer (MACS), a best-of-its-kind, high-flux spectrometer allowing ultrahigh-sensitivity access to dynamic correlations in condensed matter on length scales from 0.1 nm to 50 nm and energy scales from 0.05 meV to 20 meV; and outreach activities to educate and serve the neutron-scattering community. Flexible partnerships with universities have enabled the NCNR to carry out leading-edge research and advance the application of neutron-scattering techniques.
6. The Expansion Project is moving ahead well within the expected range of uncertainties. Given the historically exceptional reliability and performance of the NCNR, a timely and successful restart of the facility is expected by the research community after the period of outage needed to complete the Expansion Project. The maintaining of direct control of the project by the Director of the NCNR should enable rapid response to and mitigation of potential challenges for a timely restart.
7. Discretionary time on the NCNR instruments is used for calibration measurements, instrument development, and projects conducted by NIST researchers, but it is also very important for the following purposes: (1) bringing new users into the facility and introducing them to neutron-scattering techniques in general, (2) providing flexibility and rapid access for cutting-edge science, and (3) developing and retaining excellent instrument scientists and personnel at the facility.

RECOMMENDATION 2: Discretionary time on NCNR instruments should be maintained.

8. The maintenance of existing university partnerships and the development of new partnerships should continue to enhance the ability of the NCNR to advance neutron-measurement techniques and their application to science and engineering problems.
9. The NCNR has best-in-class instruments and capabilities in the area of soft condensed matter. A focus area in neutron-scattering measurements of membrane proteins has been significantly enhanced over previous years through collaborative partnerships involving the NCNR and other NIST laboratories and external collaborators, such as the Biomolecular Labeling Laboratory (involving the University of Maryland and the NIST Biochemical Science Division of the Material Measurement Laboratory); a joint hire of a research scientist with the Material Measurement Laboratory; and a proposal developed jointly by the Institute for Bioscience and Biotechnology Research (a collaborative institute involving NIST and the University of Maryland), JILA (located in Boulder, Colorado), and NCNR staff in this area. Continued emphasis and effort to ensure a successful realization of this partnership should greatly strengthen the capabilities and impact of biological work at the NCNR as well as tap into a high-growth community. The focus on membranes and membrane proteins is a reasonable approach, given the number of individuals currently spearheading this effort.
10. Synergies between the NCNR and the Polymer Division of the NIST Material Measurement Laboratory have historically led to highly productive science.

RECOMMENDATION 3: Collaborative efforts with the NIST Material Measurement Laboratory and the Physical Measurement Laboratory should be maintained to aid the NCNR in extending its leadership in cold-neutron research. Future partnerships with the NIST Center for Nanoscale Science and Technology should be explored to strengthen the capabilities and impact of the NCNR.

11. Funding of the ion mobility spectrometer (IMS) proposal to develop scintillation detectors could lead to a significant improvement in detector capabilities and help to mitigate concerns regarding the future availability of ^3He for detectors.
12. Currently, the Beam Time Allocation Committee is working well.

RECOMMENDATION 4: Care should be taken to ensure that the proposal review process continues to work effectively as the NCNR facility expands.

13. There is only one vendor for the fuel used in the NCNR reactor, and costs, which are increasing every year, will be substantially higher with the conversion to low enriched uranium. Additional operational funds will be required for the facility to maintain its high level of operating days and productivity.

14. 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 completion of the Expansion Project.
15. The development of software for facile structural biology analysis by the general user community is likely to have significant impact and will aid in promoting the conduct of neutron-scattering measurements by nontraditional users in the life sciences. Two personnel are being hired, using funds provided under the American Recovery and Reinvestment Act of 2009 (Public Law 111-5), for the further development and refinement of the SASSIE analysis software (which is used to create atomistic models of molecular systems and also to compare scattering data from these models directly to experimental data), although these hires are for only 1 and 2 years for the respective tasks. Continuing support in this area can ensure the completion of a robust analysis package for users as well as enhanced modeling and analysis capabilities in the future. For example, similar capability to include known chemistry, physics, and structural information in order to analyze scattering data from magnetic materials would be extremely helpful not only for the analysis of scattering data but also for the design of pertinent experiments.
16. The development of facilities for the growth of large single crystals suitable for neutron-scattering experiments would remove a considerable hindrance to further advancement in many areas of condensed-matter science. The addition of this capacity would be an important service to the materials community.
17. The NCNR continues to develop novel ancillary sample environments and equipment, developed in part by users, such as the development of the novel shear cell with the University of Delaware, the development of the humidity cell for membrane studies with Carnegie Mellon University, and advances in ^3He polarization capabilities. Such capabilities add to the attractiveness of the NCNR as a facility for carrying out unique studies with a convenience not yet found in other facilities.

RECOMMENDATION 5: The development at the NCNR of novel ancillary sample environments and equipment should be continued.

The Charge to the Panel and the Assessment Process

At the request of the National Institute of Standards and Technology (NIST), the National Research Council (NRC) 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 six,¹ as well as the alignment of the laboratories' activities with their missions. NIST requested that three of its laboratories be assessed in 2011: the Center for Nanoscale Science and Technology (CNST), the NIST Center for Neutron Research (NCNR), and the Information Technology 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) 2011 assessment, NIST requested that the panel focus on the following criteria as part of its assessment:

1. Assess the degree to which laboratory programs in measurement science, standards, and services achieve their stated objectives and fulfill the mission of the operating unit (laboratory);
2. Assess the technical merits and scientific caliber of the current laboratory programs relative to comparable programs worldwide; and
3. Assess the alignment between laboratory research and development (R&D) efforts and those services and other mission-critical deliverables for which the laboratory is responsible.

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 11 volunteers whose expertise matches that of the work performed by the NCNR staff.² The panel members visited the NCNR facility at Gaithersburg, Maryland, on March 14-16, 2011, for 2.5 days, during which time they attended presentations, a tour, a poster session, and interactive sessions with NCNR staff. The panel members also conducted interactive sessions with NCNR managers and with leaders of NCNR user groups and

¹ The six NIST laboratories are the Material Measurement Laboratory, the Physical Measurement Laboratory, the Engineering Laboratory, the Information Technology Laboratory, the Center for Nanoscale Science and Technology, and the NIST Center for Neutron Research.

