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

Fiscal Year 2023

Panel on the Assessment of the National Institute of Standards and Technology (NIST) Center for Neutron Research

Laboratory Assessments Board

Division on Engineering and Physical Sciences

Consensus Study Report

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PANEL ON THE ASSESSMENT OF THE NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY (NIST) CENTER FOR NEUTRON RESEARCH

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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.

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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 **DAVID W. JOHNSON**, University of Minnesota, Twin Cities, and **JENNIE S. HWANG (NAE)**, H-Technologies Group, Inc. They were 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.

An Assessment of the National Institute of Standards and Technology Center for Neutron Research: Fiscal Year 2023

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An Assessment of the National Institute of Standards and Technology Center for Neutron Research: Fiscal Year 2023

Summary

BACKGROUND AND TASK

Since 1959, the National Institute of Standards and Technology (NIST) has annually enlisted the National Academies of Sciences, Engineering, and Medicine to convene expert panels comprising individuals from academia, industry, and various scientific and engineering fields. Their primary task is to evaluate the quality and efficacy of NIST's six measurements and standards laboratories, as well as the sufficiency of resources available to these laboratories. These evaluations are carried out under contract, initiated by NIST. For the fiscal year 2023, NIST has commissioned the National Academies to assess the NIST Center for Neutron Research (NCNR). The task of the Panel on the Assessment of the National Institute of Standards and Technology (NIST) Center for Neutron Research was to assess NCNR's scientific and technical programs; its portfolio of scientific and technical expertise; the adequacy of the budget, facilities, instrumentation, and human resources; and the effectiveness of NCNR's dissemination efforts. The statement of task is presented in more detail in Chapter 1. The assessment process involved a site visit by the panel, encompassing laboratory tours, one-on-one interactions with NCNR researchers, and subsequent inquiries following the site visit. Leveraging its collective experience and expertise, the panel then appraised NCNR in accordance with the predefined scope of work and provided recommendations accordingly. NCNR was last reviewed in 2021, 2 years ago (NASEM 2021).

NCNR, situated in Gaithersburg, Maryland, is an integral part of NIST. Its primary focus is to provide neutron measurement capabilities to the research community in the United States. It serves as a national hub for research employing thermal and cold neutrons, making its instrumentation accessible to eligible applicants. Many of its instruments leverage high-intensity cold neutron beams generated from a state-of-the-art liquid hydrogen moderator. NCNR's mission encompasses the following three core objectives: to operate NCNR safely as a cost-effective national resource; to enable a broad program of research using neutron techniques and to develop and apply new neutron measurement techniques; and to operate NCNR as a national resource for researchers from industry, university, and other government agencies.

In February 2021, the NCNR reactor underwent an unplanned shutdown after fission products were detected in the helium sweep and ventilation exhaust systems. This was due to a safety event, specifically a fuel element that had unlatched from its seat in the reactor, resulting in the reactor's fuel temperature violating its safety limit. NCNR submitted a request to the U.S. Nuclear Regulatory Commission to restart the reactor on October 1, 2021, identifying the root causes of the shutdown and corrective actions. After significant clean-up efforts and corrective actions, NCNR was approved to restart reactor operations on March 9, 2023. Since June 1, 2023, the reactor has been operating at 1 MW; its normal operating power is 20 MW. Elevation to higher power levels of operation are expected to be implemented later during the summer of 2023. Testing of effluents, as well as a careful assessment of the short- and long-term fixes that were implemented as a result of this accident will occur continuously to ensure safety and performance of the reactor. NCNR leadership felt that the restart of reactor operations made an assessment of NCNR appropriate at this time.

Because the reactor was shut down during the entire assessment period, 2021 through the first half of 2023, there was no work conducted at NCNR to assess. However, the staff at NCNR have used the

time to engage with users to focus on aftercare, which entails offering assistance in data analysis and publication drafting, leading to a continued outstream of publications.

