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

FISCAL YEAR 2018

Panel on Review of the Center for Neutron Research at the
National Institute of Standards and Technology

Committee on NIST Technical Programs

Laboratory Assessments Board

Division on Engineering and Physical Sciences

A Consensus Study Report of
The National Academies of
SCIENCES · ENGINEERING · MEDICINE

THE NATIONAL ACADEMIES PRESS
Washington, DC
www.nap.edu

THE NATIONAL ACADEMIES PRESS 500 Fifth Street, NW Washington, DC 20001

This activity was supported by Contract No. SB134117CQ0017/18107 with the National Institute of Standards and Technology. Any opinions, findings, conclusions, or recommendations expressed in this publication do not necessarily reflect the views of any organization or agency that provided support for the project.

International Standard Book Number-13: 978-0-309-XXXXX-X
International Standard Book Number-10: 0-309-XXXXX-X
Digital Object Identifier: https://doi.org/10.17226/XXXXX

Copies of this publication are available from

Laboratory Assessments Board
National Academies of Sciences, Engineering, and Medicine
500 Fifth Street, NW #928
Washington, DC 20001

Additional copies of this publication 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

Suggested Citation: National Academies of Sciences, Engineering, and Medicine. 2018. *An Assessment of the Center for Neutron Research at the National Institute of Standards and Technology: Fiscal Year 2018*. Washington, DC: The National Academies Press. https://doi.org/10.17226/XXXXX

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PANEL ON REVIEW OF THE CENTER FOR NEUTRON RESEARCH AT THE NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

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Acknowledgment of Reviewers

This Consensus Study Report was reviewed in draft form by individuals chosen for their diverse perspectives and technical expertise. The purpose of this independent review is to provide candid and critical comments that will assist the National Academies of Sciences, Engineering, and Medicine in making each published report as sound as possible and to ensure that it meets the institutional standards for quality, 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 thank the following individuals for their review of this report:

Stuart Cooper, NAE, Ohio State University,
Alan Hurd, Los Alamos National Laboratory,
Peter Green, National Renewable Energy Laboratory,
Christopher Gould, North Carolina State University, and
Stephen H. White, University of California, Irvine.

Although the reviewers listed above provided many constructive comments and suggestions, they were not asked to endorse the conclusions or recommendations of this report nor did they see the final draft before its release. The review of this report was overseen by Michael Ladisch, NAE, Purdue University. He was responsible for making certain that an independent examination of this report was carried out in accordance with the standards of the National Academies and that all review comments were carefully considered. Responsibility for the final content rests entirely with the authoring committee and the National Academies.

Contents

Summary

The National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR), with an annual budget of $50 million and a total staff of 217, is one of seven NIST laboratories. In 2017, NCNR served 2,769 users at the facility. It is an efficiently run neutron-scattering facility delivering 228 days of operation in 2017 with 98 percent reliability. It has a robust safety program with no regulatory violations since the last panel assessment in 2015.[1] Its reactor's hydrogen cold source is scheduled for replacement with one based on deuterium in 2022, an operation that will require an 8- to 12-month shutdown, during which time several existing beam lines will be equipped with more efficient supermirror guides. The commissioning of the Very Small Angle Neutron Scattering (vSANS) instrument is substantially complete, with the polarization capability still in progress at the time of this writing; vSANS will significantly improve the capabilities that the NCNR can offer the soft-matter community. The Chromatic Analysis Neutron Diffractometer or Reflector (CANDOR), which is scheduled to come on line in 2019, will enable new experiments to probe shorter timescales and improved polarized neutron measurements. The NeXT (Neutron and X-Ray Tomography) system, which began operation in 2016, cements NCNR's continuing world leadership in neutron imaging. The Stress Diffractometer, which provides a platform for the noninvasive study of inhomogeneous stress and strain, is undergoing a series of upgrades that will increase its data acquisition rate by a factor of 20 and increase its value to its industrial users. The NCNR has an aggressive program to upgrade software and to make it more user friendly and deployable across platforms. The NCNR and its users conduct world-class and highly cited research in soft matter, hard matter (particularly magnetic materials), biology, and chemical and engineering physics. It runs the Center for High Resolution Neutron Scattering (CHRNS), an important partnership, the funding for which must be renewed in 2020 with the National Science Foundation. Because of its investment in beamline and special-environment staff and equipment, this partnership is critical to the NCNR's ability to offer an effective user program. The NCNR established in 2012 a unique and creative consortium, called nSoft, that is designed specifically to engage industry in neutron scattering, and it runs cooperative agreements with four universities that provide funds to support technical staff, postdoctoral researchers, and graduate students. It also has a robust education and outreach program that features a very popular neutron scattering summer school run through CHNRS.

[1] National Academies of Sciences, Engineering, and Medicine, 2015, *An Assessment of the National Institute of Standards and Technology Center for Neutron Research: Fiscal Year 2015*, The National Academies Press, Washington, DC.

KEY FINDINGS AND RECOMMENDATIONS

The Panel on Review of the Center for Neutron Research at the National Institute of Standards and Technology determined that the following issues merit attention. More detailed explanations of them appear in the final chapter of this report.

The reactor is 50 years old. Loss of this facility would have a strongly negative impact on neutron science within the United States and the scientific disciplines that NCNR serves.

RECOMMENDATION: The NCNR should commission a detailed assessment of the current facility and begin the conceptual design of a new reactor. NCNR would do well to elaborate a systematic succession plan in concert with NIST leadership.

External reviews conducted less frequently than annually are not able to provide sufficiently current or detailed evaluations of the NCNR or to track its technical and operational issues.

RECOMMENDATION: The NCNR should establish external reviews that assess its technical and operational issues on an annual basis.

The NCNR plays a critical role in both fundamental and applied industrial research within the United States but does not currently have representation on the NIST Visiting Committee on Advanced Technology.

RECOMMENDATION: The NCNR leadership should work with NIST leadership to address the absence of VCAT representation in neutron applications.

The panel was not provided with a document that clearly articulates the NCNR's vision, mission, and strategic plan complete with contingencies.

RECOMMENDATION: The NCNR should prepare a guiding document on vision, mission, and strategic plans and update it regularly.

The United States significantly lags the European Union in neutron scattering facilities, and it is in jeopardy of becoming internationally noncompetitive. NCNR represents a large fraction of the neutron scattering capability within the United States, and it remains a world-class facility, even though its funding has been stagnant in recent years. Continuation of current funding trends will inevitably lead to a trajectory of decline.

The Neutron Physics group has a long history of studying the fundamental properties of the neutron. It is currently running experiments to measure the lifetime of the neutron, which is an important parameter in models of how atomic nuclei were formed in the Big Bang, and the magnetic moment of the neutron; test the so-called Standard Model of elementary particle physics; search for new mechanisms that might help explain the matter-antimatter asymmetry in the universe; and search for a possible elementary particle called the sterile neutrino, which responds only to gravitational forces. These are important measurements that require great care and often take a long time to complete.

RECOMMENDATION: NCNR leadership should work with NIST leadership to ensure the support of the NCNR at a level of resourcing that will enable it to develop and support world-class neutron scattering instrumentation.

The nSoft consortium is developing a more facile engagement with industry.

RECOMMENDATION: The NCNR should establish quality and success metrics for nSoft.

RECOMMENDATION: The NCNR should develop an additional umbrella organization for hard matter and industrial interactions.

While this report was being prepared, a study prepared by the Panel on Public Affairs (POPA) of the American Physical Society, *Neutrons for the Nation*,[2] was released. Its findings are consistent with those presented here, although its focus includes, unlike this document, the transition from highly enriched uranium (HEU) to low enriched uranium (LEU) that is scheduled to take place in U.S. nuclear facilities on a 10-year-plus time scale.

[2] American Physical Society, 2018, *Neutrons for the Nation: Discovery and Applications while Minimizing the Risk of Nuclear Proliferation*, https://www.aps.org/policy/reports/popa-reports/heu.cfm.

1

Introduction

The special properties of the neutron and how it interacts with matter make it a unique probe of materials structure and function. Neutron scattering is a key tool for the development of next-generation materials for applications from energy to health. It is critical for optimizing existing technologies, such as oil extraction from shale; for the development of new technologies, such as practical fuel-cell power plants for vehicles; and for understanding the basic science on which completely disruptive new technologies can be built. The impact of neutron science on economic competitiveness is high because better performing advanced materials are a basis for better performing devices and systems. A highly pertinent current example is the development of safe, cheap, environmentally friendly, and earth-abundant materials and devices for energy storage—for applications from grid storage through practical electric vehicles, all the way to long-lived active medical implants. Neutron science may appear arcane, but it instead has rather direct short, medium, and long-term impacts on lifestyle and societal well-being as well as on economic competitiveness.

