An Assessment of the National Institute of Standards and Technology Center for Neutron Research

Fiscal Year 2013

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, NW 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. SB1341-12-CQ-0036 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: 978-0-309-29608-3
International Standard Book Number-10: 0-309-29608-0

Copies of this report are available from

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

Additional copies of this report are available from the National Academies Press, 500 Fifth Street, NW, Keck 360, Washington, DC 20001; (800) 624-6242 or (202) 334-3313; http://www.nap.edu.

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. C. D. Mote, Jr., 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. C. D. Mote, Jr., are chair and vice chair, respectively, of the National Research Council.

www.national-academies.org

PANEL ON NEUTRON RESEARCH

PETER F. GREEN, University of Michigan, *Chair*
PAUL A. FLEURY, Yale University
LAURA H. GREENE, University of Illinois at Urbana-Champaign
ANDREW HARRISON, Institut Laue Langevin
ALAN J. HURD, U.S. Department of State
DALE E. KLEIN, University of Texas at Austin
WAYDE KONZE, Dow Chemical Company
ROGER A. LEACH, DuPont Central Research and Development Division
TOM C. LUBENSKY, University of Pennsylvania
BRIAN MAPLE, University of California, San Diego
V. ADRIAN PARSEGIAN, University of Massachusetts, Amherst
DAVID A.WEITZ, Harvard University

Staff

JAMES P. McGEE, Director
ARUL MOZHI, 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:

Todd R. Allen, University of Wisconsin-Madison,
Susan N. Coppersmith, University of Wisconsin-Madison,
Donald M. Engelman, Yale University,
Julia S. Higgins, Imperial College London, and
Thomas P. Russell, University of Massachusetts, Amherst.

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

The National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR), with its strong tradition of hiring and developing excellent scientific and technical staff, is one of the leading institutions worldwide in neutron instrumentation, technology, and science. It is a very well-managed user facility. With the recent completion of a $95 million expansion, performed on time and on budget, it has enhanced its instrumentation capabilities and has constructed a new guide hall. This expansion further enhances NCNR's ability to meet high user demands—a factor of two higher than capacity—for experimentation to conduct cutting-edge research. NCNR's high scientific productivity is due, in part, to effective communication between the management and staff and with the internal and external user communities.

To continue to respond effectively to a changing environment and opportunities afforded by the recent reorganization of NIST, the NCNR management should pay particular attention to the considerations below to ensure that the NCNR continues to effectively serve its mission.

NCNR management has historically done an excellent job at short-term, tactical planning. The NIST reorganization now provides them with an opportunity to operate more strategically. Because in the near future some of the more senior scientific and technical staff will be retiring, formalized succession planning needs to be performed in coordination with the broader NIST management.

Recommendation 1. The NCNR should develop and maintain a strategic plan that takes into account current and anticipated NIST organizational structures, mission factors, staffing, budgets, fuel and infrastructure resources, and its user constituency.

While numerous interactions exist between NCNR staff and other NIST staff in the various laboratory units, more formalized and coordinated planning could lead to new opportunities, or at least enhance the effectiveness of the current interactions. This, for example, would ensure that collaborative projects have sufficient budget support and appropriately serve the goals of the organization.

Recommendation 2. NCNR management should establish a more formalized engagement process with other NIST laboratory units, particularly the Material Measurement Laboratory, the Physical Measurement Laboratory, and the Center for Nanoscale Science and Technology; programmatic planning involving personnel should be more formally coordinated with other areas of the laboratory.

Funding to ensure that the reactor continues to operate efficiently, with appropriate and timely upgrades, is essential.

Recommendation 3. The NCNR should develop a formal plan to address the impending ^{4}He shortage and the fuel supply costs that promise to be problematic.

The NCNR has served its internal and external users well. This is, in part, because the NCNR management and staff have been open and responsive to feedback from the internal and external user communities. One important outcome of this positive relationship is that it has enabled the NCNR to identify areas where it needs to develop new facilities and instruments, as well as technical and scientific expertise.

Recommendation 4. The NCNR should continue to develop mechanisms that enable effective communication and feedback from current and potential users. A user community workshop should be planned for the near future. Additionally, web-based communications mechanisms, where appropriate, should also be used.

The impact of travel budget restrictions on the ability of NCNR staff to travel and to communicate with other researchers hampers their ability to effectively serve the user community.

The impact of the $1 million (30 percent of the entire budget for this collaboration) permanent decrease in funding for the National Science Foundation (NSF) collaboration involving the Center for High Resolution Neutron Scattering (CHRNS) is of serious concern. This collaboration has had a positive influence on research in the field.

Recommendation 5. The potential impact of the reduction in funding for the collaboration between NIST and the National Science Foundation involving the Center for High Resolution Neutron Scattering should be carefully examined, documented, and addressed.

nSoft, the new program designed to enhance industrial collaborations and contribute toward NIST's mission, appears to be a productive model for industrial outreach and engagement.

Recommendation 6. The NCNR should continue to focus its efforts on recruiting additional companies into the nSoft program and should establish new performance metrics that differ from those used to quantify the effectiveness of NCNR interactions with academics.