In 2020, the year prior to the unplanned shutdown, more than 3,000 researchers from U.S. government laboratories, academia, and industry performed experiments at NCNR. New instruments, including the Chromatic Analysis Neutron Diffractometer or Reflector (CANDOR) and the very-small-angle neutron scattering (VSANS), were made available to researchers, initiating an era of important new advances in different areas of hard and soft matter materials research. The new instrument designs have significantly improved the efficiencies of experiments, providing significantly more data to researchers with shorter experiment durations. The resulting data provided new insights into the spatial and temporal behavior of materials at various length scales. The newly improved neutron depth profiling instrument and sample environment enhancements provided unprecedented information about in operando monitoring of lithium-ion transport processes, which is otherwise very difficult to obtain. This work will contribute to higher-capacity battery systems, increased safety, and longer lifetimes of installed batteries. VSANS has enabled observation of the flow of liquids over wider spatial and temporal scales—for the first time ever. The development of new data analysis strategies, new theoretical understandings, and machine learning (ML) and artificial intelligence (AI) tools were exploited to garner this information.

It is noteworthy that the research productivity, measured by peer-reviewed publications in highimpact factor journals, remains high despite the shutdown. This was, in part, made possible by NCNR staff who provided significant assistance to researchers to better understand, analyze, further extract information, and in some cases to develop models, from yet-to-be-published neutron data. NCNR researchers have been able to devote more time helping users to analyze their data in greater detail, uncovering new insights, and to more carefully plan future experiments. The recent shutdown also enabled the planning of new instrumental and sample environmental designs. Since the unplanned shutdown in February 2021, both instrument design and engineering improvements to the guide halls have continued and are expected to further enhance the tools available to the users of NCNR. The number of NCNR publications by year is shown in Figure S-1.

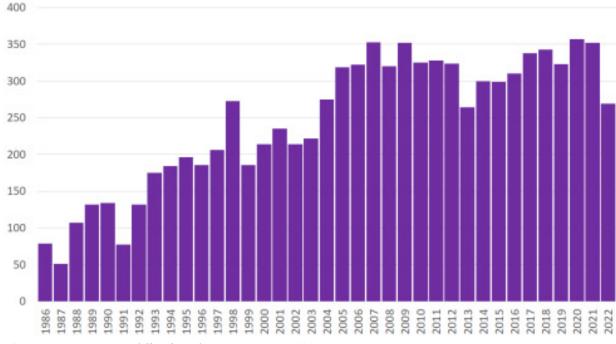


FIGURE S-1 NCNR publications by year, 1986–2022. SOURCE: NCNR.

SUMMARY

MAIN MESSAGES

Important challenges confront NCNR as it emerges from this shutdown, resumes normal operations, and prepares for future collaborative research with the user community. There are concerns about NCNR's support of and continued relevance to the U.S. neutron research community as it exits a long, unplanned shutdown and plans to enter another lengthy shutdown after perhaps less than a year of operations. Another concern is continuing the commendable progress in improving the NCNR safety culture in a way that the scientific work at the laboratory is not unduly hindered. NCNR has a number of old instruments that need either to be recapitalized or replaced. NCNR's budget has generally not kept pace with inflation and has experienced some challenges since the February 2021 shutdown. This has had a negative impact on both the technical and engineering aspects of the laboratory and on the expert workforce necessary upon which users' research critically depends. Finally, NCNR has come to rely more and more on AI and ML but does not have a coherent, organized approach to the use of these tools, nor does it have—or have access to—the high-performance computing infrastructure necessary to fully use these advanced and powerful tools. These topics are addressed below, not in order of importance—the panel did not prioritize its recommendations, as that is something more properly done by the laboratory—but in the order of occurrence of recommendations on these topics.