At the request of the National Institute of Standards and Technology (NIST), the National Academies of Sciences, Engineering, and Medicine has, since 1959, annually assembled panels of experts from academia, industry, medicine, and other scientific and engineering communities to assess the quality and effectiveness of the NIST measurements and standards laboratories, of which there are now seven,[1] as well as the adequacy of the laboratories' resources. 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. NIST laboratories conduct research to anticipate future metrology and standards needs, enable scientific and technological advances, and improve and refine existing measurement methods and services.

In 2018, the Director of NIST asked the National Academies to appoint a panel on review of the NIST Center for Neutron Research (NCNR) and provided it with a statement of task (see Box 1.1).

The director pointed out that in arriving at its assessments, the panel was to be sensitive to the overall 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 objectives of the research done at NIST laboratories are to anticipate future metrology and standards needs, enable new scientific and technological advances, and improve and refine existing measurement methods and services.

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

In order to accomplish this assessment, the National Academies assembled the Panel on Review of the Center for Neutron Research at the National Institute of Standards and Technology, a panel of nine volunteers whose collective expertise corresponds well with the research done at the NCNR. The panel members participated in an onsite review at the NCNR on July 10-12, 2018. The visit began with welcoming remarks and overview comments from the Director of NIST and from the Director of the NCNR. Their talks were followed by scientific and technical presentations by NCNR staff, a tour of the facilities, and a poster session featuring research by graduate students and postdoctoral researchers. Ample time was provided for discussions with NCNR management and for panel deliberation. The panel was provided with copies of all presentations and posters, NCNR annual reports, and copies of other studies relevant to neutron science in the United States, all of which provided valuable input for the preparation of this report.

Time constraints did not allow the panel to explore all aspects of NCNR operations. Rather, the panel focused on the research that the leadership of the NCNR chose to present to it and on a number of issues related to laboratory development that the panel identified as requiring particular attention. This report presents the panel's observations and recommendations. Because the issues this panel was asked to address differed somewhat from those considered by earlier panels, this report should be regarded as complementing their reports, rather than as replacing them.

BOX 1.1
Statement of Task

The National Academies shall appoint a panel to assess independently the scientific and technical work performed by the National Institute of Standards and Technology (NIST) Center for Neutron Research. This panel will review technical reports and technical program descriptions prepared by NIST staff and will visit the facilities of the NIST Center for Neutron Research. The visit will include technical presentations by NIST staff, demonstrations of NIST projects, tours of NIST facilities, and discussions with NIST staff. The panel will deliberate findings in closed sessions of the panel meeting and will prepare a report summarizing its assessment findings.

The Director of NIST asked that the panel consider following:

1. Assess the organization's technical programs.
    - How does the quality of the research compare to similar world class research in the technical program areas?
    - Is the quality of the technical programs adequate for the organization to reach its stated technical objectives? How could it be improved?
2. Assess the portfolio of scientific expertise within the organization.
    - Does the organization have world class scientific expertise in the areas of the organization's mission and program objectives? If not, what areas should be improved?
    - How well does the organization's scientific expertise support the organization's technical programs and the organization's ability to achieve its stated objectives?
3. Assess the adequacy of the organization's facilities, equipment, and human resources.
    - How well do the facilities, equipment, and human resources support the organization's technical programs and its ability to achieve its stated objectives? How could they be improved?
4. Assess the effectiveness by which the organization disseminates its program outputs.
    - How well are the organization's research programs driven by stakeholder needs?
    - How effective are the technology transfer mechanisms used by the organization? Are these mechanisms sufficiently comprehensive?
    - How well is the organization monitoring stakeholder use and impact of program outputs?
    - How could this be improved?

2

Adequacy of Facilities, Equipment, and Human Resources

OVERVIEW OF THE CENTER

The NCNR is one of the seven laboratories[1] of NIST. The mission of NCNR is to provide facilities, access, and assistance to members of the U.S. scientific and industrial communities interested in using neutrons for their research. It has been in operation for more than 50 years and has earned a well-deserved reputation as one of the best organizations of its kind in the world.

The NCNR has an annual budget of approximately $50 million, which can be compared to the total NIST annual budget of roughly $1.2 billion in fiscal year 2018. It has a total staff of 217, of which 103 are in condensed matter science, 44 in facilities and operations, 36 in construction, and 34 in safety and administration. There are 5 affiliated technical staff/instrument scientists per instrument to serve/collaborate with users. In addition, NCNR scientists have active research programs of their own. For comparison, the world's largest neutron user facility, the Institute Laue-Langevin (ILL) in Grenoble, France, requires on average two more staff—7 technical staff per instrument—for its operations.

In 2017, the reactor provided neutrons for 228 days of operation at full power with 98 percent reliability to 29 instruments for a total of 2,769 research participants. Among high-performance neutron sources, the NCNR has consistently led the United States in user instrument days in the past decade.[2] The process for obtaining instrument time includes twice-yearly calls for proposals. In 2017, 661 proposals requesting 3,518 days of beam/instrument time were received. About one-third of the proposals were successful, and 1,391 days of instrument time were allocated. About 20 percent of users at NCNR are foreign scientists.

An important portion of the NCNR portfolio is the Center for High Resolution Neutron Scattering (CHNRS), which is jointly funded by the National Science Foundation (NSF) and NIST. The partnership agreement for CHNRS was renewed for 5 years in 2015. Last year, CHNRS received 210 proposals for 1,235 days and awarded, on a competitive basis, 90 proposals for 384 instrument days. The NCNR User Group conducted a user survey in 2015 on new directions for CHRNS, advancing instrumentation, and diversifying the community of research users. (The survey is discussed further in the section "User Program and Obtaining User Access to the NCNR" in Chapter 0).

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

[2] R. Dimeo, NIST, "NCNR Overview to the Panel on Neutron Research," presentation to the panel on July 10, 2018.

Accomplishments

The NCNR is delivering a high return on investment, as measured by its productivity, and it is an enterprise and national asset that needs to be nurtured and supported. Its managers have been and continue to be excellent stewards of the resource entrusted to them. It has done a remarkable job in maintaining and enhancing the impact of the NCNR by promoting partnerships with NSF and industry and by making timely and bold decisions on what to support and what to reduce. The results they have obtained with an aging 50-year old reactor are laudable.

The NCNR maintains a robust safety management program that addresses radiological, occupational, and industrial hazards. Key elements of the program include management commitment and employee involvement, worksite inspections, management observations, hazard prevention and control (including planning for work involving radiological hazards), and training for staff and users. In addition to operating with a strong safety management program, the NCNR has an excellent safety record that includes no regulatory violations since the last National Academies assessment in 2015.[3]

Challenges and Opportunities

In the near term the NCNR must deal with an uncertain helium-4 (^{4}He) supply[4] and increasing security and safety demands, which place strain on current staff and threaten continuing open-access of the facility to users. The increasing cost of shipping radioactive waste to Savannah River is another of the NCNR's budgetary concerns. Because it appears that NCNR funding is likely to be flat, or to decrease, for the next few years in nominal dollars, and hence almost surely to decrease in real terms, the NCNR's ability to continue operating at current levels, let alone to develop new instrumentation and maintain international competitiveness, is at risk.

As noted, the results NCNR has obtained with an aging 50-year old reactor are laudable. However, it is clear that this success cannot continue given the flat budgets that management has had to contend with for several years. The only way a facility like the NCNR can remain competitive is by continually investing in new experimental capabilities. At the NCNR, this investment, which historically was close to 30 percent of the annual operating budget, is gradually being reduced towards zero. Absent funding increases, the facility will ultimately be forced to curtail the services it now provides the research community. The capabilities the NCNR delivers to its users are critical for both the U.S. scientific and innovation enterprise and the Nation's economic competitiveness.

The role of the NCNR in NIST's future needs to be continually and strategically examined and evolved. The NCNR currently has a rough strategic plan that needs to be regularly updated and shared with the NIST Director and the Visiting Committee on Advanced Technology (VCAT)[5] as well as the NCNR staff and user community. Although the NCNR is less than 10 percent of NIST in terms of budget, it plays a unique role in the Institute and a vital one for the nation's science. The NCNR needs to be an

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[3] National Research Council, 2015, *An Assessment of the National Institute of Standards and Technology Center for Neutron Research: Fiscal Year 2015*, The National Academies Press, Washington, DC.

[4] This issue and the importance of a helium recovery system is discussed by other authoring groups. See, for example, National Research Council, 2010, *Selling the Nation's Helium Reserve*, The National Academies Press, Washington, DC; American Physical Society, Materials Research Society, and American Chemical Society, 2014, *Responding to the U.S. Research Community's Liquid Helium Crisis*, American Physical Society, College Park, MD; M. Beattie-Moss, 2013, "Probing Question: Are We Running Out of Helium?," *Phys.Org*, August 26, https://phys.org/news/2013-04-probing-helium.html.