1

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, including two user facilities, as well as the adequacy of the laboratories' resources. In 2013, NIST requested that the NRC form a panel to assess the NIST Center for Neutron Research (NCNR). This report summarizes the findings of the Panel on Neutron Research.

For the assessment, NIST requested that the panel consider the following criteria:

1. The merit of the current NCNR scientific and technical programs relative to current state-of-the-art programs;
2. The degree to which the NCNR scientific and technical programs achieve their objectives and fulfill the mission of the NCNR; and
3. The adequacy of the NCNR facilities, equipment, and human resources, as they affect the quality of the NCNR's scientific and technical programs. The panel should consider the potential impact of facility modifications completed during the recent outage as well as the ongoing facility developments.

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.

To accomplish the assessment, the NRC assembled a panel of 10 volunteers whose expertise matches that of the work performed by the NCNR staff. The panel members visited the NCNR facility at Gaithersburg, Maryland, for a day and a half, during which time they attended presentations, tours, demonstrations, and interactive sessions with NCNR staff. Subsequently, the panel members assembled for another day during which they 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.

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 scientific and technological research presented 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 the NCNR's definition of its mission, and specific elements of the NCNR's resource infrastructure that are intended to support the work and the users of its facilities. These highlighted examples are intended collectively to portray an overall impression of the laboratory, while preserving useful suggestions specific to projects and programs that the panel considered to be of special note within the set of those examined. The assessment is currently scheduled to be repeated annually, which will allow, over time, exposure to the broad spectrum of NCNR activity. While the panel applied a largely qualitative approach to several elements of the assessment, 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 and focuses on representative programs and projects relevant to those 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 Management and Operation

The NCNR is one of the world's premiere neutron science user facilities. To maintain its leadership position and to continue to serve the science and technology communities and the larger NIST mission, it is essential that the NCNR excel in both the physical and managerial aspects of its operation.

The NCNR has developed a strong managerial tradition that is well suited to its mission, dating back at least three decades. NCNR line management has been rightly characterized as open, honest, candid, and exceptionally capable technically. Evidence of this is found in their very successful recruitment and hiring of creative, motivated, enthusiastic, and highly capable early-career scientific and instrument staff over the years, most of whom have entered initially as limited-term hires or postdoctoral staff.

While only a small fraction of these people stay on for long terms, the majority have gone on elsewhere to quite successful careers in industry, academia, and other national laboratories, contributing significantly to the scientific user community in the United States and elsewhere. NCNR management conducts rigorous and regular performance reviews of the staff and provides candid feedback to them. These management practices have enabled the NCNR to build and maintain a cadre of senior scientists who are among the best in their fields and who both conduct their own in-house research and, significantly, collaborate with and assist the broader user community.

The more technically oriented NCNR staff have been essential in meeting the NCNR mission objectives related to advancing both neutron instrumentation and techniques. A particularly striking example of this is the recent $95 million instrument expansion and new guide hall project, which was completed on time and within budget. With its expanded capabilities, it is important that the NCNR continue and evolve processes to solicit user input and provide technical support to outside users.

As the customer base and mission of NIST itself have evolved, the NCNR has similarly evolved. The reorganization of the NIST laboratory programs and line organizations in 2010 brought both challenges and opportunities, some of which are discussed here. The number of NIST laboratory units was recently reduced from nine to six and reconfigured to enable better cross-organizational planning, coordination, and collaboration. The position of Associate Director for Laboratory Programs and Principal Deputy for NIST was created to oversee and implement the reorganization. Although the reorganization's goals are being vigorously pursued, achieving many of the more strategic goals remains a work in progress.

The NCNR does its recruiting, hiring, and performance evaluations largely as a stand-alone unit, although performance review results are shared among all six NIST laboratories. Similarly, coordination and collaborations involving the NCNR with the other laboratories (Material Measurement Laboratory [MML], Physical Measurement Laboratory [PML], and the Center for Nanoscale Science and Technology [CNST], in particular) currently remain primarily at the tactical rather than the strategic level. Although there are dozens of scientific and technical staff from these other laboratories who work closely and are even collocated with NCNR staff, their budgets and programmatic planning appear to remain coordinated mainly on an ad hoc basis.

The reorganization itself, as well as an increased focus at NIST on mission areas such as advanced manufacturing, present the need and opportunity for NCNR management to participate more strongly in NIST-wide strategic planning, with particular emphasis on more formalized engagement with the MML, PML, and CNST. Opportunities appear potentially fruitful in areas like recruiting, promotions, succession planning, and facilities planning. Succession planning should be an area of focus to ensure continued positive operations.

NCNR management and operational practices over the years have resulted in excellent relations with the broad and diverse user community. The innovative formation of the “expertise transfer” paradigm for industry interactions, embodied in the nSoft program, is an example of best practices. CHRNS outreach and educational collaboration with NSF shows promise in building the neutron user community as well as in more general awareness and appreciation of the value of neutron science. The NCNR should be proactive in sharing, establishing, and maintaining cross-organizational activities that include the development of paradigms applicable across NIST laboratories.