NCNR Availability and Relevance

As noted above, impressive things were accomplished during the recent reactor shutdown, both in instruments and the facility as well as in scientific productivity. Yet, the fact remains that NCNR has not been able to support new work by researchers and students since February 2021. This has had a significant impact on the neutron user community and on the ability of students to conduct research. The NCNR reactor should be very close to resuming normal operations by the time this report is published. But a cold source upgrade, to replace liquid hydrogen with liquid deuterium as a moderator to produce cold neutrons, is planned less than a year after the reactor resumes normal operations in support of NCNR's users. The liquid deuterium will enable an enhancement of the long-wavelength flux of cold neutrons when the reactor is converted from highly enriched uranium to low enriched uranium fuel. This cold source upgrade is expected to take approximately 11 months and is planned to occur in 2024. The obvious concern is that scientific progress will no doubt be undermined if NCNR undergoes yet another shutdown for a prolonged period after the recent shutdown of more than 2 years. In addition to the further disruption to the neutron research community, the panel is concerned about the impact of this plan on NCNR's continued relevance to that community. A further concern is that the members of user community might be discouraged from reengaging with NCNR due to uncertainty associated with future shutdowns; this is something that deserves careful consideration.

Recommendation 2-1: The National Institute of Standards and Technology Center for Neutron Research should delay the proposed shutdown to install the cold source by up to a year, starting no earlier than the first quarter of 2025.

Recommendation 2-2: The National Institute of Standards and Technology Center for Neutron Research leadership should develop a plan to demonstrate how the time during the future planned shutdown for the cold source upgrade will be used to ensure that the user base will be maintained and engaged currently and in the future.

Safety

One of the outcomes of the accident is that despite a strong safety record over the decades, new safety processes and protocols are being introduced. The safety organization now directly reports to the

NCNR director, elevating the oversight of this part of operations and improving the safety culture of the facility. The panel notes that the overall procedures for safety and security include the hosting of guest researchers performing experiments and are not restricted to NCNR staff. It is important that the new rules that are being considered to ensure the safety of the guest users and NCNR personnel not unreasonably impede the scientific productivity of the facility. Hence, a collaborative effort between personnel responsible for safety and those responsible for accomplishing the mission is needed in implementing the new rules.

Recommendation 2-3: The National Institute of Standards and Technology Center for Neutron Research leadership should ensure that the new procedures implemented for the safe operation of the facility also serve to support the achievement of mission objectives.

Aging Instruments

The Multi-Axis Crystal Spectrometer (MACS)-II spectrometer is the best in its class, but the BT-4¹ and Spin Polarized Inelastic Neutron Spectrometer (SPINS) spectrometers and the BT-1 powder diffractometer need to be upgraded to be competitive with similar instruments around the world. Hence, based on its performance metrics, the SPINS spectrometer is ranked seventh in the world compared to other similar instruments. The BT-1 diffractometer is 30 years old. While it continues to provide very valuable information, the experiments take an unreasonable amount of time and require specialized expertise. The BT-4 thermal triple-axis instrument is 40 years old and is in need of an upgrade or replacement. Instruments such as BT-1 and BT-4 support a tremendous amount of work and will be particularly important for users during the period of the planned upgrade of the Spallation Neutron Source at Oak Ridge National Laboratory. Finally, the MACS spectrometer alone is not sufficient to meet the future needs of the U.S. hard condensed matter research community. Despite the new instruments that have come online, there is a dire need for new instrumentation.

Recommendation 2-4: To support the hard condensed matter science community, the National Institute of Standards and Technology Center for Neutron Research (NCNR) should

- Upgrade the BT-1 power diffractometer and BT-4 instruments to make them relevant again.
- Fully upgrade the Spin Polarized Inelastic Neutron Spectrometer (SPINS), including the backend of the instrument, to provide a fully upgraded instrument; to accomplish this, NCNR should make the SPINS upgrade a central part of its hard condensed matter science portfolio and fund it accordingly. NCNR should not rely on funding vehicles like the National Science Foundation Major Research Instrumentation grants to accomplish this.