[5] "The VCAT reviews and makes recommendations regarding general policy for the National Institute of Standards and Technology, its organization, its budget, and its programs, within the framework of applicable national policies as set forth by the President and the Congress, and submits an annual report to the Secretary of Commerce for submission to the Congress" (NIST Office of the Director, "Visiting Committee on Advanced Technology," https://www.nist.gov/director/vcat, accessed September 14, 2018).

essential element of NISTs' strategy and strategic planning. The longevity and relevance of its research enterprise necessitates strong communication of the NCNR's strategic planning with the NIST management including, for example, a regular annual formal briefing to the NIST Director and VCAT. Participation of the VCAT in the NCNR's planning and budgetary activities would also be beneficial.

THE REACTOR

Current Status

The panel received a presentation about the current status of the reactor.[6] There is an ongoing program to replace all of the reactor's old electronic control panels with new ones, an upgrade to the cold neutron source, and a fuel conversion for the nuclear reactor core. The two major modifications to the reactor are envisaged to occur in the next decade. First, the replacement of the hydrogen cold neutron source inside the reactor vessel with a deuterium cold neutron source will significantly enhance the capabilities of the NCNR. During the shutdown required for this upgrade, the NCNR will replace several existing beam guides with more efficient supermirror guides. The installation of the new cold neutron source will require approval by the U.S. Nuclear Regulatory Commission. The licensing issues involved with this upgrade were not discussed. The nuclear reactor will be shut down in 2022 for this upgrade, and the shutdown will last for 8 to 12 months. During that period, the only neutron facilities available to users in the United States will be the High Flux Isotope Reactor (HFIR) and Spallation Neutron Source (SNS) at Oak Ridge National Laboratory (ONRL). It would be wise for the NCNR to initiate a discussion with HFIR and SNS management about how best to meet the needs of NCNR users during the shutdown.

Second, a major nuclear fuel modification is planned for the reactor core involving the conversion of the reactor from an HEU (highly enriched uranium) fuel to a LEU (low enriched uranium) fuel, which is currently planned for 2028. NIST indicated that no changes will be required inside the reactor vessel, although at the same time, the conversion is contingent on the development of a suitable LEU fuel. Much technical work remains to be done for this fuel conversion.

The NIST nuclear reactor is essential to the NCNR; no reactor means no NCNR. Furthermore, with the effective closure of the Lujan Center at the Los Alamos Neutron Science Center (LANSCE) to the broader scientific community, the neutron beams provided to the scientific community at the NCNR are more important today than they ever were in the past, and thus, it is essential that the NIST reactor be kept in operation for as long as possible.

Accomplishments

The reactor is being operated in a safe and reliable manner, and the status of the reactor and the reactor vessel is being monitored in an effective and conscientious manner. The NCNR has made plans to replace the hydrogen cold-neutron source inside the reactor vessel with a deuterium cold-neutron source—an upgrade that will significantly enhance the capabilities of the NCNR. Recognizing the importance of NIST being able to continue to provide a high-performance neutron source, the NCNR in 2017 completed a preliminary study of options,[7] some key findings of which are listed in Box 2.1. The NCNR would do well to elaborate this preliminary study into a systematic succession plan. Such a plan might touch upon not only the research services provided to the user community but also the benefits delivered in the associated application space, such as drug-delivery systems or practical fuel-cell power plants for vehicles.

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[6] T. Newton, NIST, "Reactor Operations and Improvements," presentation to the panel on July 10, 2018.

[7] NIST Center for Neutron Research, 2017, *Future Options for the Neutron Source at the NIST Center for Neutron Research*, June 15.

BOX 2.1
Key Findings of NIST Study of Future Options for the Neutron Source

In 2017, NIST elaborated three possible future options for its neutron source:

- Maintain NBSR [National Bureau of Standards Reactor] in its current configuration. No new neutron beams could be added.
- Major upgrade to the NBSR to increase flux in conjunction with conversion to low enriched uranium (LEU) fuel. Would allow some optics optimization but no increase or numbers of beams. Would necessitate 3- to 4-year shutdown and cost $550 million to $700 million (design, fabrication and construction).
- Building a replacement reactor. Would double the number of cold beams and allow five-fold increase in cold flux. No loss in continuity as NBSR could continue to operate concurrently. Would require 10- to 15-years and cost upwards of $1 billion.

SOURCE: NIST Center for Neutron Research, 2017, *Future Options for the Neutron Source at the NIST Center for Neutron Research*, June 15; T. Newton, NIST, "Reactor Operations and Improvements," presentation to the panel on July 10, 2018.

Opportunities and Challenges

The NCNR research reactor is one of only two high-performance, reactor-based neutron sources in the United States, and it is over 50 years old. It will require recertification in 2020, and it has already-known problems. Several of the cooling tubes in the reactor's thermal shield are plugged, and this could impact its longevity and maintenance. The ramifications become apparent when one realizes that it would take more than 15 years to replace the NIST reactor with a new one. Other research reactors of similar age have either been shut down or have plans to do so (e.g., the National Research Universal [NRU] reactor in Canada, the Petten reactor in the Netherlands, and the Halden reactor in Norway).

In 2017, the NCNR, as noted, completed a preliminary study of options for provision of neutrons for users for the long term.[8] Options elaborated by the study included continued operation of the current reactor, refurbishment of the current reactor, or replacement of that reactor with a new, modern, more powerful one. This study, and the more detailed one that is expected to follow, deserves the full support of NIST and the NIST Director, including, if necessary, funding for the design of a new reactor.

GLOBAL COMPETITIVENESS OF THE NCNR

The NCNR continues to be among the world's best facilities by all of the standard metrics, as can be seen from the data in Table 2.1.

Over the past decade, the U.S. position in the world neutron enterprise has eroded, and the future looks no better. Europe is well ahead of the United States in the production and delivery of neutron scattering capabilities, and China, as well as other parts of Asia, are expanding theirs, while the United States has closed the neutron facilities it once operated at Brookhaven National Laboratory and at Argonne National Laboratory.[9] There are currently three operational neutron sources in accessible user

[8] NIST Center for Neutron Research, 2017, *Future Options for the Neutron Source at the NIST Center for Neutron Research*, June 15.

[9] Argonne National Laboratory, undated, "Neutron Scattering Facilities," available at http://www.neutron.anl.gov/facilities.html, accessed August 28, 2018.

facilities the United States: two of them reactors, including the HFIR (High-Flux Isotope Reactor) at ORNL and the NCNR at NIST; and one spallation source, the Spallation Neutron Source, also at ORNL. A fourth might be included—the Lujan Center at LANSCE, which has four spallation beam lines, but whose only current user program is run through the NNSA (National Nuclear Security Administration). Both of the reactor-based sources are more than 50 years old. They are well regulated and safe, but a planned, or unplanned, closure of either facility would have a major and instantaneous negative impact on U.S. capabilities for developing advanced materials that drive future innovation, as well as important research on fundamental properties of the neutron, like its lifetime or an upper limit on its electric dipole moment. At present, there are no plans in place to replace either reactor. Moreover, were such a plan to be developed, replacement is a process of 15 years or more, at which point both reactors would be at least 65 years old. In comparison, Europe now has two spallation sources and four high-performance reactors,[10] although two of the latter are scheduled for decommission in 2019. The advantage the European Union now enjoys will become even greater when the European Spallation Source (ESS) comes on line around 2025. China[11] has two reactors that are less than 10 years old and a new spallation source that is coming up to power. Compared to its competitors, the United States is under-investing in neutron science, and this is eroding U.S. leadership, capabilities, and competitiveness. Scientific and industrial users based in the United States who apply for time at overseas facilities are bound to be treated less generously that those based in the countries that are paying for them. Thus, were the NIST facility to shut down, the economic benefits that derive from neutron research would increasingly accrue to other nations. Thus, it is more important than ever that NCNR plan for, and receive support for, securing future, internationally competitive neutron facilities—to include upgrades (e.g., the anticipated deuterium cold neutron source) and instrumentation—for the U.S. scientific and industrial communities. NIST would be well advised to articulate a succession plan for the future of its neutron source—the reactor itself. NIST would do well to remain in contact with the other U.S. facilities to coordinate and plan.

[10] Europe, spallation sources: ISIS, PSI (SINQ); reactors: ILL, FRM-II, LLB, BER-II.
[11] China, spallation: CSNS (first beam obtained); reactors: CARR (60MW), CMRR (20MW).