The operations of the beam facilities have been very good. Continuous enhancements to the research programs have been achieved. It is equally important that the reactor itself continue to be maintained and staffed appropriately. Attention should be given to both the nuclear facilities and the staff. It was noted that several of the long-term reactor staff are eligible for retirement. Succession planning and recruiting efforts are especially important in this arena. Upgrades to the reactor should receive the same attention and funding as the research equipment for the research facilities. If the reactor is not properly maintained and modernized, the NCNR incurs the risk of having great research facilities but no reliable source of neutrons.

The area of most concern for the reactor is the fuel supply. There are two specific areas of concern: the cost and funding for the current fuel design and the potential cost and reduced capabilities with a new fuel design. Appropriate funds need to be made available for the current fuel so that the reactor operation does not get in a situation of having to choose between buying the fuel or providing proper maintenance. There is also uncertainty about the cost of the fuel as the Department of Energy moves toward the development of low enriched uranium (LEU) fuel.

In summary, the management and operation of both the NCNR research facilities and activities and the NCNR reactor are well done. Continued vigilance and NIST management attention will be required to maintain this excellent track record.

3

NCNR in Relation to Neutron Facilities Nationally and Internationally

A number of metrics are commonly used to provide some measure of performance of a user facility such as NCNR. Among them are the degree of user demand—or oversubscription—as well as the quantity and quality of published output. Other measures of performance include the number of students trained, beam-days sold to industry, and case studies that illustrate the impact on society at large of the research carried out.

The level of user demand is not in itself a measure of performance, but rather an indicator of the size and strength of the community that chooses to use a particular institute where there is a choice. Levels of demand tend to self-regulate when they start to rise significantly, with users becoming discouraged if success rates drop too low. The over-subscription level at NCNR of approximately 2.1 indicates that it is in good health.

Performance indicators based on published output are difficult to establish and interpret. Gathering reliable data is a challenge. The institute itself can use a combination of searches in electronic databases and information received from users and instrument scientists as they share news about their recent publications. Such measures of quality will vary between various scientific domains; for example, impact factors of journals in the life sciences are significantly higher than in fundamental physics.

Probably the most widely used measure of quality by neutron scattering centers is the Vettier index, established by a former Institut Laue Langevin (ILL) science director, Christian Vettier.[1] For the purposes of this report, a pragmatic approach has been adopted; the Vettier approach is used as one indicator of quality and is provided alongside the total number of publications in Table 3.1 for all user facilities in the United States, together with some of the other leading centers worldwide.

---

[1] This was based on a "shopping basket" list containing a number of relatively high-impact journals in which science performed at neutron scattering centers is commonly published. (The list was revised in 2008 and comprises the following journals: *Nature, Nature:Physics, Nature:Materials, Science, Physical Review Letters, Physical Review B,C,E, JACS, Macromolecules, Langmuir, Journal of Molecular Biology, European Physics Journal:E, European Physics Letters,* and *Chemistry of Materials*. The appearance of few European publications is due to political pressure to support such journals by members of the ILL scientific council but does not have a significant impact on the final values.) ILL takes charge of this process, first gathering papers through an electronic search (Thomson Web of Science) for the occurrence of the word "neutron" in papers from the shopping basket that bears the name of each institute. Each paper found in this way is checked manually to ensure that it is appropriate. The fact that at present only one institute gathers the data and checks each paper manually means for practical reasons that the number of journals considered is relatively small and does not evolve quickly with time, so it may not reflect changes in the journals in which scientists chose to publish. So, for example, not all of the strongest work in soft condensed matter and chemistry—areas of particular strength at NCNR—is captured by this approach. A better approach would be for each neutron scattering center to contribute a complete list of its publications every year to a common database, ensuring that the impact of every publication may be taken into consideration—an initiative to do this was launched at the last International Conference on Neutron Scattering meeting.

Comparisons of neutron scattering centers should also take into account the relative size of operations, such as the number of instrument days, the number of staff associated scientifically or technically with each instrument, and the budget, noting that there is generally a delay of a year or two between performing an experiment and publishing the results. For example, noting the relative scale of the operations (in terms of instrument days, budget—that for the ILL is at least twice as large as that for the NCNR—and staffing levels per instrument, with 4.5 and 7.0 full-time equivalent staff [FTEs] for NCNR and ILL respectively), the NCNR scores very highly for the quantity and quality of its output and, together with ISIS (the pulsed neutron and muon source at the Rutherford Appleton Laboratory in Oxfordshire, U.K.), is comfortably among the top three centers in the world in terms of the number of high-impact publications. It will take a few more years before SNS (Spallation Neutron Source at the Oak Ridge National Laboratory), HFIR (High Flux Isotope Reactor at the Oak Ridge National Laboratory), MLZ (Meier-Leibnitz Zentrum, based at the FRM-II reactor in Germany), and ANSTO (Australian Nuclear Science and Technology Organisation) reach a steady state in terms of the number of instrument days, after which a more meaningful comparison can be made between different institutes.

The success of the NCNR over the years is largely attributable to their strategy of building on areas of strength, matching instruments with support facilities, fostering in-house scientific and technical expertise, and attracting a strong user community to bring their science there as well. The instrumentation is particularly strong for the study of large-scale structures (SANS [small angle neutron scattering], incorporating USANS [ultra-small angle neutron scattering], and reflectometry), with complementary sample-environment equipment such as rheometers. Spectroscopy has also benefitted from strong instrumentation, with MACS-II (Multi Axis Crystal Spectrometer) a world-leading addition to the stable, and is matched by very strong user groups and in-house scientists in this field. This combination of strong users and in-house scientists has also ensured excellent output in diffraction, despite instrumentation that is not world-leading; even stronger science could emerge with a modest investment in an upgrade here.