Budget and Workforce

There are concerns about loss of staff, and the associated scientific and instrument expertise, at NCNR due to the shutdown and decreasing operational funding budgets. The 2018 and 2021 reports (NASEM 2018, 2021) noted that core financial support for the program has decreased steadily for many years, and the number of scientists per instrument has been decreasing. This has been described as a potential crisis. However, while the base funding has increased, and funding for the Center for High

¹ BT stands for beam tube. But the instruments are referred to as "BT" and that is the nomenclature used in this report.

SUMMARY

Resolution Neutron Scattering (CHRNS), a partnership between the National Science Foundation (NSF) and NIST, increased slightly since its renewal and 11 permanent staff have been lost since 2018. Hence, after adjusting for inflation, the annual base, or core, funding for largely operating, maintaining, and advancing instrument design has been decreasing since 2015. Despite this challenge, NCNR staff are to be commended for continuing to support the high-quality user program, while also making important and new innovations in instrument design and efficiencies. The productivity of the external users has remained high due largely to support from NCNR staff. Staff continue to work long hours to achieve the mission, which will eventually negatively affect their morale. Staffing challenges for instruments, particularly for small-angle neutron scattering, are daunting.

Also, at the time this report was drafted, the number of licensed engineers and technicians is insufficient to operate the reactor 24 hours per day, continuously. However, NCNR is working to address the reactor operations staffing issue by training additional personnel, and these individuals are expected to have successfully passed their licensing exams by the time normal operations resume. Still, non-competitive pay and a lack of opportunities for professional development are obstacles to attracting and retaining the best talent. The panel concluded that NCNR's scientific and technical research services appropriations need to increase by at least 20 percent to correct for inflation-driven budget erosion since 2018 and allow NCNR to address its instrument and workforce challenges.

It is the understanding of the panel that, due to the shutdown, NSF's financial support for CHRNS is currently halted, hopefully temporarily. Some educational efforts have continued, but the lack of support does pose important potential challenges. NSF funding for this collaboration provides support for instrument upgrades, scientific staff to help users, and user services. It also supports reactor operation and the cold neutron source as well as beamlines for MACS, the Neutron Spin Echo spectrometer, CANDOR, the High Flux Backscattering Spectrometer, and VSANS. These are considered the best-in-class instruments for studies of nano-magnetism, quantum magnetism, and the structure and dynamics of soft matter. This research has broad societal applications (see Chapter 3), and the termination of NSF funding to CHRNS (see Chapter 5 for impact of CHRNS) would be a blow to neutron research vital to the United States and its industry.

Major efforts are needed to address this shortcoming in support from NSF, because the implications are significant. Another shutdown is proposed for the reactor in order to carry out an upgrade to the cold source. The panel does not believe that this is a reason to halt financial support; many of the activities that are supported by the collaboration can and should continue, regardless of whether neutrons are available to users.

Recommendation 4-1: The National Institute of Standards and Technology Center for Neutron Research (NCNR) leadership should address its funding challenges. The recommendations and potential from the CHIPS and Science Act of 2022 may be significant. However, the funds have not been appropriated and the timing of new resources remains unclear. NCNR should provide information about the return on investments in neutron characterization and measurement capabilities to science and industry. It should also provide insights into lost opportunities, over the coming years, associated with the limited availability of neutrons. The goal here is to demonstrate the urgent need for additional financial support.

Recommendation 4-3: The National Institute of Standards and Technology Center for Neutron Research should continue to fund and execute an adequate suite of capital improvement projects to better exploit the instrument suite.

Recommendation 4-4: The leadership of the National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR) should engage with NIST leadership to secure the funding necessary to hire more world-class scientific staff to meet the demands of resuming normal operations, prevent a degradation in NCNR's capabilities due to

understaffing, and to allow for growth in NCNR's work in the future. NCNR should explore special pay rates to help it recruit and retain the best available staff. That will, of course, require an adequate budget.