TABLE 2.1 Comparison of the NCNR with Other Neutron Facilities

	NCNR	HFIR	SNS	CMRR	HANARO	J-PARC	LANSCE[e]	ILL	ISIS	MLZ	PSI	ANSTO
n instruments (total-all types)	29	15	19	9	9	20	12	50	33	29	17[b]	14
Scattering	17	11	18	6	7[c]	16[a]	3	33	26[a]	23	11	13[a]
Imaging	2	1	0	2	2	1	2	1	1	2	2	1
Neutron Physics	6	0	1	0	0	1	5	9	0	0	0	0
Test Stations	1	0	0	0	0	1	2	7	1	2	4	0
Other[d]	3	3	0	1	0	1	0	0	5	2	0	0
d days	220	165	197	123	0	146	126	121	174	149	153	302
Type	Reactor (HEU)	Reactor (HEU)	Spallation (60 Hz)	Reactor (LEU)	Reactor (LEU)	Spallation (25 Hz)	Spallation (20 Hz)	Reactor (HEU)	Spallation (50 Hz)	Reactor (HEU)	Spallation (50 MHz)	Reactor (LEU)
MW	20	85	1.0	20	30	0.4	0.1	56	0.175	20	1.0	20

[a] One additional instrument is being commissioned or under construction.
[b] There is in addition a cold-neutron source.
[c] There are a further eight sources not/yet operational.
[d] "Other" could include PGAA (prompt-gamma neutron activation), for example.
[e] Statistics include Lujan Center and Weapons Neutron Research Facility.

NOTE: ANSTO, Australian Nuclear Science and Technology Organisation; CMRR, China Mianyang Research Reactor in Sichuan Province, China; *d*, days of operation per year (average of 2015, 2016 and 2017); HANARO, High-Flux Advanced Neutron Application Reactor of the Korea Atomic Energy Research Institute; HEU, highly enriched uranium; HFIR, High Flux Isotope Reactor at the Oak Ridge National Laboratory; ILL, Institut Laue-Langevin; ISIS, Spallation Neutron Source in the United Kingdom; J-PARC, Japan Proton Accelerator Research Complex; LANSCE, Lujan Neutron Scattering Center at the Los Alamos Neutron Science Center; LEU, low enriched uranium; MLZ, Meier-Leibnitz Zentrum based at the FRM-II reactor, Germany; *n*, number of instruments; NCNR, NIST Center for Neutron Research; PSI, Paul Scherrer Institute in Switzerland; SNS, Spallation Neutron Source at the Oak Ridge National Laboratory.

3

Adequacy of Facilities, Equipment, and Human Resources: Instrumentation Advances at the NCNR

MULTI-AXIS CRYSTAL SPECTROMETER

Accomplishments

The Multi-Axis Crystal Spectrometer (MACS), which has been operating for 8 years, is currently a world-class instrument for studying magnetic dynamics with high flux and low backgrounds, allowing a sensitivity in detecting small signals that is unmatched anywhere in the world. This instrument is critical in the search for quantum spin liquids, a phase of quantum matter that has long been predicted, but whose existence has never fully been established. Recent experiments on MACS are bringing us closer than ever before to establishing its existence. MACS is also critical for the study of unconventional superconductivity.

Opportunities and Challenges

Planned developments of MACS include lowering the background for better signal-to-noise ratio (e.g., it is critical for weak magnetic signals in the quantum spin liquid) and the development of event-mode neutron detection, which will greatly increase experimental throughput, enable instruments to collect data while the instrument is moving, and provide tools to study time-dependent phenomena.

MACS is losing its leading-edge because of the development of competing capabilities at both spallation-based and reactor-based neutron sources around the world—for example, instruments at the Spallation Neutron Source, Paul Scherrer Institute, and the European Spallation Source (ESS). The putative MACS-II upgrade of MACS is needed to turn MACS into a polychromatic multi-plexed instrument. Importantly, however, funds have not been secured for this project. The existing MACS instrument will continue to be the one of choice for experiments that require a few fixed-energy cuts in reciprocal-space, so a complementary suite of MACS-II, which would reside on the revamped NG4 line after the replacement of the cold-source, and MACS-I, on its dedicated cold-source with highly optimized optics, will leave the NCNR well-placed to tackle the emerging challenges in quantum magnetism.

NEUTRON IMAGING

Neutrons and photons interact with matter differently and, thus, provide complementary information about its structure and properties. While this has been widely understood and exploited to do absorption, emission, and scattering experiments, the advantages of neutron imaging have been far less appreciated than have those of photon imaging. the NCNR is now, and continues to be, a world leader in neutron imaging.

Accomplishments

NIST's Neutron and X-Ray Tomography (NeXT) system has been available to users since June 2016 and has already contributed to advances in the study of novel batteries, concrete degradation, geologic flows, and shale composition. This instrument—the only one of its kind—can simultaneously carry out neutron and X-ray tomography experiments on samples. This instrument makes it possible to do structural, compositional, temporal, and functional experiments on essentially any sample under a variety of environments and operational conditions. Substantial improvements in both the spatial and the temporal resolution of the NeXT instrument are expected to materialize over the next 4 years**.** Improvements in spatial resolution obtained using the 1.5 micron detector on this instrument have already led to new insights into fuel-cell operation, owing to the neutron's unequalled sensitivity to water. Later in 2018, this detector will be upgraded with a higher frame-rate camera and other improvements in its optics.

Opportunities and Challenges

Introduction of Wolter optics to the NeXT instrument in coming years will enable improved time and spatial resolution, permitting more detailed exploitation of more complex sample environments. The neutron phase-imaging option on this instrument provides enhanced sensitivity to structural thickness and other structural properties by more than an order of magnitude. New neutron-grating interferometers are under development and will permit even greater sensitivity. Far-field interferometry is a promising tool for a wide variety of materials science problems, but its development faces significant challenges in the near term. New gratings will be required for improved fringe visibility, and a dynamic source grating also has to be developed. New data analysis strategies and software will be needed. All of these require increased funding over what is now available. The NCNR is now seeking internal funding through NIST's Innovation in Measurement Sciences (IMS) Program for these initiatives, which needs to be given appropriate attention by NIST decision makers.

STRESS DIFFRACTOMETER

Opportunities and Challenges

The BT8 beam guide, along with the residual stress diffractometer it feeds and its associated instrumentation, was introduced in the mid-1990s. It is currently undergoing a series of upgrades that will increase its data acquisition rate by a factor of 20 or more. It provides a platform for the noninvasive study of inhomogeneous stresses and strains produced in materials by industrial processes such as stamping of automotive hoods, fastening two metals together, or additive manufacturing. Its strain-measuring devices were built to support the NIST Center for Automotive Lightweighting, an industrial consortium led by the NIST Material Measurement Laboratory (MML). Users of this facility include academic researchers, industrial laboratories, and the U.S. Army.

SOFTWARE DEVELOPMENT

Accomplishments

Software is essential for interpreting data. In many instances, the lack of consensus across the scientific community about how best to analyze particular types of data creates confusion. The NCNR is to be commended for leading efforts to develop consensus by developing software that can analyze scattering data measured at any facility (globally). This software includes the packages SASSIE, SASView, and Refl1D, widely used by the user community, for analyzing small-angle scattering and reflectivity. Reductus, a browser-based online analysis platform for reflectivity data, has been rolled out and looks promising.

Challenges and Opportunities

Software development is absolutely essential for instrument control and data acquisition. The NCNR has a small, but effective, software group of five people, although it is facing a challenge, which is unlikely to disappear anytime soon, in recruiting and retaining talent in this area, because enticing opportunities abound for people skilled in software development. On the controls/data acquisition side, the staged rollout of the NICE software platform continues, and it is now used to control nine instruments, apparently with good user satisfaction overall. This rollout will continue in the upcoming period.

Developments are in progress to improve the analysis of polarized, time-resolved, and two-dimensional (2D) anisotropic data. There is a significant need to develop software that will make it easier to relate real-space structures to scattering measurements in Fourier space and to complement scattering measurements with simulations.

NIST actively seeks outside resources to support software development through joint development projects with other facilities and through direct government funding. Refl1D, the NCNR reflectometry program, was initially developed under the DANSE (Distributed Data Analysis for Neutron Scattering Experiments)[1]-reflectometry National Science Foundation grant. It is arguably the most complete and versatile package for analyzing specular reflection data, but it has not been embraced globally. The DANSE project also supported the precursor to SasView, and SasView itself is in the process of being transitioned into what is being called the “community collaborative” software project. It currently has European Union funding through 2020 under the SINE2020 (Science and Innovation with Neutrons in Europe in 2020).[2] Further development will likely come in the form of programming resources from three main facilities: NCNR, ESS, and the ISIS Neutron and Muon Source.

NEW INSTRUMENTS

Very Small Angle Neutron Scattering

The commissioning of the Very Small Angle Neutron Scattering (v-SANS) instrument will markedly improve the capabilities that the NCNR can offer the soft-matter community. This long-awaited, long-in-development instrument will give researchers access to length scales from 1 micron down to 1 nm using a three-detector system, with high flux on the sample. Using either a white beam, a velocity selector, or a graphite monochromator, the wavelength and wavelength resolution can be selected by the user to optimize the beam either for time-resolved studies or for very high spatial resolution.