The NCNR's instrumentation and neutron technology are among the best in the world. It is world-leading in the SEOP (spin-exchange optical pumping) technology for ^{3}He polarisation optics, and it has a small but high-quality activity in neutron optics and detector developments. The multiplexed reflectometer, CANDOR (chromatic analysis neutron diffractometer or reflectometer), promises a step-change in capability in its field and is likely to be of great interest to those at other steady-state sources; NCNR staff described exciting prospects in very-high-resolution imaging using a novel neutron microscope that borrows from concepts developed for the Chandra X-ray Observatory; a collaboration has been established between NIST, the Massachusetts Institute of Technology, and NASA with the aim of reaching 1 μm spatial resolution. All of this is indicative of an NCNR culture in which creative thinking is encouraged and thrives.

TABLE 3.1 Comparison of NCNR with Other Neutron Facilities

	NCNR[a]	HFIR[b]	SNS[b]	LANSCE[c]	ILL[d]	ISIS[e]	MLZ[f]	ANSTO[g]
Number of instruments	23	12	15	8	40	28	26	5-7
Days of operation per year	267	150	200	125	200	120	240	285
Number of publications in 2010	323	307	231	131	552	436	172	92
Number (and percentage) of high-impact publications (using the Vettier index)	62 (19)	49 (16)	36 (16)	28	133 (16)	70 (16)	42 (24)	32 (17)
Measure of facility output = (number of instruments x number of days) ÷ number of papers	19.0	5.8	13.0	7.6	14.5	7.7	36.3	9.8
Type of neutron source	Reactor	Reactor	Spallation	Spallation	Reactor	Spallation	Reactor	Reactor
Megawatts	20	85	1.0	0.1	58	0.25	20	20

NOTE: Figures represent data for 2012.
[a] NIST Center for Neutron Research, available at http://www.ncnr.nist.gov/AnnualReport/FY2012/AR_2012_large.pdf. Data reported here are for mid-2011 to mid-2012.
[b] High Flux Isotope Reactor at the Oak Ridge National Laboratory; Spallation Neutron Source at the Oak Ridge National Laboratory, available at http://neutrons.ornl.gov/media/pubs/2012-published.shtml.
[c] Lujan Neutron Scattering Center at the Los Alamos Neutron Science Center Spallation Neutron Source at the Oak Ridge National Laboratory. Data supplied by Lujan.
[d] Institut Laue-Langevin, available at http://www.ill.eu/fileadmin/users_files/Annual_Report/AR-12/page/publications.htm.
[e] Spallation Neutron Source in the United Kingdom, available at http://www.isis.stfc.ac.uk/about-isis/annual-review/2012/isis-annual-review-2012-pdf13438.pdf.
[f] Meier-Leibnitz Zentrum based at the FRM-II reactor, Germany, available at http://www.mlz-garching.de/annual-reports.
[g] Australian Nuclear Science and Technology Organisation, available at http://neutron.ansto.gov.au/Bragg/proposal/PublicationList.jsp?year=2012&type=1.

4

External Engagement of the NCNR

ROLE OF THE NCNR IN THE INTERNATIONAL NEUTRON-SCATTERING COMMUNITY

NCNR is active in the meetings of the Neutron Facility Directors (NFD) in North America, including Chalk River, which have met annually since the inaugural meeting at Los Alamos in January 2003. A valuable aspect of the meeting is rotational hosting, allowing leadership from all laboratories to see sister facilities. This group was established by a recommendation in a report by the Office of Science and Technology Policy (OSTP) Interagency Working Group on Neutron Science to foster inter-facility cooperation, mutual planning, and strategic planning, as well as collaboration and communication. NFD has fostered excellent coordination in outages, outreach activities such as schools, and policies relevant to user needs. There has also been good coordination in adopting facility metrics suitable to both the Department of Energy (DOE) and the Department of Commerce (DOC) cultures.

Recently the NFD has taken the strategic planning recommendation more seriously than in the past. This is welcome news; continued coordination in instrumentation to meet the needs of the user community with both capacity and uniqueness is encouraged. As budgets slim down, technique development may be vulnerable to loss of attention; the NFD could have a role in formulating effective teamwork for advancing techniques in neutron-based research.

In view of its strong standing among facilities for North America, the NCNR has a leadership obligation within NFD, perhaps superseding that of the SNS at this point in time. While this balance may change, the weight of NCNR's staff expertise, its user group, and its advocacy power should be utilized to the best advantage of the broad neutron and materials research communities.

The NCNR also plays a role in the international neutron scattering community through its participation in meetings of the directors of the world's major neutron scattering centers. Such meetings are generally held in conjunction with the principal gatherings of the neutron scattering community, such as the quadrennial International Neutron Scattering Conference (ICNS), with the aim of discussing issues of common concern. For example, at the most recent ICNS meeting in Edinburgh in July 2013, the NCNR director led the discussion of future needs and supply of ^{3}He, and he participated actively in debate on other issues, such as detector development and a more coherent approach to establishing meaningful performance metrics for neutron centers.