² See <http://www.ncnr.nist.gov/> for more information on NCNR programs. Accessed June 14, 2011.

met in closed sessions to deliberate on the panel's findings and to define the contents of this assessment report.

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 degree to which the NCNR programs achieve their stated objectives and fulfill the NCNR mission, the technical merit and scientific caliber of the NCNR work, and the alignment between NCNR R&D efforts and NCNR services and other mission-critical deliverables. 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 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.

For its assessment, the panel relied primarily on presentations made by NIST and NCNR managers and staff and by other researchers associated with NIST projects and programs, and on informational notes prepared by NIST and NCNR staff for use by the panel. Posters by various researchers involved with NCNR activities were also presented to the panel during its visit to the NCNR. This report does not contain extensive citations of technical articles and reports. Other documents and resources used by the panel are cited in the report, as appropriate.

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 non-exhaustive 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.

The preceding Summary highlights major issues that apply to the center as a whole and presents the panel's key findings and recommendations for the NCNR. Chapter 2 presents a more detailed overall assessment of the NCNR, including a comparison of the center with other neutron research centers. Chapter 3 provides an assessment of the scientific and technological research conducted at the NCNR. Chapter 4 discusses the adequacy of the facilities and human resources that support the center, and Chapter 5 discusses the center's role as a user facility. The panel's general conclusions are presented in Chapter 6.

General Assessment of the NIST Center for Neutron Research

The timing of this review of the NIST Center for Neutron Research coincided with a time of considerable change for the U.S. neutron community: namely, the coming online of the Spallation Neutron Source (SNS) at the Oak Ridge National Laboratory (ORNL) and the approaching 10.5-month shutdown of the NCNR facility for upgrades and the installation of a new guide hall and new instruments. It is, therefore, an appropriate time to put in perspective the role that the NCNR has played in the field of neutron-scattering science in the United States and to discuss the NCNR facility in comparison with other leading neutron sources worldwide.

ROLE OF THE CENTER IN THE NEUTRON-SCATTERING COMMUNITY

For the past decade, the NCNR can claim to have been the flagship of American neutron-scattering facilities, and it ranked high among all international facilities in neutron scattering. In fact, after the Institut Laue-Langevin (ILL) in France, which is the largest neutron facility in the world (as measured by the number of beam lines and staff), the NCNR is, by almost all measures, the next most productive and effective scientific neutron facility in the world. This is borne out by statistics measuring its performance according to several criteria: number of instruments; number of operating days per year (with a 20-year average of 233 days per year and a record 267 full-power operating days in 2010); number of participants per year; number of publications per year; an enviable safety record;³ a staffing level of 4 or 5 scientists, technicians, and engineers per instrument (acknowledged worldwide as the desirable and required staffing level); and a high level of user satisfaction as shown by surveys of users.

The facility, which was originally a research reactor meant at the time to serve the needs of NIST and industry, grew in the 1980s, with the addition of a cold-neutron guide hall, into a true national user facility, driven by the vision of its scientist-managers. Their hands-on and effective management helped to develop the spirit of dedication, efficiency, and scientific excellence that persists to this day. These qualities enabled the NCNR (along with the Intense Pulsed Neutron Source, or IPNS, at the Argonne National Laboratory) to maintain U.S. competitiveness in the field during the long “neutron drought” at Department of Energy (DOE) sources in the 1980s and 1990s. That drought resulted from the shutdown of the High Flux Beam Reactor (HFBR), the long periods of shutdown at the High Flux Isotope Reactor (HFIR) at the ORNL, and, during that period, the erratic performance of the Lujan Neutron Scattering Center at the Los Alamos Neutron Science Center (LANSCE) facility. (The IPNS itself was shut down in 2005.)

It also opened up an era in which industrial firms including Exxon, DuPont, and others, together with various universities, were able to operate Participating Research Teams at the Cold Neutron Research Facility (CNRf, the original name for the NCNR)

³ National Institute of Standards and Technology, *The NIST Center for Neutron Research: 2010 Accomplishments and Opportunities*, NIST Special Publication 1110, December 2010. Available at http://www.ncnr.nist.gov/AnnualReport/FY2010/AR_2010_large.pdf. Accessed June 14, 2011.

and to use neutron scattering as one of their R&D tools. The presence of several experienced and renowned scientists on the staff of the CNRF who were willing to work closely with these users and to help them with their problems was crucial to the success of this effort.

Industrial involvement at the NCNR, which has continued to the present day, and the involvement of the Polymers Division at NIST—which brought in industrial consortia made up of groups such as Sematech and Exxon that use small angle scattering, neutron reflectivity, and powder diffraction, and which, in partnership with General Motors, has used the Neutron Imaging Facility for imaging hydrogenous matter in large components—help the NCNR to fulfill its role of being a resource for industry. Thus, over the past decade (and longer), the NCNR has amply carried out its role as a scientific and technical resource for U.S. industry and the U.S. scientific community. In this context, gauging the scientific impact of the NCNR facility by comparing the citations to published scientific work done at the NCNR to those of other facilities would be one means to quantify the role of the facility on the world stage.

The management philosophy, scientific tradition, and user satisfaction continue to be a focus of the facility. Personnel development and strategic promotion from within the NCNR have enabled this culture to continue. It is also gratifying to see that a respected retired NCNR director is still actively involved in the technical design of the new cold source and that several of the excellent and experienced retired scientists at the NCNR still take part in the scientific life and activities at the center.

The plans for the upgrade appear to be well thought out and are being implemented satisfactorily. The designs for new instruments such as the very small angle neutron scattering (vSANS) spectrometer, the chromatic analysis neutron diffractometer or reflectometer (CANDoR), and the new materials diffractometer are imaginative and sound, and it is hoped that the required increase in staffing will not be disrupted by the uncertain fiscal plans of the U.S. government.