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[1] Further information is available at the Distributed Data Analysis for Neutron Scattering Experiments (DAMSE) website at http://danse.us/.

[2] SINE2020 is a consortium of 18 partner institutions from 12 countries, funded by the European Union through the H2020 programme. Further information is available at the SINE2010 website at https://www.sine2020.eu/.

Experiments can be performed either with multi-pinhole focusing optics, which requires large samples, or with a single-pinhole or a slit geometry, in which case the data must, by default, be de-smeared. The versatility and flexibility designed into this instrument will make it suitable for carrying out a wide variety of experiments such as the study of membrane proteins or of micelles for use in drug-delivery systems.

Preliminary data indicate that v-SANS can achieve the ultrahigh resolution it was designed for while at the same time delivering a high-flux beam to the samples. In fact, initial experiments indicate that, for otherwise similar operating conditions, the flux on the sample in the v-SANS instrument is about twice that provided by existing SANS instruments at the NCNR. During the next cycle, the instrument will be made available to users for one-third of the beam time and in the following cycle for two-thirds of the beam time.

Chromatic Analysis Neutron Diffractometer Or Reflector

The Chromatic Analysis Neutron Diffractometer Or Reflector (CANDOR) instrument, scheduled to be fully operational in 2019, has a novel reflectometer design for reactor sources that involves the delivery of multiple streams of neutrons with different wavelengths onto the sample at the same area using an array of monochromators. A single CANDOR detector array consist of 54 highly oriented pyrolytic graphite crystals set at different takeoff angles to diffract neutrons into 6 LiF:ZnS(Ag) proportional counters. Specular reflectivity at multiple scattering vectors can be measured simultaneously, greatly reducing the time of measurement, and opening the possibility of performing time-resolved reflectivity studies or allowing measurement on very small samples, which is particularly important for polarized reflectivity measurements on magnetic systems. The science that will be enabled with CANDOR will include time-resolved interfacial and thin-film behavior of soft matter and polarized reflectivity measurements on very small magnetic multilayer samples.

4

Assessment of Technical Programs: Scientific Areas Investigated at the NCNR

CONDENSED MATTER PHYSICS: SOFT MATTER

The comprehensive suite of scattering instruments at the NCNR, including uSANS, vSANS, two 30-meter SANS, MAGIK,[1] Polarized Beam Reflectometer (PBR), and horizontal reflectometer (soon to be sunset), provide soft matter researchers in condensed matter physics (CMP) with a comprehensive world-class set of instruments to address both fundamental and applied problems for which the use of neutrons is necessary and critical. The novel Chromatic Analysis Neutron Diffractometer Or Reflectometer (CANDOR), when fully realized in 2019, will be a game changer for diffraction and reflectivity measurements at a reactor source. Through the simultaneous use of multiple wavelengths, large effective enhancements of the neutron flux on the sample will be achieved. The High Flux Backscattering Spectrometer (HFBS) has been enhanced by near doubling of its flux by the improvement in focusing optics. Together, HFBS and the Neutron Spin-Echo Spectrometer (NSE) enable molecular-level motion to be correlated with soft-matter structure. The partnership with the National Science Foundation to operate the Center for High Resolution Neutron Scattering (CHRNS), which supports the operation of these spectrometers, is a crucial component for the NCNR's continued leadership in soft matter research.

Accomplishments

The NCNR continues to carryout leading-edge research in the area of complex fluids and flow, covering diverse areas of structure, dynamics, and functionality. Scanning Narrow Aperture Flow uSANS (SNAFUSANS) is a robust sample environment available for users to measure structure along the flow gradient. Such measurements, for example, enabled concentration gradients induced by shear stress to be measured in shear-banding fluids. These flow-induced concentration gradients govern and provide desired flow properties in commercial products ranging from shampoos to fluid additives for drag reduction and enhanced oil recovery.

Neutron-scattering measurements continue to provide important new insight for controlling complex fluid systems. The SANS rheology sample environments were developed at the NCNR with the

[1] Further information available at https://www.nist.gov/ncnr/spin-filters/spin-filter-instruments/magik.

University of Delaware's Center for Neutron Science. The team has also provided assistance for SANFUSANS to be implemented on the D22 beamline at the Institut Laue-Langevin (ILL).

Research on the structure of nanoparticle grafted polymer chains[2] has clearly demonstrated the power of neutron scattering to provide information that is otherwise difficult, or impossible, to obtain. The synthesis of nanoparticles may provide new ways of catalyzing a wide variety of chemical reactions in both laboratory and industrial contexts. By selectively deuterating the inner-only versus outer-only portion of the grafted polymer chains (corona), the variation in polymer chain stretching away from the nanoparticle surface was directly measured by SANS. The structure, thus determined, matched well with theoretical predictions, and these structure models are being incorporated into the SASSIE analysis software. Importantly, the integrated and complementary instruments of the NCNR CHRNS facility enabled researchers to go beyond static structure and to measure chain dynamics in two polymer-corona regions, which differed significantly, on the same samples using the NSE spectrometer. These are the first measurements of their kind.

A second research presentation on lipid membranes[3]—barriers that separate cells from the surrounding environment and that delimit their internal compartments—demonstrated additional efforts to couple neutron scattering measurements of structure and dynamics. It is believed the dynamical properties of these membranes play a critical role in determining their functional properties. In this case, the change in dynamic fluctuations of two-component lipid membranes as a function of composition and temperature were determined. The decrease in fluctuations could be directly mapped onto changes in the bending modulus of the membrane. Although the membrane composition was relatively simple, these measurements are compelling for continuation work to measure the impact of composition and inclusions such as raft domains, proteins, and so forth on membrane dynamics.

Opportunities and Challenges

With the recent demonstration of Dielectric RheoSANS, SANS rheological measurements can now be carried out simultaneously with dielectric spectroscopy. This novel sample environment enables (di)electric properties to be directly coupled to changes in structure/morphology and flow/stress. Syncing the three simultaneous data sets—structure/morphology, flow/stress, and dielectric properties—is well under way and will lead to fundamental insights into structure-property relationships in conducting systems under steady and dynamic flow conditions. Plans are in place to make this sample environment available to users.

CONDENSED MATTER PHYSICS: HARD MATTER

Accomplishments

The scientific impact of the NCNR in the area of CMP is very high. Measurements being done at the NCNR on magnetism, superconductivity, and multiferroics continue to produce new insights that advance our understanding of these materials. Strong electron correlations in materials lead to emergent properties that result in unusually large material responses to external stimuli. This makes these materials of interest for the construction of transducers and non-volatile memories. A particularly exciting recent development is the verification of topological effects in materials. Neutrons have had a large impact in the study of skyrmions— topological spin-texture objects that are studied using SANS—and the NCNR has

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[2] M. Hore, Case Western Reserve University, "Structure and Dynamics in Polymer-grafted Nanoparticle Systems," presentation to the panel on July 11, 2018.

[3] E. Kelley, NIST, "Insights into the Dynamics of Heterogeneous Lipid Membranes from Neutron Scattering," presentation to the panel on July 11, 2018.

been in the forefront of these developments. An exciting study reports the generation of ground-state skyrmions created by patterning a planar vortex configuration within cobalt nanodots of diameter 560 nm and height of 30 nm that are placed on top of a magnetic thin film.[4] The nanodots produce boundaries that favor a planar vortex configuration of spins in the film, but the spins lower their energy by "escaping to the third dimension" toward the center of the dot to yield a skyrmion.

The NCNR has excellent capabilities on a number of beamlines for producing polarized neutron beams that are ideally suited for measurements of spin and spin fluctuations in traditional magnets and in exotic quantum magnetic systems. The Multi-Axis Crystal Spectrometer (MACS, as noted in Chapter 0), has been operating for 8 years and is currently a world-class instrument for studying magnetic dynamics with high flux and low backgrounds, allowing a sensitivity to detecting small signals that is unmatched anywhere in the world. This instrument is critical in the search for quantum spin liquids, a phase of quantum matter that has long been predicted, but whose existence has never fully been established. Recent experiments on MACS are bringing us closer than ever before to establishing its existence.

Experiments on unconventional superconductivity have utilized the MACS to show strong interactions between itinerant electrons and magnetic spins in $CeCoIn_5$ cause an unusually high critical temperature (Tc).[5] These imply a direct role of spins in the superconductivity and a change in the magnetic exchange energy on entering the superconducting state that leads to a novel incommensurate entwined magnetic/superconducting state called Q-phase. Planned developments of MACS include lowering the background for better signal-to-noise (critical for weak magnetic signals in the quantum spin liquid for example) and the development of event-mode neutron detection, which will greatly increase experimental throughput.