NCNR INTERACTION WITH THE INDUSTRIAL COMMUNITY

The NCNR has a sizable and diverse industrial user community that includes more than 40 companies with direct access to the facility to perform both publishable and proprietary scientific experiments. These companies span a range of technology space from petrochemicals to materials and electronics, and, increasingly, to biotechnology and pharmaceuticals as well. The NCNR's heavy focus on the development of sample stages that allow for the manipulation of sample temperature, pressure, strain, or moisture/humidity is extremely useful for industrial researchers needing to understand performance of materials in situ. These sample manipulation capabilities, along with the performance of the experimental beam lines, place the NCNR among the leaders of neutron science facilities for industrial users.

Many of the industrial user companies access the facility through partnerships with NIST scientists that are tied to larger collaborative programs ongoing within other NIST laboratories, and several companies access the NCNR beam lines directly through the general proposal process. Many industrially relevant problems are being explored in this facility, either through direct collaborations with industry or in partnership with academic researchers. The level of measurement science being developed and expanded is impressive and highly relevant for solving these industry problems. In addition, proprietary research of particular value to many industrial partners is underway. It is impossible to know precisely how many companies benefit from the value of NCNR research either through indirect collaboration with academic or national laboratories scientists who are NCNR users, or through the study of the published scientific output from non-industrial NCNR users, but the number and impact of these initiatives are substantial. The NCNR should work closely with industrial partners to identify and highlight the impact that this facility has had on technology advances and innovation that have resulted in financial benefits for these companies.

Efforts should continue to enhance the impact of the NCNR in supporting the development of new technologies to drive the U.S. economy. For example, over the past 3 years, a new user consortium model for industrial access based on the CRADA (cooperative research and development agreement) framework has been developed, which may prove to be a preferred way to introduce industrial researchers to the value of the NCNR. The first embodiment of this, called nSoft, was initiated in late 2010 and has grown to eight member companies, with at least four more in the process of joining. The goal of nSoft is to develop and share new scientific capabilities based on the consensus priorities of the member companies. Currently, significant progress has been reported. It is too early in the nSoft consortium's life cycle to assess the impact on its industrial users; this model should be carefully studied and replicated if it is deemed successful over the next few years.

USER GROUP CONSIDERATIONS

The panel discussed many aspects of NCNR User Group (NUG) activities with both NCNR facility management and with the NUG chair. The NUG Executive Committee, about half of whose members were recently elected, evinced an impressive vibrancy and commitment to the work of the committee. Three areas of NUG activity were assessed: advocacy of user needs to NCNR management, advocacy of NCNR facility needs to the U.S. government, and facilitation of the user needs survey.

Users find NCNR management to be receptive and responsive to many and varied concerns, from data acquisition to office space to child care. Since the NCNR expansion, there have been few user concerns to report; nevertheless, several aspects of user experience have been improved. For example, the facility has implemented a new data access policy that will make retrieval easier from offsite. More significantly, the user community expressed the desire to be more involved with strategic planning and setting a long-term vision for NCNR, perhaps through a user group meeting that could be held despite difficulties arising from current federal travel budget restrictions. Possible approaches include working through regular meetings convened in the areas of materials (MRS [Materials Research Society] and APS [American Physical Society]) and neutron scattering (ACNS [American Conference on Neutron Scattering] and ICNS) to bring NCNR users and potential users into the planning process.

The chair of the NUG Executive Committee evinced the NUG's impressive commitment to advocacy for neutron science in Washington, D.C. Better articulation of NUG's role in the National User Facility Organization (NUFO) will help NUG to amplify its voice to law and policy makers. The Neutron Scattering Society of America, in which NUG members are quite active, provides additional advocacy flows to the benefit of neutron scatterers and facilities. The NUG Executive Committee has a good mixture of practitioners and early-career and experienced people for effective advocacy.

The NUG is ready and eager to create a new user-needs survey as a follow-up to surveys in 2007 and 2011. The needs of industrial, academic, and government users should be identified to capitalize on the NCNR's special mission advantages in serving industry. The NIST deputy director for laboratory programs confirmed an increased emphasis at NIST on serving the manufacturing community.

Beam Time Allocation Committee

In general, the merit review of beam time proposals is effective and efficient. The Beam Time Allocation Committee (BTAC) chair discussed her committee's work with the panel by phone. The NCNR's practice to group proposals by similar instruments is working well. The BTAC carries an extraordinarily heavy load in SANS (38 percent) and Large Scale Structure (57 percent) proposals, but recruitment to the committee appears to meet the needs well. Although the BTAC is advisory to the NCNR director, the committee feels empowered in the review process by the openness and freedom in ranking proposals; the chair conveyed the impression that BTAC decisions are not overruled by management.