The planned 10.5-month shutdown of the NCNR and decrease of neutron-scattering capabilities in the United States will adversely affect the neutron-scattering community, particularly university users whose research grants and students' dissertations depend on current programs at the NCNR. It is hoped that NIST management and scientists will help facilitate for their current users alternative arrangements at the HFIR, LANSCE, and SNS. After the NCNR restarts with its suite of new instruments—it is hoped, as scheduled in September 2012—it is expected that the NCNR will continue to be one of the world's leading neutron facilities and will provide to the U.S. neutron community a resource comparable to the SNS. The maintaining of direct control of the Expansion Project and restart by the Director of the NCNR should enable rapid response to and mitigation of potential challenges for a timely restart.

COMPARISON OF THE CENTER WITH OTHER USER FACILITIES

The comparison between reactor sources and continuous and pulsed spallation sources is technically complicated by different power and neutron flux issues, since continuous and pulsed flux optimize different experiments. Utilization metrics including “users” are complicated by non-uniform definitions throughout the neutron community and therefore are excluded from the comparison of the NCNR and other user facilities. Similarly, oversubscription is not compared because user-requested time is not under

facility control. (Oversubscription is the number of days requested by users divided by the total number of days available.)

The NCNR oversubscription rates by beam line are in a healthy range, averaging 2.2 over the facility, indicative of a robust and vibrant user community. To provide a means to evaluate the NCNR relative to other comparable user facilities and to allow for a straightforward and direct comparison, the average number of beam days that a user team requires in order to develop a publication was considered here. In most cases, a 2010 figure, if available, is reported for each metric shown in Table 1. In order to provide comparable data for sources undergoing change, a consistency check was performed to determine whether the 2010 figure was representative of a 5-year average. Thus, for example, the ISIS publications in 2010 (209) were considered representative in spite of the low 2009 (108) figure, which may have been depressed by the outage that occurred in order to bring up the second-target station; 2010 SNS and HFIR metrics were also estimated. When publication lists were available, conference proceedings were removed from counts; otherwise, publications numbers from the facilities were used directly. The definition of “high-impact publications” as specified by the respective facilities was accepted; otherwise the “Vettier List” was used—namely, *Nature*, *Science*, *Proceedings of the National Academy of Sciences (PNAS)*, *Physical Review Letters (PRL)*, *Physical Review E (PRE)*, *Physical Review B (PRB)*, *Journal of Molecular Biology (JMB)*, and *Journal of the American Chemical Society (JACS)*. (The high-impact fraction was found to be consistent with a 2004 report by Christian Vettier for 19 neutron facilities.⁴)

On the international scene, the clearest point of comparison is with the Institut Laue-Langevin, a reactor source of comparable power and flux to that of the NCNR. ILL is the consensus gold standard for neutron-scattering and neutron science user programs. With $n = 47$ instruments operating and $d = 200$ days of operation per year, ILL produces over $p = 630$ (585 for its 5-year average) publications per year and claims $h = 12$ to 16 percent high-impact papers. The NCNR currently has 22 instruments operating about 250 days per year (~233 days, 20-year average), 325 publications per year, and approximately 11 percent high-impact papers. Productivity $P = nd/p$, the average beam time required to produce a refereed publication, is 18 instrument days for NCNR, comparable to 14 instrument days at ILL. The productivity P depends on source, instrument, and user service factors.

The ILL is at or near the top in budget and staffing for reactor sources. In 2010, the overall ILL staffing of 489, which includes an in-house theory group, is supported by a facility budget of 88.5 million euros, or \$124 million. By comparison, the NCNR fields 134 core full-time-equivalent (FTE) staff members with a budget of \$46 million; the larger NCNR staffing is 260 FTEs (including staff deployed from other NIST laboratories).

⁴ See Robert M. Briber, Henry Glyde (Chair), and Sunil K. Sinha, *Access to Major International X-Ray and Neutron Scattering Facilities*, Committee on International Scientific Affairs of the American Physical Society, April 30, 2009. Available at http://www.aps.org/programs/international/resources/upload/Facilities_Access_All_2009.pdf. Accessed August 15, 2011.

TABLE 1 Comparison of the NCNR with Other Representative Neutron Facilities

	ILL	NCNR	HFIR	ANSTO	Lujan	SNS	ISIS TS1 +muons	ISIS TS2	ISIS Total
<i>n</i>									
instruments	45	22	7.5 ^a	9	11	7.5 ^a	28	13	41
<i>d</i> days	200	267	168	340	125	177	201	179	194
<i>p</i> papers									
2010	630	325	66 ^b	89	109	53 ^b	209	50	259
<i>h</i> % high impact	12%	11%	45%	11%	12%	45%	11%	—	—
<i>nd/p</i>	14.3	17.9	18.9 ^c	34.4	12.6	25.0 ^c	26.9	46.5	30.7
Type	reactor	reactor	reactor	reactor	spallation	spallation	spallation	spallation	spallation
MW	60	20	85	20	0.1	1.0	0.3	0.1	0.4

NOTES: ILL, Institut Laue-Langevin; NCNR, NIST Center for Neutron Research; HFIR, High Flux Isotope Reactor at the Oak Ridge National Laboratory; ANSTO, Australian Nuclear Science and Technology Organisation; Lujan, Lujan Neutron Scattering Center at the Los Alamos Neutron Science Center (LANSCE); SNS, Spallation Neutron Source at the Oak Ridge National Laboratory; ISIS TS1 +muons, ISIS Spallation Neutron Source in England; ISIS TS2, ISIS Spallation Neutron Source in England; *n*, number of instruments; *d*, days of operation per year; *p*, number of publications in 2010; *h*, percentage of high-impact publications; *nd/p*, measure of facility output = number of instruments x number of days ÷ number of papers; type, type of neutron source; MW, megawatts.