Artificial Intelligence, Machine Learning, and High-Performance Computing

National laboratories around the United States have made significant investments in advanced computing, including high-performance computing, to support their programs. This has been necessary because of the adoption of new advanced analytical tools, including increasingly sophisticated AI and ML tools requiring huge amounts of computational power, to solve problems across diverse fields. The world's first exascale computer, Frontier, is now operational at Oak Ridge National Laboratory. Other Department of Energy national laboratories—including the Pacific Northwest National Laboratory, National Renewable Energy Laboratory, Argonne National Laboratory, and Lawrence Berkeley National Laboratory—have high-performance computers to solve a range of science and engineering problems. In talking with many NIST staff about their research, it became apparent to the panel that most NCNR programs take advantage of AI and ML for data analysis. They accomplish this in suboptimal ways, using disparate and unrelated efforts across different groups in an ad hoc manner. Unfortunately, this is not sustainable for NCNR and the growing sophistication of state-of-the-art algorithms required for data analysis.

Recommendation 4-2: The National Institute of Standards and Technology Center for Neutron Research should develop a plan for access to, and use of, high-performance computing resources to support initiatives in scientific computing, artificial intelligence, and machine learning and to ensure the ability to scale up to meet the needs of scientist-driven initiatives.

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NASEM. 2021. An Assessment of the Center for Neutron Research at the National Institute of Standards and Technology: Fiscal Year 2021. Washington, DC: The National Academies Press. https://doi.org/10.17226/26418.

Overview of the National Institute of Standards and Technology Center for Neutron Research

The mission of the National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR) is to "provide safe and reliable operations in service to the neutron science community, supporting U.S. economic and technological advancement." NCNR is a user facility that provides neutron beamtime and instruments to investigators. It is a world-leading institution for neutron research with a history of high-impact scientific and technological advances in areas of broad societal importance, including fundamental advances in measurement science, hard and soft matter science, quantum information science, artificial intelligence, cybersecurity, and the foundations of neutron science. In addition to thousands of contributions to high-impact scientific and technical publications, more than 1,200 patents have been informed by research conducted at NCNR; in recent years, the average has been approximately 50 patents per year.

The NCNR reactor underwent an unplanned shut down in February 2021. Fission products were detected in the helium sweep and ventilation exhaust systems, owing to a safety event. A fuel element had unlatched from its seat in the reactor, resulting in the reactor's fuel temperature violating its safety limit and partially melting some fuel. Significant clean-up efforts and corrective actions resulted in an approval to resume limited reactor operations on February 1, 2023. Since June 1, 2023, the reactor has been operating at 1 MW; its normal operating power is 20 MW. It is expected that the reactor will resume full-power operations in the fall of 2023. Effluents will be continuously monitored to ensure reactor safety and performance.

NCNR is one of seven NIST laboratory programs, with partnerships that include the National Science Foundation's (NSF's) Center for High Resolution Neutron Scattering (CHRNS) and nSOFT, a consortium of corporate entities. The NCNR budget for fiscal year (FY) 2023 is \$87 million, which supports 170 federal employees and 70 associates who enable and support the work of more than 2,500 investigators. NCNR hosts and operates 30 beam instruments, 5 of which are operated by CHRNS. Its collaboration with NSF presents a unique opportunity to train many researchers who go on to become experts in neutron science, including academics in institutions in the United States and around the world, as well as corporate researchers who have played an important role in the applications of neutrons to industrial projects. CHRNS is also responsible for introducing undergraduates, teachers, and high school and middle school students to the impact and overall societal value of neutron science. Applications of work conducted at NCNR include processing and manufacturing in the automobile, chemical, and pharmaceutical industries as well as the production of vaccines. Moreover, the successful launch of the nSOFT consortium is complementary to the CHRNS partnership.

Figure 1-1 shows the NCNR budget from FY 2015 through FY 2023. It shows several categories of funding. Base scientific and technical research services (STRS) funding is the regularly appropriated funding that NCNR receives to conduct its work. Non-base (NB) STRS funding represents time-limited appropriations in addition to the base STRS funding. These NB STRS funds have principally been for recovery from the reactor incident. The funds from the NIST program Innovations in Measurement Science (IMS) are awarded competitively through a NIST-wide process. NCNR leads two IMS projects. Funding from the NIST working capital fund is shown for FY 2022. Other government agencies (OA) funding is from reimbursable work done for other federal agencies.