BIOLOGY

Neutron scattering is used by biological scientists to obtain low-resolution information about the structural organization of biological materials that would be challenging to secure by other means. It can also be used to obtain insights into the dynamic properties of biological systems of all kinds. Many of these experiments exploit the difference in scattering lengths between hydrogen ($b = -0.374 \times 10^{-12}$ cm) and deuterium ($b = +0.667 \times 10^{-12}$ cm) either to produce differences in contrast between components of large biological structures that otherwise would not exist, or to alter those that already do. It is also used to control the contrast between these structures and the solvents in which they are dissolved. The NCNR facility, as noted, includes several kinds of instruments useful for doing experiments of this sort: SANS diffractometers, neutron reflectometers, and an NSE spectrometer (i.e., the NG-A). For example, the SANS spectrometers have been used recently to characterize the structure of nucleosomes and to investigate the time-averaged structure of immunoglobulins. Neutron reflectometers are used to determine the transverse distribution of scattering-length density in lipid membranes. This allows for better understanding of the three-dimensional structure and dynamics of macromolecules with health care and other applications.

Accomplishments

The reflectometers at the NCNR have been used recently to investigate the organization of the complexes that lipid bilayers form with specific proteins and polypeptides. Inelastic neutron scattering is

[4] D.A. Gilbert, B. Maranville, A.L. Balk, et al., 2015, Realization of ground-state artificial skyrmion lattices at room temperature, *Nature Communications* 6:8462.

[5] C. Stock, J.A. Rodriguez-Rivera, K. Schmalzl, F. Demmel, D.K. Singh, F. Ronning, J.D. Thompson, and E.D. Bauer, 2018, From Ising resonant fluctuations to static uniaxial order in antiferromagnetic and weakly superconducting $CeCo(In_{1-x}Hg_x)_5$ (x = 0.01), *Physical Review Letters* 121:037003.

the only experimental technique available for characterizing the large-scale conformational changes associated with the activities of biological structures of all kinds. The NSE spectrometer has been used to good effect recently to study the dynamics of both cytochrome P450, and a series model phospholipid bilayers.

Opportunities and Challenges

Biological scientists are regular consumers of beam time at neutron scattering facilities all over the world, and they have long been members of the user community at the NCNR, which has several first-class instruments suitable for biological experiments. Nevertheless, although biological scientists consume approximately 15 percent of the beam time at the NCNR, only approximately 6 percent of the most highly cited papers that have emerged from the NCNR over the past decade describe work done on biological samples, as determined by the web of Science.[6] Consistent with these statistics, the leadership of the NCNR did not indicate that it believed biological science is one of the facility's strong suits. In fact, most of the biology-related posters presented to the panel described studies directed at bioengineering issues, rather than biology per se. This work may well be useful to those concerned about the specific applications to which they pertain, but it is unlikely to attract much attention from the wider scientific community. All of the above notwithstanding, the measurements of lipid bilayer dynamics that have been done recently at the NCNR did much to reassure the panel that neutron-scattering experiments can produce important information about biological systems that cannot be obtained in any other way.

Three conditions must be met if a biological neutron scattering experiment is to have a large impact: (1) the system examined must be scientifically significant; (2) the experiments must yield information that could not easily be obtained by any other means, if at all; and (3) the information must materially alter the way biological scientists think about the system. Many of the opportunities for doing high-impact neutron experiments on biological systems have been, and continue to be, missed. The problem is that the vast majority of the biological macromolecular systems under investigation today are studied by biological scientists well trained in X-ray techniques but not in those using neutrons and, hence, are oblivious to the opportunities it offers. Moreover, until one of the groups working on such a system is persuaded of the value of the information neutron-scattering experiments might provide, no one is going to make the investment required to do those experiments. Furthermore, it is unrealistic to expect that groups already working at the NCNR will start doing experiments on a system unrelated to the one they are already studying, just because it looks promising. The grant support system discourages such changes in direction. It would be worthwhile, therefore, for the NCNR to make a special effort to educate the larger biochemical and biophysical communities about neutrons. If just a few of the groups that are studying systems that might yield high-impact neutron data could be persuaded to do work at the NCNR, both the quantity and the quality of the biological papers produced at the NCNR would improve considerably.

CHEMICAL PHYSICS

Many of the systems that chemical physicists study at the NCNR are relevant to today's economy and to technical innovation. Importantly, the pursuit of basic scientific challenges in the NCNR program has also been thriving, so it is impossible to capture the full range of the chemical physics problems addressed at the NCNR in just a few sentences. The systems investigated include materials for capturing and storing Cl_2, Br_2, H_2, and methane. Substances that are superconducting or that have interesting magnetic properties have also been receiving considerable attention lately, as have some novel polymer physical chemistry challenges.

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[6] NIST, "Highly Cited Publications: 2008-2017," background paper transmitted to the panel, June 27, 2018.

Opportunities and Challenges

It is important to note that the most important instrument at the NCNR for these investigators is BT-1, which is a powder diffractometer. This is the oldest instrument now operating at the NCNR, and while it is unquestionably true that a better powder diffractometer could be built today, there are no plans to replace it. Lack of resources, rather than lack of need, appears to be the reason.

ENGINEERING PHYSICS

The NCNR has an engineering physics effort focused primarily on stress analysis of industrially important materials using the RT8 Residual Stress Diffractometer. In the past few years, this effort has responded to two important new manufacturing developments: (1) the ongoing transition in passenger vehicles from steel-based structures to bodies composed partially of aluminum, magnesium, and advanced high-strength steel brought about by commitments to increase fuel efficiency and (2) the introduction of additive manufacturing (AM) (often referred to as 3D printing) into a variety of industries, most notably the aircraft industry. Both developments create internal stresses that need to be characterized and understood, because they can lead to long-term degradation. The transition to lighter metals requires methods for joining different metals beyond spot welding.

Accomplishments

Experiments at RT8 measured stresses in joined sheets of different materials produced by three alternatives fasteners: self-piercing, flow-drill screw driving, and composite friction rivets. Another series of experiments measured internal stresses in additively manufactured steel cylinders of different sizes.

NEUTRON SCIENCE

The Neutron Physics Group of the NIST Physical Measurement Laboratory performs experiments at the CNR, but being as they are from a different NIST laboratory, the group was not under review. The group leader nonetheless provided an informative presentation on the group's work on neutron science and metrology.

The basic science could be summarized as focusing on fundamental neutron physics, neutron interferometry, and reactor and solar neutrinos.[7] The neutron undergoes beta decay—into a proton, beta-minus particle (i.e., an electron), and an anti-neutrino—in accord with the Standard Model. The lifetime of the neutron is not however known to good precision; there remain discrepancies between beam- and bottle-type experiments. The physics of this electro-weak interaction is being investigated using cold beam neutrons. The aCorn experiment measures electron and proton momenta to permit inferences of the angular correlation of these two subatomic particles. The group reports the most precise measurement of the angle—the dimensionless parameter "a"—to date following a 15-month data run at the CNR.[8] In its experiments using neutron interferometry, the group conducts experiments to observe phase-coherent neutron waves. The group's work on neutrinos is searching for what are dubbed sterile neutrinos, a fourth flavor of this particle such as might explain anomalies such as the reactor neutrino deficit. The Li6-doped liquid scintillator they are developing is operational at HFIR at the Oak Ridge National Laboratory.[9]

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[7] J.S. Nico, NIST, "Recent Results in Neutron Physics," presentation to the panel on July 10, 2018.

[8] Darius, G., W.A. Byron, C.R. DeAngelis, M.T. Hassan, F.E. Wietfeldt, B. Collett, G.L. Jones, et al. 2017, Measurement of the electron-antineutrino angular correlation in neutron β decay, *Physical Review Letters* 119:042502.

[9] J.S. Nico, NIST, "Recent Results in Neutron Physics," presentation to the panel on July 10, 2018.

The group also undertakes investigations on the neutron magnetic dipole moment as a proof-of-concept for work on setting an upper limit on the neutron's *electric* dipole moment, the ultimate value of which cannot be non-zero without violating time reversal symmetry in the Standard Model. The group also provides metrology services—for example, the recalibration of the NBS-1 national neutron standard.[10] (Discussion of neutron research services at CNR may be found in Chapter 3, in the section "Neutron Imaging.")

[10] J.S. Nico, NIST, "Recent Results in Neutron Physics," presentation to the panel on July 10, 2018.