SOURCES:

- ILL: *ILL Annual Report*, Available at http://www.ill.eu/fileadmin/users_files/Annual_Report/AR-10/index.htm. Accessed June 30, 2011.
- NCNR: National Institute of Standards and Technology, *The NIST Center for Neutron Research: 2010 Accomplishments and Opportunities*, NIST Special Publication 1110, December 2010. Available at http://www.ncnr.nist.gov/AnnualReport/FY2010/AR_2010_large.pdf. Accessed June 30, 2011.
- HFIR and SNS: Allen Ekkebus, Oak Ridge National Laboratory; and Oak Ridge National Laboratory, *ORNL Neutron Sciences, Neutron Review*, ORNL/TM-2011/88, April 2011. Available at <http://neutrons.ornl.gov/media/pubs/pdf/2010neutronreview.pdf>. Accessed June 30, 2011.
- ANSTO: *ANSTO Annual Report 2009-2010*, September 2011. Available at http://www.ansto.gov.au/_data/assets/pdf_file/0006/48912/AR_2010_online.pdf. Accessed June 30, 2011.
- Lujan: for LANSCE, 2010 publications were obtained from ISI Web and Google Scholar.
- ISIS: *ISIS 2010*, September 2010. Available at <http://www.isis.stfc.ac.uk/about-isis/annual-report/2010/isis-annual-review-201011462.pdf>. Accessed June 30, 2011.

^aInstruments available to general users:

- SNS: 7.5 available throughout 2010 (8 instruments *fully* available in general user call for one cycle and 7 for the other); 12 instruments on the floor
- HFIR: 7.5 available throughout 2010 (8 instruments *fully* available in general user call for one cycle and 7 for the other); 9 instruments on the floor

^bPapers are only those involving research performed on or describing SNS or HFIR instruments. Publications involving all HFIR and SNS resources, including staff using other techniques and facilities and irradiation and accelerator activities, number 156 for HFIR and 250 for SNS.

^cPublications in 2010 result from experiments performed in 2008 and 2009 while the SNS and HFIR were constructing and commissioning many new instruments and ramping beam days. Therefore, the number of instrument days per publication metric, "*nd/p*," is an overestimate using the 2010 data.

A straightforward measure of user service is the level of beam-line staffing. The NCNR fields approximately 5 FTEs per instrument; ILL claims to field 7 FTEs.⁵ The NCNR is competitive with the best facilities in the world in user support. Thus, the NCNR program is currently about 50 percent of ILL in size and scope from instruments to staff. In this context, the NCNR productivity metric is excellent.

⁵ Colin Carlisle, Director of the ESS Scandinavia Secretariat Lund, personal communication to the panel, March 23, 2011.

Science and Technology at the Center

Research conducted at the NIST Center for Neutron Research continues to be highly collaborative, and the facility continues to attract a diverse cross section of users from academia, national laboratories, and industry in the United States and from Europe. Whereas academic and national laboratory researchers comprise 67 and 13 percent of the participants, respectively, industrial researchers currently account for only 5 percent. Plans are being developed and implemented to increase the number of industrial participants. The formation of the nSoft consortium to involve industry in using neutron scattering in the area of soft materials is an attempt to formalize and continue collaborations with industry, and it is hoped that it will result in successful collaborations. A workshop on industrial uses of neutron scattering is being planned for industrial scientists. This is an excellent idea, with the laudable goal of improving industrial participation.

Partnerships with universities and other agencies have strengthened the scientific impact and capabilities of the NCNR. For example, the Center for High Resolution Neutron Scattering (CHRNS) represents a long-standing partnership between the NCNR and the National Science Foundation. It provides funds for scientific staff to support users on the CHRNS instruments; instrument development such as the multi-angle crystal spectrometer (MACS), a best-of-its-kind, high-flux spectrometer allowing ultrahigh-sensitivity access to dynamic correlations in condensed matter on length scales from 0.1 nm to 50 nm and energy scales from 0.05 meV to 20 meV; and outreach activities to educate and serve the neutron-scattering community. Flexible partnerships with universities have enabled the NCNR to carry out leading-edge research and advance the application of neutron-scattering techniques. The maintenance of existing university partnerships and the development of new partnerships should continue to enhance the ability of the NCNR to advance neutron-measurement techniques and their application to science and engineering problems.

One of the primary reasons that the NCNR continues to be one of the best places in the world for performing neutron experiments is the quality of the research staff and the availability of state-of-the-art instrumentation for measuring the structure and dynamics of diverse materials systems. The capabilities and continuous improvement of the instruments, which currently enable measurement of the structure and dynamics over a wide range of length scales (0.01 nm to 10 microns) and timescales (0.01 picoseconds to 100 nanoseconds), respectively, make the NCNR facility competitive on the world stage. The instruments continue to be oversubscribed, as evidenced by the proposal pressure, which is between two and three proposals offered for each one accepted. The research continues to be at the forefront, covering a number of areas of soft and hard condensed-matter science, as well as measurement science. These areas include structural biology (particularly membranes and vesicles), neutron radioactive decay experiments, ferroelectricity, dynamics of complex fluids, high critical-temperature (T_c) materials, and magnetism. The highest level of proposal oversubscription and the most

publications currently arise from experiments utilizing small angle neutron scattering (SANS) and powder diffractometry.

An important metric of performance is the number and quality of publications annually and the percentage of experiments performed at the facility that lead to publications. At 325, the number of publications in 2010 remains high; 76 percent of the papers are published in journals with impact factors equal to or greater than 2. Moreover, 50 percent of the experiments performed at the facility resulted in publications. This indicates that the experiments are well planned and that the proposal review process is effective. Notably, most of the publications are in the area of soft-matter science, reflected by the fact that four of the top five journals in which publications appear emphasize topics involving soft matter.