EDUCATION AND OUTREACH

The NIST education and outreach program is particularly strong and effective. Several NCNR outreach initiatives were highlighted. For K-8, NIST implements a variety of tried-and-true programs (e.g., USA Science and Engineering Festival and Bring Your Sons and Daughters to Work Day); and innovative programs (e.g., Adventures in Science and a Boy Scout nuclear science merit badge). The NCNR's high school summer intern program has hosted 25 students since 2008, and its strong undergraduate summer research fellowship has hosted 85 students since 2000 with impressive records: 23 publications and 82 percent of eligible students have gone to graduate school. Another vital education program for U.S. science is the CHRNS Summer Neutron Scattering School. NIST also fosters outreach through laboratory tours for a range of student ages.

Other important and innovative outreach activities include a Summer Institute for Science Middle School Teachers and a Research Experience for Teachers. These programs are self-propagating: teaching the teachers is always an efficient way to promote science education in K-12 schools—an area that is important and in need of support in this country. NIST's efforts in this area are commendable.

5

Science and Technology

HARD CONDENSED MATTER

The NCNR hosts an excellent mix of outstanding senior investigators and early-career, energetic, talented researchers. The early-career researchers who presented their research to the panel were very knowledgeable, enthusiastic, and articulate and gave clear descriptions of their research projects.

Magnetism, Superconductivity, and Correlated Electron Phenomena

The general direction of research in magnetism, superconductivity, and correlated electron physics is toward timely and important research problems at the forefront of condensed matter/materials physics. Research in this area is driven by both senior scientists and users of the NCNR facility.

The NCNR is supporting a powerful program on quantum magnetism that is based on the unique MACS II spectrometer. The focus of this research program is on frustrated two-dimensional quantum magnets, and the primary interest is on exotic states of matter, such as spinons in Kagome antiferromagnets and resonating valence bonds in a triangular lattice. In this project, frustration is used as a tuning parameter to drive a quantum phase transition from a magnetically ordered state to an exotic nonmagnetic state. Eight papers based on this program have been published in high-impact journals, such as *Physical Review Letters*, *Nature*, and *Science,* during the past 3 years. Highlights include the first observation of spinons in two-dimensions and the observation of a collective continuum in a molecular magnet.

The NCNR has also supported recent progress in neutron scattering studies of magnetism, superconductivity, and correlated electron phenomena in novel materials. This excellent and broad-based program has been very successful over the years and has had a significant impact in condensed matter/materials physics. One of the recent efforts focused on various phenomena in Mn-based compounds, for example (Ba-Sr)MnO_3—multiferroic, (Ba-K)Mn_2As_2—itinerant half-filled ferromagnet, and LaMnPO—antiferromagnetic insulator. The compound LaMnPO, which has the same structure as the LaFePnO (Pn = P, As) superconductors, was studied under applied pressure to determine whether it would be possible to suppress the magnetic order and induce a correlated electron metallic state that would exhibit superconductivity. It was found that only modest pressures are required to transform LaMnPO from an insulating tetragonal structure with a large moment to a gapless orthorhombic structure with a small moment and no long-range order. However, no superconductivity was observed to emerge upon suppression of the magnetic order.

Superconductivity in Fe-pnictides and Chalcogenides

NIST was an early world leader in the area of Fe-based superconductors. They had access to the first high-quality crystals outside of Japan and China and were the first to determine the magnetic structure of one of the "122" compounds, $BaFe_2As_2$ (parent compound), revealing the novel antiferromagnetic structure of that compound. That was only a few months after the discovery of the Fe-based superconductors in Japan. The paper that reports these results, as obtained by neutron scattering, remains highly cited. The NIST Superconductivity Group continues its world leadership and has done fundamental work on over a dozen families of Fe-pnictides and Fe-chalcogenides. They continue their leadership in the growth of large single crystals of all three of the 122 families of materials, $(Ba,Ca,Sr)Fe_2As_2$, through their own work and external collaborations. In the Sr122 system, they identified early the low-energy spin waves and magnetic interactions. In the Fe-chalcogenide system (FeTeSe), they detected a spin resonance that bore a surprisingly close parallel to the magnetic resonance studied in the high-temperature superconducting cuprate Bi2212 more than 10 years earlier. This solid work over time is helping the field to compare and contrast the role of spin fluctuations in the mechanism of these two distinct families of high-temperature superconductors (cuprates and Fe-based). NIST included one of the early laboratories to start to test the S± theory for the order parameter symmetry in the Fe-based superconductors.

Related to the work on the superconductivity is the outstanding research on quantum criticality in other materials that exhibit phase diagrams (carrier concentration versus temperature) similar to the high-temperature superconductors. They all exhibit a dome under which there is strong evidence for a quantum critical point (QCP). Superconductivity may be arising from this proximity to the magnetic state at the QCP. Most of the work presented was accomplished by the MACS II spectrometer—a noteworthy success in neutron scattering design. One of the many impressive results is the detection of collective molecular magnetism in $LiZn_2Mo_3O_8$ at 1.5 K. The resonating valence bond detection on a triangular lattice is equally impressive. It is not clear how far MACS will take the field of strong electron correlations in condensed matter systems, but the future is quite promising.

The entire neutron group and the condensed matter community benefit from a symbiotic relationship that substantially strengthens both. The experiments done on MACS II and SANS and neutron reflectivity experiments are impressive and deserve continued strong support.