6

Portfolio of Scientific Expertise

NCNR PARTNERSHIPS

User Program and Obtaining User Access to the NCNR

The NCNR is dedicated to providing neutron beams for use by the scientific user community in keeping with the scope and mission of its parent agency NIST. Through the NCNR, NIST maintains and operates the nuclear reactor and some associated instrumentation. The NCNR also supports a large user program. Twice a year, there is an open call for user proposals, which are submitted via an online portal. Users have commented that the web-based interface, which they must use, has improved over the past few years, making it more intuitive, stable, and user friendly. Proposals are peer-reviewed by three to five external referees for technical merit and by the NCNR beam scientists for feasibility. Proposals are required to include a list of recent publications from previous beam-time allocations. The proposals are then ranked, and awards of beam time are made by the Beam-Time Allocation Committee (BTAC). Proposals not awarded beam time are returned to the user with comments received from the referees to improve subsequent submission. The number of participants and proposals have been increasing at a rate of 6 and 10 percent per year, respectively, since 1991—a testament to the quality of the facility, the outreach efforts of the NCNR staff scientists, and the growth of the neutron-scattering community in the United States.

Accomplishments

The NCNR User Group conducted a survey of its users in 2015 to determine what the NCNR could do to improve its service to the user community. The panel was provided with the results of that survey and the NCNR's response to it, which was deemed satisfactory by this review panel. The chairperson of the User Group, Associate Professor Megan Robertson of the University of Houston's Department of Chemical Engineering, described the User Program, the proposal submission and review process, and the interactions between the User Group and the NCNR management, and she provided very positive feedback on the overall operation of the NCNR and the User Program.[1]

[1] M. Robertson, University of Houston, presentation to the panel on July 10, 2018.

Center for High Resolution Neutron Scattering

The Center for High Resolution Neutron Scattering (CHRNS) is as noted a partnership between the National Science Foundation (NSF) and the NCNR that supports seven of the NCNR's premier neutron-scattering instruments. This partnership is critical to the NCNR's ability to offer an effective user program because of its investments in beamline and special-environment staff and equipment. The main mission of CHRNS is to develop and operate state-of-the-art neutron-scattering instrumentation with broad applications in materials research for use by the general scientific community. Its mission, in keeping with that of the NSF and its education and outreach mission, differs slightly from that of NIST but in important ways. The ability of the NCNR, through this partnership, to meet the needs of both agencies greatly enhances the impact of the facility on the community.

CHRNS is also responsible for a significant effort in scientific support services, not least of which are the Helium-3 (^3He) spin filters that are critical to the spin polarized measurements on MACS and SANS. These filters, which will also be installed on vSANS and CANDOR, require considerable technical support made possible by the CHRNS partnership.

Accomplishments

The main mission of CHRNS is as noted to develop and operate state-of-the-art neutron-scattering instrumentation with broad applications in materials research for use by the general scientific community. The development of new capabilities provide significant benefits for the NCNR and all of its stakeholders. It also has a significant impact on the scientific output of the NCNR by providing and supporting sample environments and by providing user support before, during, and after experiments. Finally, it supports the NSF missions of education and outreach, which increases the nation's expertise and enhances the NCNR education and outreach activities, particularly through the Summer Undergraduate Research Fellowship (SURF) and the Summer High School Intern Program (SHIP) programs as well as neutron-scattering schools run at the NCNR have helped educate students and active scientists about neutrons, thereby increasing the pool of potential users.

CHRNS also leads in user training on CHRNS instruments and in user-environment support, including ancillary laboratories and devices for controlling sample temperature (including milli-Kelvin [mK] cryogenics), pressure, magnetic field, humidity, and fluid flow. In addition, CHRNS is the epicenter of the NCNR's education and outreach efforts, which have had high impact. NCNR staff presented a number of anecdotes of people who attended a school or summer experience at the NCNR, loved it, made their way into a doctoral program that involved neutron scattering, and became young faculty building their own neutron-scattering active groups. The large size of the neutron community in Europe, compared to that in the United States, is often attributed to the fact that European universities are much more willing to support neutron-scattering groups than are their U.S. counterparts. The fact that 33 percent of the NCNR postdoctoral researchers have made their way into faculty positions is not only an amazing feather in the NCNR's cap, but it also bodes well for the future of neutron scattering in the United States.

Opportunities and Challenges

The current CHRNS agreement with NSF runs through 2020, and every effort needs to be made by the NCNR to ensure that it is renewed. Without CHRNS, the effectiveness of the User Program at the NCNR would suffer. The NCNR needs to act, in consort with the user community, to increase the visibility of CHRNS, to ensure that NSF and CHRNS are appropriately acknowledged in publications resulting from research performed on CHRNS instruments, and to continue and broaden the education and outreach components of CHRNS, which are absolutely essential to NSF.

The suite of CHRNS instruments, which includes many of the most exciting at the facility (MACS(II), HFBS, NSE, vSANS, and CANDOR, and so forth), is continually evolving. The vSANS is just entering the user program, and CANDOR is being installed, although its high-resolution, fixed, small-angle detector at the end of the secondary flight path has not yet been installed. The vSANS will make it possible to measure the scattering profiles of samples over an unusually wide Q-range, opening the way to studies of samples that exhibit structure at many different length scales. CANDOR is a high-throughput reflectometer that utilizes a polychromatic incident beam that provides large gains in measurable intensity. Its introduction into operations has been delayed, in part owing to the discovery that the signal from inelastically scattered neutrons in the analyzers was having a (detrimental) effect on the performance. This necessitated a redesign with cryogenically cooled analyzer crystals. The decision to halt the project and fix it, rather than to take the alternative approach to make post-hoc corrections was bold but correct. While it delays deployment of the instrument, the redesign will give much higher quality data.

User Program—nSoft

nSoft is an industrial consortium, unique among neutron-scattering user facilities, designed specifically to engage industry in neutron scattering. The consortium was inaugurated in 2012 and has since grown to include 15 companies. Member companies pay $25,000 per year to participate in this program, which focuses on the development of

- Advanced measurements of industrially relevant materials and manufacturing processes and
- Member companies' own measurement technologies, including their analytical research programs.

The nSoft director schedules beamtime on the 10 m SANS and arranges beamtime on other instruments for member companies. All nSoft research is nonproprietary, since, by law, all proprietary research must be done on a full-cost-recovery basis. Proposals for nSoft research projects that are to be performed on nSoft's beamlines do not pass through the normal user proposal review process; instead they are approved by the member companies and NIST personnel. This procedure overcomes significant impediments to industrial use of national facilities by reducing the time required to get beam time and perform experiments and by implementing less stringent guidelines for scientific originality. The intent is to be more useful to the industrial sector, which often has to deal with significant time constraints. nSoft is an innovative concept that provides an excellent way to educate industrial concerns about the utility of neutron science and to encourage them to add it to their research toolboxes.

Though the nSoft consortium has published a few papers, including one in *Nature Communications*, its overall publication rate is far below that of the NCNR's general user program. This could reflect nothing more than the newness of the program, but it could also reflect inherent reluctance of industry to publish, even though the research is nonproprietary. (The value of the research to the company's business plan or to its customers was not judged by the panel.) Nevertheless, there are apparently no protocols in place to evaluate the effectiveness of the nSoft program, and it would be well to develop metrics which would include parameters other than publication number and citations that are acceptable to the nSoft member companies, the NIST personnel involved in nSoft, and the NCNR and NIST management. These need to be publicly available, and an independent assessment of the progress of the program needs to be made from time to time. This will provide nSoft with the information it will need to justify its continued existence. As the NCNR's programs continue to grow, and more and more demands are placed on existing beamlines, it will be necessary for nSoft and the NCNR to develop strategies for deciding future directions.

NCNR/University Cooperative Agreements

The NCNR has cooperative agreements with the University of Delaware, the University of Maryland, the University of Indiana, and Carnegie Mellon University. Some of these agreements are quite long-standing, while others are more recent. Other universities can apply for their own cooperative agreement when calls for proposals are announced. The agreements provide NCNR funding to universities for the support of technical staff, postdoctoral researchers, and graduate students engaged in neutron science and instrumentation at the NCNR. Technical staff, including beam-line scientists and software developers, hired under this program help run the NCNR facility and are stationed at the NCNR. Most postdocs and graduate students, in contrast, are stationed at their host universities. At the moment, this program supports 9 graduate students, 6 postdocs, and 23 technical staff. It has the added benefit of outreach to university students, both undergraduate and graduate, with many postdocs being recruited to the NCNR following their graduate work. While students must focus on their thesis research to graduate, they and post-doctoral fellows do provide the NCNR with extra people to carry out research, to engage in instrument developments, and, to a lesser extent, to contribute to the operation of instrumentation on beamlines. Faculty involved in these agreements have the advantage of having an on-site representative from their group at the NCNR. It would be beneficial for the NCNR to consider increasing the number of these agreements to expand on the research being done at the facility and further diversify the academic engagement.

NIST STAFF

The NCNR fields a staff of 217, of which 103 are in condensed matter science, 44 in facilities and operations, 36 in construction, and 34 in safety and administration. There are 5 affiliated technical staff/instrument scientists per instrument to serve/collaborate with users. In addition, NCNR scientists have active research programs of their own, discussed in Chapter 0. For comparison, the world's largest neutron user facility, the Institute Laue-Langevin in Grenoble (ILL), requires 7 technical staff/instrument scientists per instrument.