The NCNR has best-in-class instruments and capabilities in the area of soft condensed matter. A focus area in neutron-scattering measurements of membrane proteins has been significantly enhanced over previous years through collaborative partnerships involving the NCNR and other NIST laboratories and external collaborators, such as the Biomolecular Labeling Laboratory (involving the University of Maryland and the NIST Biochemical Science Division of the Material Measurement Laboratory); a joint hire of a research scientist with the Material Measurement Laboratory; and a proposal developed jointly by the Institute for Bioscience and Biotechnology Research (a collaborative institute involving NIST and the University of Maryland), JILA (located in Boulder, Colorado), and NCNR staff in this area. Continued emphasis and effort to ensure a successful realization of this partnership should greatly strengthen the capabilities and impact of biological work at the NCNR as well as tap into a high-growth community. The focus on membranes and membrane proteins is a reasonable approach, given the number of individuals currently spearheading this effort. In addition, synergies between the NCNR and the NIST Polymer Division have historically led to highly productive science. Collaborative efforts with the NIST Material Measurement Laboratory and the Physical Measurement Laboratory should be maintained to aid the NCNR in extending its leadership in cold-neutron research. Future partnerships with the NIST Center for Nanoscale Science and Technology should be explored to strengthen the capabilities and impact of the NCNR.

The NCNR continues to develop novel ancillary sample environments and equipment, developed in part by users, such as the development of the novel shear cell with the University of Delaware, the development of humidity cell for membrane studies with Carnegie Mellon University, and advances in ^3He polarization capabilities. Such capabilities add to the attractiveness of the NCNR as a facility for carrying out unique studies with a convenience not yet found in other facilities. The development at the NCNR of novel ancillary sample environments and equipment should be continued.

The section below contains an assessment of the potential impact of ongoing projects presented to the panel.

CAPABILITY DEVELOPMENT: USANS, VSANS, AND POWDER DIFFRACTION

The ultra-small angle neutron scattering (USANS) instrument at the NCNR continues to attract new users needing the world-leading capabilities of this unique instrument. New users, including those from industry, interested in topical areas such as

carbon sequestration, and concrete and explosives research present new opportunities for the SANS program. The development of vSANS, which will extend the momentum transfer vector (Q) range to overlap USANS and SANS, is a particularly noteworthy development. The vSANS instrument should allow for efficient measurements with low background, and, given appropriate samples, be as convenient as conventional SANS measurements. With the addition of vSANS, the NCNR instruments will provide the capability of carrying out measurements over multiple length scales, covering five orders of magnitude in a single facility. Such a capability is especially important in real-world problems; for example, size distribution of voids is important to the shock resistance of explosives and to the integrity of concrete used in nuclear waste storage.

The powder diffraction program continues to be internationally competitive as well as forward looking, owing largely to excellent management support and high-quality external and internal collaborators. Currently, research is devoted to iron superconductors, hydrogen, CO_2 , and other gas sorption/separation experiments. A preconceptual design for a high-flux materials diffractometer was presented to the panel. This is an important development, as its existence will enable measurements such as time-resolved powder diffraction and diffraction from small samples, which might allow more routine study of hydrogenated materials. If fully realized, such capabilities are likely to be utilized by a large number of users, as it will be much more tractable to study pure samples of novel compounds when only small volumes of material are required. The new materials diffractometer also will enable the study of materials under extreme conditions of, for example, pressure (up to 2.5 GPa), temperature (30 milli-kelvin to 700 K), and magnetic field (10 and 15 tesla), with sample environments available at the NCNR with higher temporal resolution. It might well return prominence to the NCNR, where the modern era of high-pressure science began with the invention of the diamond anvil cell at NIST/National Bureau of Standards in the 1950s through the 1970s (<http://nvl.nist.gov/pub/nistpubs/sp958-lide/100-103.pdf>). The development of such an instrument should be supported.

RHEOLOGY

The work done in the area of rheology is diverse. It includes the structure and properties of polymers for fuel cells, organic materials for solar cells, and polymers for microelectronics, as well as the flow and rheology of complex fluids. Collaborations with universities through the Center for High-Resolution Neutron Scattering have been very successful. These collaborations have been responsible for the development of a commercial rheometer that enables the in situ study of complex fluids under shear, while simultaneously probing the structure using SANS. Exciting results using scanning narrow aperture flow-USANS (SNAFUSANS) were presented to the panel and were also featured in the 2010 annual report of the NCNR. The construction of a novel sample cell, now available in the pool of ancillary equipment at the NCNR, allowed observation of compositional and structural differences in complex fluids under shear. This new capability enabled the establishment of “non-equilibrium phase diagrams” for complex fluids that are used for a wide range of applications, from health care products to drug delivery.

THIN-FILM STRUCTURE

Another area of active investigation involves off-specular neutron scattering to develop an understanding of the structure of two-dimensional ordered materials and the extracting of orientational nanophase information from thin films. The technique is complementary to more conventional atomic force microscopy and grazing-incidence small angle x-ray scattering (GSAXS) measurements. Software is being developed to analyze data taken from a position-sensitive detector in order to gain information laterally about the structure of the sample within the film. Success of this program should lead to more widespread use of this technique for studying two-dimensional complex fluid films, such as ordered block copolymer thin films subject to geometrical constraints, and biomimetic membranes. Reflectivity measurements continue to be used to address important research problems.

CORRELATED ELECTRON AND MAGNETIC MATERIALS

Research on correlated electron materials continues to be an area of strength at the NCNR for its internal researchers as well as for the vigorous national and international user community. The NCNR continues to make key advances on the iron pnictide superconductors, having made important alliances with leading sample growers. There continue to be important advances in the understanding of the magnetic excitations and structures of the 122 compounds, and the position-sensitive detectors and spin polarization on the BT-7 double focusing triple-axis spectrometer have proven instrumental for these advances. Of particular note in the past year have been the diffraction and inelastic scattering experiments on the iron chalcogenide compounds that clarify the role of iron interstitials and strain on the magnetic structure of Fe_{1-x}Te , and also the evolution of magnetic excitations with doping.

The U.S. quantum magnetism community, with interests in compounds such as heavy fermions and geometrically frustrated insulators, remains headquartered at the NCNR. The MACS is becoming increasingly important for these users. The incorporation of spin polarization analysis into inelastic scattering and diffraction experiments is just starting to make its mark, as evidenced by the recent results on the magnetic shell structure of nanoparticles and magnetic domains in a multiferroic compound. The NCNR's continued emphasis on providing reliable sample environments makes it competitive with the SNS in retaining these users, although this situation is likely to become less tenable as SNS capabilities increase in the next few years. NCNR management is providing appropriate and unique capabilities that will keep the NCNR relevant to the correlated-electron user community, even as more intense sources come online elsewhere. The CHRNS has played an especially important role in the continued vitality of this field, both in providing resources and in recruiting and training new practitioners. The NCNR continues to attract excellent junior scientists whose research interests reside in these correlated electron materials, which bodes very well for the continued preeminence of NCNR research in this area.