Fundamental Neutron Science: aCORN

A very interesting poster titled "aCORN ['a' correlation in neutron decay]: A Measurement of the Electron-Antineutrino Correlation (Little "a")" described an innovative fundamental physics experiment incorporating a new approach to measure a dimensionless parameter a within uncertainties of about 0.5 percent, which represents the angular correlation between the beta electron and antineutrino in neutron beta decay ($n \rightarrow p + e^- + \bar{\upsilon}_e$). When combined with other neutron decay parameters, the value of a for free neutron decay can be used to determine the weak vector and axial vector coupling constants g_v and g_A and to test the validity and self-consistency of the

Electroweak Standard Model. Previous experiments measuring a relied on precise proton spectroscopy and were limited by systematic effects at about the 5 percent level.

Crystallography

Although the NCNR suite of instruments for crystallography is not extensive (comprising the powder diffractometer BT-1 and the residual stress diffractometer BT-8) and has no dedicated instrument for single-crystal diffraction, in the hands of a team of crystallographers with a broad profile in experience and a strong and varied user community, the scientific output is nevertheless very strong. Highlights include research featured in recent highly cited papers in the fields of porous systems and functional materials such as superconductors and multiferroics. Particularly striking examples include the location of different molecules in microporous materials used to process or separate different molecular species. These provide unique insights into the absorption mechanisms to aid their exploitation in chemical processes. This research also impacts industrially relevant problems, with close links to a number of companies both in chemical crystallography and engineering.

SOFT CONDENSED MATTER

Neutron scattering is a very powerful technique for studying soft matter systems. Because scattering contrast arises from interactions between the scattering neutron and the nucleus, useful scattering intensity can be obtained from common soft materials or biomaterials. By contrast, X-ray scattering can often be too weak, and light scattering (multiple scattering) can be too strong for useful experiments. Furthermore, neutron scattering has the unique advantage that contrast can be adjusted through deuteration to limit the contrast to a specific portion of the structure, further enhancing the capabilities of the scattering. Several examples that exploited these features were presented to the panel.

By far the most widely used scattering technique of those presented was small-angle scattering, and there are three SANS instruments at NCNR. In addition, neutron reflectivity was used for interfacial studies, and spin-echo scattering provided information about dynamics.

One of the most impressive efforts in soft matter science at NCNR is the work on rheo-scattering, in which neutron scattering is combined with rheological measurements. There are several tools that enable the neutron beam to probe all three independent directions required for Couette flow in a rheometer. These are tools that have been constructed at NCNR in response to user needs, and NCNR leads the world in this field. The work on shear-thickening colloidal suspensions, which have potential as body armor, particularly benefits from neutron scattering. The NCNR staff developed a creative way to utilize all the neutrons in a SANS experiment done on an oscillatory measurement to isolate the scattering at specific times during the oscillation. This enabled the team to confirm the underlying mechanism of the shear thickening—the formation of transient hydro-clusters for which lubrication forces, which lead to the large increase in stress observed at high shear rates, become dominant. These experiments are an excellent example of a case in which neutron scattering data provides essential insight into the underlying physical processes.

Another good example of collaboration between NCNR and users is the study of monoclonal antibodies, which is supported in part by Genentech and is an attempt to help solve an important problem that could limit the use of some new biologic, antibody-based drugs, which are becoming increasingly important and common. The NCNR studies attempted to determine the origin of a large increase in viscosity, which makes injection difficult, with increased monoclonal antibody concentration. There were studies using both small angle-scattering and spin-echo scattering to help resolve the origin of this increase. In both cases, the results support the hypothesis that at high concentrations the antibodies interact to form trimeric clusters that can further interact to form larger structures that lead to the increased viscosity. The results seem solid, but the data depend quite strongly on modeling the behavior, particularly in the case of the SANS data.

Polymer glasses and composites of polymers and small particles are important industrial materials. The transition temperature of the materials from the liquid phase to the glass phase is often smaller in thin films in the bulk. This may be a result of interactions between the polymer and the interface, making it important to investigate interfacial properties of polymer glasses. Neutron reflectivity measurements by the NCNR group from thin films with one or more deuterated layers provided a direct measure of the roughness of the layer interfaces and of their self-diffusion coefficient and, thus, provide valuable insight into the glassy properties of these films and the effects of the interface.

Membranes constitute a form of soft matter of importance both to biology and to complex fluids. Using the unique capabilities of the spin-echo technique, an NCNR-university collaboration produced high-quality measurements of dynamical correlations in lipid membranes arising from both their shape and their thickness fluctuations.

Systems of relevance to biology, including membranes and proteins, tend to be quite complex, and interpreting neutron data about them is often a challenging undertaking. NCNR staff realize this and have begun to develop in-house modeling expertise. As the soft matter effort grows, however, it would benefit from more theoretical and modeling input.

6

Challenges and Opportunities

The major challenges facing NCNR are associated with constraints based on shrinking budgets, a growing user base, growing competition, and factors relating to maintaining a dynamic workforce. At the same time, there exist opportunities to increase the size and disciplinary diversity of the user base, particularly by increasing the number of industry users, and thereby have a notable impact on industry and manufacturing.