Accomplishments

The NCNR maintains a robust safety management program that addresses radiological, occupational, and industrial hazards. Key elements of the program include management commitment and employee involvement, worksite inspections, management observations, hazard prevention and control (including planning for work involving radiological hazards), and training for staff and users. In addition to operating with a strong safety management program, the NCNR has an excellent safety record that includes no regulatory violations since the last panel assessment in 2015.

The NCNR also supports a large user program. The number of participants and proposals have been increasing at a rate of 6 and 10 percent per year, respectively, since 1991—a testament to the quality of the facility and the outreach efforts of the NCNR staff scientists

Opportunities and Challenges

Increasing security and safety demands will place strain on current staff and threaten continuing ease of access of the facility to users.

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Dissemination of Outputs

CENTER FOR HIGH RESOLUTION NEUTRON SCATTERING-SPONSORED SUMMER SCHOOL

The NCNR has been very active in outreach activities over a broad spectrum of educational levels. This is an important component of the overall facility's program, and NCNR staff reported that the researchers at the NCNR are enthusiastically engaged in it. The flagship outreach program is the highly oversubscribed Center for High Resolution Neutron Scattering (CHRNS)-sponsored summer school for graduate students and young scientists. The emphasis of the school varies from year-to-year with content ranging from elastic scattering to inelastic scattering to imaging. The focus on neutron imaging, neutron spectroscopy, neutron reflectometry, and SANS at this school is more intense than it is at the National School on Neutron and X-ray Scattering offered each year by the Argonne National Laboratory and Oak Ridge National Laboratory.

Accomplishments

The CHNRS school provides students with significant hands-on time with instrumentation, and in several cases, has enabled them to later gain access to NCNR facilities through the standard proposal mechanism. While the school has a strong record of engaging, educating, and exciting students about the possibility of using neutrons in their own research, it has also been used more recently to reach out to communities—for example, the geosciences community—whose members may be unaware of what neutrons could bring to their research. Consequently, this school is expanding the pool of possible neutron users, which benefits the entire neutron community. Participation in the CHRNS summer school is capped at 35 persons, comprising graduate students, postdoctoral researchers, and junior faculty.[1] The return rate on this school— that is, the number of students who actually return to perform experiments, is quite high, of order 75 percent—a testament to the school's effectiveness.

[1] NIST Center for Neutron Research, undated, "Summer School on the Fundamentals of Neutron Scattering," https://www.ncnr.nist.gov/summerschool/ss17/index.html, accessed August 29, 2018.

OTHER EDUCATION AND OUTREACH

In addition to the summer school, outreach activities include a component of the NIST Summer Institute for middle-school science teachers at CHRNS. The goals are (1) to provide them with enough information about neutrons and neutron experiments that they will be able to incorporate neutron science into their curriculum and (2) to allow them to experience the excitement of participation in a real experiment, an excitement that they can pass on to their students, thus multiplying the impact of the summer school. Middle schoolers are at the age when exposure to new ideas can have its greatest impact, and exposure to the mysteries of neutrons can broaden their horizons and possibly lead them to a career in science.

The NIST Summer Undergraduate Research Fellowship, part of the Research Experience for Undergraduates program, is geared toward undergraduate students who spend time at the NCNR engaged in research with an NCNR advisor. Hosted at CHRNS, it has seen over 160 students take advantage of the program with approximately 70 percent of the attendees advancing on to graduate school.

NCNR staff also engage with the community through school demonstrations and presentations and the Adopt-a-School and Adventures in Sciences programs. These activities are also augmented by tours of the facility for students and professional groups, lectures by the staff at universities, and participation in national and international conferences. These latter activities are particularly important because they provide a venue for the staff to interact one-to-one with professional scientists and possibly convince them to pursue neutron research.

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Key Findings and Recommendations

REACTOR

The nuclear reactor on which the NCNR depends is 50 years old, and as a matter of simple prudence, a plan needs to be developed that will ensure that NCNR users have the neutrons they need into the indefinite future. In June 2017, the NCNR issued a report describing the results of a brief study of the following available options: (1) continued operation of the existing reactor, (2) upgrade of that reactor, and (3) its complete replacement. This report needs to be updated and a much more detailed plan developed. Options 1 and 2 are inferior to Option 3. The NCNR report indicated that Option 3 is likely to cost about $1 billion and take more than 15 years to complete. A project of this magnitude will not be undertaken without a substantial planning effort and support from the neutron and the general scientific communities. An advantage of building a new reactor is that the current reactor could continue running, and thus serve the user community, while the new reactor is being built. If Option 1 were to be pursued, the United States will become increasingly noncompetitive internationally. If Option 2 were chosen, user services will be interrupted for at least 2 years, risking permanent loss of the user community.

The reactor is 50 years old. Loss of this facility would have a strongly negative impact on neutron science within the United States and the scientific disciplines that CNR serves.

RECOMMENDATION: The NCNR should commission a detailed assessment of the current facility and begin the conceptual design of a new reactor. NCNR would do well to elaborate a systematic succession plan in concert with NIST leadership.

OPERATION

While external reviews of the NCNR that are conducted less frequently than annually have been and continue to be useful, they do not provide sufficiently current or detailed evaluations and tracking of the center's technical and operational issues. In particular, there is no apparent formal, regular assessment connecting the NCNR to NIST overall and to the NIST Visiting Committee on Advanced Technology (VCAT) in particular. External reviews of the NCNR consisting of scientists and managers familiar with the international neutron communities and landscape, need to be conducted annually. Their annual reports to the NCNR director and to the cognizant NIST Director would be beneficial. Such annual reviews are especially needed at this time in view of the major strategic issues facing the NCNR in the execution of its strategic objectives:

External reviews conducted less frequently than annually are not able to provide sufficiently current or detailed evaluations of the NCNR nor to track its technical and operational issues.

RECOMMENDATION: The NCNR should establish external reviews that assess its technical and operational issues on an annual basis.

The NCNR plays a critical role in both fundamental and applied industrial research within the United States but does not currently have representation on the NIST VCAT.

RECOMMENDATION: The NCNR leadership should work with NIST leadership to address the absence of VCAT representation in neutron applications.

The panel was not provided with a document that clearly articulates the NCNR's vision, mission, and strategic plan complete with contingencies.

RECOMMENDATION: The NCNR should prepare a guiding document on vision, mission, and strategic plans and update it regularly.

The United States significantly lags behind the European Union in neutron-scattering facilities, and it is in jeopardy of becoming internationally noncompetitive. The NCNR represents a large fraction of the neutron scattering capability within the United States, and it remains a world-class facility, even though its funding has been stagnant in recent years. Continuation of current funding trends inevitably leads to a trajectory of decline.

RECOMMENDATION: NCNR leadership should work with NIST leadership to ensure the support of the NCNR at a level of resourcing that will enable it to develop and support world-class neutron scattering instrumentation.

nSoft

nSoft is an industrial consortium, unique among neutron scattering user facilities, designed specifically to engage industry in neutron scattering. It embodies an innovative strategy for getting U.S. industries involved in neutron science by making it easy for industrial users to realize benefits that neutron scattering can provide to their research programs. What is missing today is a means to assess the impact of nSoft. Metrics need to be established to assess its effectiveness.

The nSoft consortium is developing a more facile engagement with industry.

RECOMMENDATION: The NCNR should establish quality and success metrics for nSoft.

RECOMMENDATION: The NCNR should develop an additional umbrella organization for hard matter and industrial interactions.

Acronyms

ANSTO	Australian Nuclear Science and Technology Organisation
CANDOR	Chromatic Analysis Neutron Diffractometer or Reflector
CARR	China Advanced Research Reactor
CHRNS	Center for High Resolution Neutron Scattering
CMP	condensed matter physics
CMRR	China Mianyang Research Reactor
CSNS	China Spallation Neutron Source
DANSE	Distributed Data Analysis for Neutron Scattering Experiments
ESS	European Spallation Source
HEU	highly enriched uranium
HFBS	High Flux Backscattering Spectrometer
HFIR	High-Flux Isotope Reactor
J-PARK	Japan Proton Accelerator Research Complex
KAERI	Korea Atomic Energy Research Institute
LANSCE	Los Alamos Neutron Science Center
LEU	low enriched uranium
MACS	Multi-Axis Crystal Spectrometer
MML	Materials Measurement Laboratory (NIST)
NCNR	NIST Center for Neutron Research
NeXT	Neutron and X-Ray Tomography
NRU	National Research Universal reactor
NSE	Neutron Spin-Echo Spectrometer
SINE2020	Science and Innovation with Neutrons in Europe in 2020
SNAFUSANS	Scanning Narrow Aperture Flow uSANS
uSANS	ultra small angle neutron scattering

vSANS	very small angle neutron scattering