LIPID MEMBRANES

The work with the membrane diffractometer (advanced neutron diffractometer/reflectometer [AND/R]) on lipid membrane multilayers continues to be of high quality and is geared toward studying the structure of proteins inside lipid membranes. One surprising result from recent measurements carried out by a group at the NCNR is that the disorder due to fluctuations in the multilayers is much larger than previously thought. Another group has carried out some impressive neutron spin-echo work to study the fluctuation dynamics of unilamellar vesicles to obtain their elastic moduli. There are very few results of this type in the field at present.

The hiring of a leader for the joint team involving the NIST Material Measurement Laboratory and the NCNR is an excellent move that should strengthen the collaborative efforts with strong groups outside of the NCNR in this area. As the Biomolecular Labeling Laboratory with the Biochemical Science Division comes online, the ability to use neutron-scattering techniques to address biological questions of interest will grow, positioning the NCNR to serve a high-growth community in the biological sciences. In a similar vein, the transition of SASSIE to a robust, user-friendly analysis software package has the potential for significantly aiding the expansion of neutron-scattering techniques in the life sciences.

The development of software for facile structural biology analysis by the general user community is likely to have significant impact and will aid in promoting the conduct of neutron-scattering measurements by nontraditional users in the life sciences. Two personnel are being hired, using funds provided under the American Recovery and Reinvestment Act of 2009 (Public Law 111-5), for the further development and refinement of the SASSIE analysis software (which is used to create atomistic models of molecular systems and also to compare scattering data from these models directly to experimental data), although these hires are for only 1 and 2 years for the respective tasks. Continuing support in this area can ensure the completion of a robust analysis package for users as well as enhanced modeling and analysis capabilities in the future. For example, similar capability to include known chemistry, physics, and structural information in order to analyze scattering data from magnetic materials would be extremely helpful not only for the analysis of scattering data but also for the design of pertinent experiments. The positive impact of robust and user-friendly software to the existing potentially growing user community is substantial.

FE-BASED SUPERCONDUCTORS

The NCNR science in the area of Fe-based superconductors is competitive with efforts anywhere in the world, and the MACS and spin polarization are special capabilities that the NCNR offers. The NRC's 2009 assessment report⁶ noted how rapidly the NCNR pursued this new family of Fe-based superconductors that had been discovered; the NCNR group's work had been based on samples brought to it by a group from the ORNL. Together, the NCNR and ORNL groups published the first report of antiferromagnetic order in one of the compounds and showed that it occurred close to, but not coincidentally with, a structural phase transition. Work on these materials has

⁶ National Research Council, *An Assessment of the National Institute of Standards and Technology Center for Neutron Research: Fiscal Year 2009*. Washington, D.C.: The National Academies Press, 2009.

continued, even though many other groups around the world, and at the SNS in particular, are also carrying out neutron-scattering experiments on these materials. Some of the NCNR researchers are also part of collaborations involving work carried out elsewhere. The focus at the SNS has been mainly on the study of the spin excitations by inelastic neutron scattering, whereas much diffraction work (both powder and single crystal) and some inelastic scattering is being carried out at the NCNR. The current efforts at the NCNR have been partly focused on the iron-tellurium compounds, doped with lighter chalcogenides, selenium, and sulfur, using both neutron diffraction and inelastic scattering.

The powder diffraction work mentioned above concentrated on studying the consequences for nuclear and magnetic structure of controlled depopulation, by de-intercalation with I₂ vapor, of the interstitial iron, which also controls the superconductivity. The inelastic scattering on the MACS has observed an energy resonance and a spin gap at the Fermi surface nesting vector. The other focus has been on the compound CaFe₂As₂ as a function of rare-earth doping, to simulate the effect of pressure. This compound is known to undergo a volume collapse under pressure, and Lynn and coworkers at the NCNR showed that this also exists as a function of temperature in rare-earth doped compounds. They have also studied spin-wave excitations in SrFe₂As₂. Overall, the NCNR maintains considerable momentum in this very competitive area of research.

In the well-trodden field of ferroelectrics, the NCNR group has studied the ferroelectric phase transition in lead zirconate titanate (PZT) and identified the soft modes associated with the corresponding structural phase transitions, and clarified the differences in behavior with the well-studied relaxor ferroelectric PMN (Pb(Mg_{1/3}Nb_{2/3})O₃). This work is a continuation of a long tradition of studying soft modes in ferroelectrics (primarily at the Brookhaven National Laboratory); through the use of large, vertical focusing monochromators, the work has been successful in spite of the limited size of available single crystals.

FUNDAMENTAL QUESTIONS IN NEUTRON SCIENCE

The research group at the NCNR continues to develop unique capabilities for probing the properties of the neutron, for using the neutrons for imaging and interferometry applications, and for the development of ³He spin filters and imaging techniques. The group recently completed a new measurement of the parity-violating spin rotation of neutrons in ⁴He, and for the first time it has observed the radiative decay branch of the neutron with a precision that may allow the group to begin testing detailed models of the bremsstrahlung processes involved. The group's work with three-blade single-crystal silicon interferometers has long set the standard for precision measurements of neutron-scattering lengths and tests of quantum mechanics with neutrons. By adding two more blades to the standard configuration and employing a quantum error correction code, the researchers have shown that they can suppress vibration effects, potentially allowing more widespread use of the technique. The group achieved a world-record 85 percent polarization for a ³He glass cell and developed imaging capabilities for fuel cells and lithium batteries.