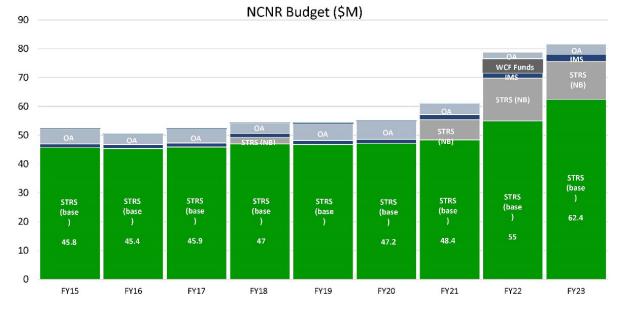


FIGURE 1-1 NCNR budget by year, not adjusted for inflation. NOTE: Base, regular funding; NB, nonbase, time-limited funding; IMS, Innovations in Measurement Science funding; OA, funding from reimbursable work performed for other agencies; STRS, scientific and technical research service funding; WCF, working capital fund. SOURCE: NCNR.

STATEMENT OF TASK

In 2023, responding to a request from the director of NIST, the National Academies established the Panel on the Assessment of the National Institute of Standards and Technology (NIST) Center for Neutron Research (referred to as the "panel") with the statement of task reprinted below.

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. The panel will review technical reports and technical program descriptions prepared by NIST staff and will visit the facilities of the Center for Neutron Research. Visits 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 and will prepare a report summarizing its assessment findings and recommendations.

NIST has requested that the laboratories be assessed against the following broad criteria:

- 1. Assess the NCNR's scientific and technical programs.
 - How does the quality of the research performed at the NCNR compare to that of similar world-class neutron facilities?
 - Is the quality of reactor operations, neutron instrumentations, and scientific utilization of the NCNR adequate for it to reach its stated objectives? How could it be improved?
- 2. Assess the portfolio of scientific and technical expertise within the NCNR.
 - Does the organization have world-class expertise in reactor operations and the development and utilization of advanced neutron instrumentation? If not, in what areas should it be improved?
 - How well does the organization's scientific and technical expertise support the research programs and the organization's ability to achieve its stated objectives?

OVERVIEW OF NCNR

- 3. Assess the adequacy of the NCNR's budget, facilities, instrumentation, and human resources.
 - How well do the facilities, instrumentation, and human resources support the NCNR's technical programs and its ability to achieve its stated objectives? How could they be improved?
- 4. Assess the effectiveness by which the NCNR disseminates its program outputs.
 - How well are the NCNR's instrument development activities and research programs driven by stakeholder needs?
 - How effective are the mechanisms by which the NCNR provides access to its instrument suite by a broad subset of the scientific community? Are these mechanisms sufficiently comprehensive?
 - How well does the NCNR monitor the scientific use and impact of the facility? How could this be improved?

CONDUCT OF THE ASSESSMENT

The panel, which consisted of 11 volunteers with expertise corresponding to the research done at NCNR, conducted an in-person review of NCNR in Gaithersburg, Maryland, from June 21 to 23, 2023. During that visit, the panel engaged with NCNR leadership and staff, who delivered comprehensive presentations. These presentations were complemented by tours of the NCNR facilities and interactive discussions between NCNR staff and the panel. Written responses to inquiries raised by the panel were also provided by NCNR staff.

In developing its assessment, the panel relied on the collective experience, technical expertise, and knowledge of its members. The assessment primarily adopted a qualitative approach, relying primarily on the materials provided—as well as presentations, poster sessions, and tours—by NCNR staff and leadership. It is important to note that the exclusion of specific NCNR projects from this report does not imply a negative perspective; the panel focused on the points it judged most significant in the information provided to it. The report centers on NCNR's ongoing work, highlighting opportunities and challenges associated with it.