An additional challenge is associated with the projected long-term shortage of ^{4}He. Addressing this challenge needs to be accomplished through understanding how to effectively exploit the strengths of the new organizational structure. Concern was also expressed regarding the eventual change from the high-enriched uranium (HEU) reactor fuel to LEU with potential negative impact on costs, fuel availability, and reactor performance. The NCNR is rightly tracking developments closely and developing appropriate contingency scenarios.

The budget constraints also require addressing the increases in the reactor fuel costs, as well as funding the effective maintenance of the facility to ensure that it operates at the highest levels of efficiency. Additionally, the budget shortfall in the resources for the collaboration with NSF and CHRNS could be problematic. The opportunities lie in increasing the scientific and industrial user base and in developing a broader strategic plan with NIST management that addresses long-term hiring plans, the current challenge of an aging workforce, and limited-term hires. Other opportunities would arise from enhancing collaborations with internal NIST users, as mentioned above.

7

Findings and Recommendations

The NCNR, with its strong tradition of hiring and developing excellent scientific and technical staff, is one of the leading institutions worldwide in neutron instrumentation, technology, and science. It is a very well-managed user facility. With the recent completion of a $95 million expansion, performed on time and on budget, it has enhanced its instrumentation capabilities and has constructed a new guide hall. This expansion further enhances NCNR's ability to meet the high user demands—a factor of two higher than capacity—for experimentation to conduct cutting-edge research. NCNR's high scientific productivity is due, in part, to effective communication between the management and staff and with the internal and external user communities.

With the recent reorganization of NIST, new budget constraints, and a combination of limited-term and permanent staff, NCNR management is operating in a changing environment. One important change that resulted from the recent reorganization is that the number of laboratory units within NIST was reduced. The goal of the reorganization was, in part, to enable NIST to more effectively fulfill its mission, which includes advanced manufacturing and measurement science. While the direct impact of the reorganization on NCNR personnel and NCNR's internal management structure were minimal, there are associated challenges and opportunities. These are especially important due to the highly specialized nature of NCNR's mission. To this end, NCNR management should pay particular attention to the considerations below in order to ensure that the NCNR continues to effectively serve its mission.

NCNR management has historically done an excellent job at short-term, tactical planning. The NIST reorganization now provides them with an opportunity to operate more strategically. Because in the near future some of the more senior scientific and technical staff will be retiring, formalized succession planning needs to be performed in coordination with the broader NIST management.

Recommendation 1. The NCNR should develop and maintain a strategic plan that takes into account current and anticipated NIST organizational structures, mission factors, staffing, budgets, fuel and infrastructure resources, and its user constituency.

Potential opportunities for recruiting and promotions need to be explored. While numerous interactions exist between NCNR staff and other NIST staff in the various laboratory units, more formalized and coordinated planning could lead to new opportunities or at least enhance the effectiveness of the current interactions. This, for example, would ensure that collaborative projects have sufficient budget support and appropriately serve the goals of the organization.

Recommendation 2. NCNR management should establish a more formalized engagement process with other NIST laboratory units, particularly the Material

Measurement Laboratory, the Physical Measurement Laboratory, and the Center for Nanoscale Science and Technology; programmatic planning involving personnel should be more formally coordinated with other areas of the laboratory.

Funding to ensure that the reactor continues to operate efficiently, with appropriate and timely upgrades, is essential.

Recommendation 3. The NCNR should develop a formal plan to address the impending ^{4}He shortage and the fuel supply costs that promise to be problematic.

The NCNR has served its internal and external users well. This is, in part, because NCNR management and staff have been open and responsive to feedback from the internal and external user communities. One important outcome of this positive relationship is that it has enabled the NCNR to identify areas where they needed to develop new facilities and instruments, as well as technical/scientific expertise.

The most recent prior user community workshop was held in 2007. This 2007 meeting had a significant impact on future planning and outcomes; facility upgrades and new instrument development were important outcomes. Now with the completion of the $95 million expansion, another workshop is necessary in order to ensure that these new resources effectively serve the academic and industrial communities.

Recommendation 4. The NCNR should continue to develop mechanisms that enable effective communication and feedback from current and potential users. A user community workshop should be planned for the near future. Additionally, web-based communications mechanisms, where appropriate, should also be used.

The impact of travel budget restrictions on the ability of NCNR staff to travel and to communicate with other researchers hampers their ability to effectively serve the user community.

The impact of the $1 million (30 percent of the entire budget for this collaboration) permanent decrease in funding for the National Science Foundation collaboration involving The Center for High Resolution Neutron Scattering (CHRNS) is of serious concern. This collaboration has had a positive influence on research in the field.

Recommendation 5. The potential impact of the reduction in funding for the collaboration between NIST and the National Science Foundation involving the Center for High Resolution Neutron Scattering should be carefully examined, documented, and addressed.

nSoft, the new program designed to enhance industrial collaborations and contribute toward NIST’s mission, is off to a great start. It appears to be a productive model for industrial outreach and engagement. The industrial members perform collaborative and proprietary research. The number of members (companies) continues to increase. There are specific examples where the scientific interactions have been of important commercial benefit, and there is need for metrics that manifest these outcomes.

Recommendation 6. The NCNR should continue to focus its efforts on recruiting additional companies into the nSoft program and should establish new performance metrics that differ from those used to quantify the effectiveness of NCNR interactions with academics.