SUMMARY

In summary, with the new instruments and improvements becoming available through the Expansion Project, there is an emphasis on the continued development and enhancement of the neutron-scattering techniques available at the facility. The new instruments will have an important impact on studies of hard and soft matter and will enable the NCNR and its research output to remain at the forefront of the field for many years. To further augment the scientific productivity of the NCNR, the development of facilities for the growth of large single crystals suitable for neutron-scattering experiments would remove a considerable hindrance to further advancement in many areas of condensed-matter science. The addition of this capacity would be an important service to the materials community.

Facilities and Human Resources

The NIST Center for Neutron Research has earned a reputation for reliable operation and outstanding service to the research community. In 2010, the NCNR successfully operated on 267 days, well above its target of 250 days. This performance is best in class among similar neutron research facilities. The NCNR is robustly staffed with reactor operators, reactor engineers, and technicians to support these activities. The staff has a healthy demographic composition, with a mix of very experienced personnel and recent hires, who will stay on after the upgrade is completed. This staffing asset positions the NCNR to maintain operational excellence in the future. The Director of the NCNR estimates that there are about 4 or 5 staff personnel supporting each instrument, which leads to a high level of satisfaction in the user community.

The NCNR is about to suspend reactor operation for 10.5 months in order to complete its Expansion Project. Five new beam lines will increase its cold-neutron measurement capacity by more than 25 percent, and the reconfiguration of existing instruments will enable better optimization of their performance. The Expansion Project schedule is aggressive and has been analyzed in detail both by NCNR staff and by visiting advisory committees. The critical-path elements are well understood by staff. Removal of the CO₂ seal on the BT-9 cold source (a remote handling project) could be problematic.

Some of the reactor refurbishments that were planned for the Expansion Project have been deferred. A new refrigerator for the cold source and an upgrade of the control room will be done at a later time. Only 4 safety shim arms will be procured initially, rather than the planned 24. Detailed planning for these activities revealed that they are more complex than originally thought, and anticipated funding from the American Recovery and Reinvestment Act of 2009 was redirected to other items at NIST. The NCNR management decided to reduce the scope of the Expansion Project in order to maintain the schedule. This adjustment demonstrates an admirable commitment to supporting the user community. However, it does increase the risk that equipment failure could force an unplanned interruption of reactor operations in the future.

The NCNR Safety Assessment Committee (SAC) recently examined the safety culture of the NCNR. As indicated to the panel, the SAC reported that “the NCNR exhibits the highest regard for safety culture at every level and is implementing the Technical Specifications as required.”⁷

Coinciding with the NRC panel’s current review of the NCNR in March 2011, Japan was struggling to control four nuclear power reactors crippled in a magnitude 9.0 earthquake. Explosions blew the roofs off three of the Japanese reactors. Nearby residents were ordered to stay inside because of dangerous releases of radioactive material. This disaster will likely lead to an intense scrutiny of hazards associated with nuclear facilities. The NCNR should be prepared to answer questions about the

⁷ Robert Dimeo, NCNR Director, “NCNR Overview to the Panel on Neutron Research,” presentation to the panel, Gaithersburg, Maryland, March 14, 2011.

consequences of low-probability but extreme events that might exceed the design criteria of the reactor building that was built in 1967.

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 completion of the Expansion Project.

Continuing concern about the security of nuclear facilities is driving the replacement of highly enriched uranium fuel with low enriched uranium (LEU) fuel in research reactors. No date for the conversion of the NIST reactor has been scheduled, but current projections by the Convert program of the Department of Energy's National Nuclear Security Administration (NNSA) suggest that conversion could take place in the 2015-2016 time frame. Changing to LEU fuel will reduce the neutron flux from the reactor, but the NNSA will mitigate this impact to performance by funding a D₂ cold-source system to replace the current H₂ cold source and refrigerator with the additional cooling capacity required for the D₂ cold source. Additionally, refurbishing the control room and the planned development of a formal software quality program have broad applicability for contributing to safe operation and constitute a key element of a comprehensive security program.

There is only one vendor for the fuel used in the NCNR reactor, and costs, which are increasing every year, will be substantially higher with the conversion to low enriched uranium. Additional operational funds will be required for the facility to maintain its high level of operating days and productivity.

The Center as a User Facility

The NIST Center for Neutron Research is a state-of-the-art facility that serves a wide range of national and international needs regarding various aspects of neutron-based science and technology. A primary purpose of the NCNR is to foster scientific research by users from universities, industry, and other national laboratories and across myriad disciplines, including condensed-matter physics, materials science, chemistry, biology, several types of engineering, and fundamental neutron science. The NCNR plays a leading role in developing new measurement techniques along with offering access to state-of-the-art instrumentation that serves basic and applied research needs, while addressing critical technological needs.

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”⁸—is evident in the breadth of the neutron science program at the NCNR, including both scattering and neutron physics, with U.S.-based and international users. The NCNR is an island of stability in the U.S. neutron science scene. One reason for this stability is the empowerment of local leadership over two decades to mold the program into a true user facility without dissipative oversight. Empowerment may be a cultural value within the Department of Commerce; it is nonetheless true that alignment of NCNR to the NIST mission has established a high level of trust. As an example, the NCNR is recognized as an international user facility because NCNR management has had the freedom to optimize the NCNR’s scientific program irrespective of the institutional origin.

In 2011, the NCNR offered a total of 4,272 instrument days through peer-reviewed proposals, which far exceeds the total instrument days offered through peer-reviewed proposals by any other U.S. neutron source. The number of proposals has risen over the past 20 years, with a near-record total of 357 proposals submitted in response to the most recent call. Overall the oversubscription rate is 2.2, and while there is clearly some variation among instruments, this figure has remained approximately constant over the past 5 years.

The number of NCNR participants continues to grow, with the 2,290 researchers in 2011 originating from every research sector: NCNR, other NIST laboratories, universities, other government agencies, and industry. The diversity of the participant base is one of the unique strengths of the NCNR, supported by the flexibility of the instrument suite, by the commitment of the NCNR staff to education and reaching out to new users, and by the NCNR’s favorable location. University participants remain the largest cadre, and the usage modes include long-standing collaborations with the University of Maryland and the University of Delaware, for example, as well as participation by researchers from other respected U.S. universities. The NCNR’s ability to meet the research needs of committed neutron-scattering users as well as those of more casual users is key to its continued success, and this mix should be preserved as the

⁸ See <http://www.nist.gov/publicaffairs/mission.cfm>. Accessed June 16, 2011.