It is worth mentioning that NIST has a distinct review body known as the Visiting Committee on Advanced Technology, which addresses the broader question of the direction that NCNR or any other NIST laboratory should be taking. Hence, deliberations on whether NCNR is pursuing appropriate research fall beyond the scope of this particular review.

STRUCTURE OF THE REPORT

After this introductory chapter, the report has four additional chapters addressing the major points 1–4 in the statement of task above; that is, NCNR's scientific and technical programs (Chapter 2); NCNR's portfolio of scientific and technical expertise (Chapter 3); NCNR's budget, facilities, instrumentation, and human resources (Chapter 4); and NCNR's dissemination of its program outputs (Chapter 5). There is a certain amount of unavoidable overlap between chapters—for instance, aspects of NCNR's instruments are discussed in both Chapter 2 and Chapter 4—but each chapter is focused on the specific questions raised in the relevant portion of the statement of task. Chapter 3 discusses the use of instruments in the context of scientific research. Accordingly, each chapter contains conclusions and recommendations focused on the particular aspect of NCNR that it addresses; so, for instance, recommendations regarding NCNR's scientific and technical expertise are found in Chapter 3.

Assessment of Scientific and Technical Programs

In this chapter, the panel addresses the first issue in the statement of task (see Chapter 1), assessing the scientific and technical programs at the National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR). That portion of the statement of task asked two sets of questions: How does the quality of the research performed at the NCNR compare with that of similar world-class neutron facilities? Is the quality of reactor operations, neutron instrumentation, and scientific use of the NCNR adequate for it to reach its stated objectives? The statement of task also asked for recommendations for how the quality of these various aspects of the NCNR could be improved.

NCNR RESEARCH COMPARED WITH SIMILAR WORLD-CLASS NEUTRON FACILITIES

Around the world, the breadth and impact of neutron science, including characterization and measurement and fundamental research, are severely limited by a lack of experimental capacity. The world's major neutron facilities, including NCNR, are significantly oversubscribed. NCNR provides a broad suite of instruments, while focusing its effort on several key areas that take advantage of the technical strengths of the facility. This allows for world-class—and, in some cases, world-leading—impacts in a wide range of areas, including neutron studies of soft matter, quantum materials, manufacturing and engineering, and energy-storage materials. The research performed at NCNR has a breadth and depth that is world-leading and that builds on decades of work by highly competent, creative, and dedicated scientists and technical staff.

During the period of this assessment—the past assessment was in fiscal year 2021 (NASEM 2021), there has been no neutron production at NCNR, and as such the research output has been declining as data collected prior to the unplanned outage are being analyzed and published. A positive effect of the unplanned reactor outage is that instrument scientists, not being fully occupied supporting users at ongoing experiments, have been able to engage with users and with early-career staff onsite to focus on aftercare—that is, providing post-experiment support to collaborate on data analysis and drafting publications. This has delayed the inevitable reduction in journal publications based on NCNR-generated data, although signs are now emerging that publication metrics are beginning to decrease sharply, as expected. Figure 2-1 shows NCNR publications by year.

The scientists at NCNR have continued their research activities by making applications for beamtime at other facilities. It is a testament to the quality of the research program that the team has been extremely successful in receiving beamtime at highly competitive, world-leading facilities, such as the Institut Laue-Langevin (ILL) in France and Oak Ridge National Laboratory (ORNL). They have also been successful in supporting users and onsite early career staff in developing beamtime proposals at other facilities.