NCNR moves forward. It is significant that the number of NCNR participants has not changed in the past few years, despite the growing user base of the SNS.

The quality of participant research at the NCNR is very high. Of the 367 publications produced in 2011 through work at the NCNR, 75 percent appeared in journals with high-impact factors, which is competitive with international sources such as the ILL, which offers many more instrument hours per year. Impressively, 13 different instruments produced high-impact papers (Journal Impact Factor [JIF] ≥ 7) in 2011, with powder diffraction and SANS responsible for more than half. Taken together, the continued degree of oversubscription and the high quality of participating user science at the NCNR confirm that there is continued high demand for neutron-scattering facilities in the United States. This demand is broad, spanning different research areas and neutron-scattering techniques, and it is very promising that there continue to be many researchers in the United States who want to use neutron scattering.

There are several reasons for the outstanding success of the NCNR's user program. At the most basic level, users decide where to carry out their experiments depending on beam flux and availability, the suitability and accessibility of sample environments, and the quality of staff support. It is clear that the NCNR management and staff understand very well what impels these decisions; it is also clear that the Expansion Project will provide extremely important new capabilities that will enable new science for existing participants as well as attracting new NCNR participants.

The NCNR is also a very reliable source, providing more instrument hours than any other U.S. source at present, which is very important for attaining the high levels of user satisfaction. To assess the level of user satisfaction with the NCNR, the center conducted a user survey in 2007. In response to questions regarding (1) instrument performance, (2) sample environments and support facilities, and (3) capabilities and assistance from the NCNR staff, more than 75 percent of the 327 respondents reported that the NCNR was "very good" or "excellent." Participants were only slightly less complimentary of the NCNR's health physics services. The survey showed that commitment to developing new sample environments and to providing the needed level of support to ensure that the environments work during experiments is widely viewed as a defining feature of NCNR's success. In addition, the long-running summer school and the various workshops on special topics were viewed by survey participants as being very effective in bringing students up to speed quickly on the capabilities of neutron-scattering measurements.

Interviews that the panel conducted with the chair of the NCNR users group and the chair of the Beam Time Allocation Committee (BTAC) reinforced these findings. Both attested to the general satisfaction of the user community with the process and practices associated with granting beam time, including the roles played by NCNR staff members in obtaining proposal reviews. Both also expressed concern over the increase in the number of proposals anticipated with the upgrade of the facility, which will strain the current system. Each expressed the belief that the NCNR's collaborative programs with universities, such as the University of Delaware and the University of Maryland, encouraged the development of sample environments and facilities that benefited all users. The chair of the BTAC noted in particular that she had access to new in situ shearing equipment recently placed in operation through the collaboration between the NCNR and the University of Delaware. Care should be taken to ensure that the proposal review process continues to work effectively as the NCNR facility expands.

NIST senior scientists are crucial to the NCNR's success. They have the experience and scientific perspective necessary to make sure that all the pieces are present to make experiments successful, to identify promising new scientific projects, to work with researchers to refine the experiments, to optimize the scientific output, and to use their considerable scientific reputations to seek out new and timely collaborations. These individuals also have the inclination and ability to train new users, forming the long-term mentorships that in many cases underlie the loyalty and continued association of many long-term users and their students. Most importantly, these senior researchers set much of the tone at the NCNR, making it a very attractive and productive place for young researchers, who in turn embrace the values of scientific excellence and education that define the NCNR's central mission. The continued scientific excellence of the NCNR scientific staff is critical for maintaining the quality and impact of neutron-scattering science by the facility and its users and for developing new measurement techniques and applications. The NCNR management should continue to take care that the next generation of senior researchers continues to develop and remain excited about their research and that they are not overly burdened with administrative and other duties that are not characterized as research.

Discretionary time on the NCNR instruments is used for calibration measurements, instrument development, and projects conducted by NIST researchers, but it is also very important for the following purposes: (1) bringing new users into the facility and introducing them to neutron-scattering techniques in general, (2) providing flexibility and rapid access for cutting-edge science, and (3) developing and retaining excellent instrument scientists and personnel at the facility. Discretionary time on the NCNR instruments should be maintained.

This is a rather volatile time in the international neutron-scattering community, made complex by widespread financial uncertainties, the possible loss of capabilities at the Japan Proton Accelerator Research Complex (J-PARC), and the SNS's increasing capabilities. It will be challenging to maintain the excellent and broad scientific user base at the NCNR in this changing landscape, and it will be challenging for the NCNR to maintain its important institutional values given these considerable external forces. It is important that the NCNR not become complacent about its ability to attract the best neutron-scattering science. Special attention should be paid to maintaining the strong connections with participants over the approaching long shutdown, particularly if delays in the construction schedule lead to a delayed user cycle. As stressed above, the breadth and depth of the NCNR user research portfolio are crucial to its mission success, and care should be taken that this balance is maintained. There is a balance of user relationships, and university and—increasingly—industrial collaborations are very important for attracting both science and resources to the NCNR. There appears to be no current cause for concern. The NCNR management should remain mindful that the user perception of open access must not be compromised as the center serves the diverse communities that depend on the NCNR.

6

Conclusions

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

The NCNR continues to provide a reliable, high flux of neutrons to a suite of high-quality instruments and sample environments that continue to evolve. The suite of thermal- and cold-neutron instruments at the NCNR enables important measurements over a broad range of time, energy, and length scales.

The NCNR is an excellent facility, with outstanding management and staff and with programs that serve well the research community and the nation. The capabilities of the NCNR play a crucial role in advancing science and in developing new technologies in the United States. They also enable NIST to satisfy its role in promoting science, standards, and technology. The upgrades and new instruments associated with the Expansion Project will enable the NCNR to continue to provide its users with access to internationally competitive instruments and to continue its preeminence as a neutron-scattering facility.