The lack of available beamtime and loss of collaborative opportunities with users associated with the shutdown are making NCNR a less attractive workplace for instrument scientists, resulting in several key staff departures. This had not yet had an impact on the research output during the review period, but it is a cause for concern as the organization prepares to start the reactor up again and restart the user program. ASSESSMENT OF SCIENTIFIC AND TECHNICAL PROGRAMS

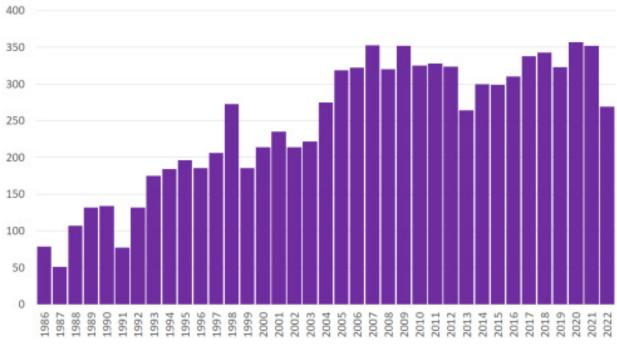


FIGURE 2-1 NCNR publications by year, 1986–2022. SOURCE: NCNR.

QUALITY OF REACTOR OPERATIONS, NEUTRON INSTRUMENTATION, AND SCIENTIFIC USAGE OF NCNR

Reactor Operations

As explained in Chapter 1, the NCNR reactor underwent an unplanned shutdown in February 2021 and was not approved for resumption of operations until March 2023. Beginning on June 1, 2023, the reactor started operating at a greatly reduced power—1 MW, or 5 percent of its usual operating power—with an elevation to higher operating power levels expected sometime during the summer. The goal of these reduced-level operations was to make sure that the reactor would perform safely and efficiently with the modifications that have been made. Given this situation, the panel was unable to assess current reactor operations at NCNR because there were none, but panel members were able to get a sense of the reactor's future through conversations with various members of the NCNR management and staff.

Recently, a cold source project to replace liquid hydrogen, used as the moderator to produce cold neutrons, with liquid deuterium was proposed. The liquid deuterium will enable an enhancement of the long-wavelength flux of cold neutrons when the reactor is converted from highly enriched uranium to low enriched uranium. This cold source upgrade is estimated to take approximately 11 months and is proposed to occur in 2024. The panel acknowledges NCNR's reason for wanting to accomplish this upgrade soon—namely, to mitigate the risk of the growing possibility that those who service and maintain the current cold source will retire, impacting NCNR's ability to maintain its current cold source. However, the proper use of work planning and controls will minimize the impact of such knowledge loss, should it occur. The panel does not feel this concern is sufficient to justify a long interruption of the scientific program and is deeply concerned about the impact of another outage so soon after restarting on the U.S. neutron research community and NCNR's ongoing relevance to that community. The panel believes that it would be prudent to delay the outage to install the cold source by up to a year to mitigate the impact of the second outage.

The reasons for this are the following. First, it is important for NCNR to use this additional time to work with all users—NIST, academic, and corporate—so that they can conclude as many experiments as possible. Some students may need to conclude doctoral dissertations. During the past shutdown, many users were allotted limited time on beam lines around the world; this is of course not optimal. Other users temporarily worked on complementary, or different, topics. It should be emphasized that because neutrons provide unique insights in the spatial and temporal behavior of virtually all kinds of materials, for a plethora of applications, users will always depend on neutron scattering techniques. Hence, users look forward to taking advantage of the technique when it is available. The panel interviewed members of the executive community for the user group, and they were clear that despite the shutdown, they were committed to continuing to exploit neutrons to study materials behavior. Neutrons provide unique insights into the behavior of condensed matter that are not available from other techniques. Second, the Spallation Neutron Source (SNS) at ORNL will not be available to users from August 2023 until July 2024. A shutdown of NCNR that coincides with the SNS outage would have a devastating impact on the U.S. neutron scattering community.

Recommendation 2-1: The National Institute of Standards and Technology Center for Neutron Research should delay the proposed shutdown to install the cold source by up to a year, starting no earlier than the first quarter of 2025.

Recommendation 2-2: The National Institute of Standards and Technology Center for Neutron Research leadership should develop a plan to demonstrate how the time during the future planned shutdown for the cold source upgrade will be used to ensure that the user base will be maintained and engaged currently and in the future.

A new reactor design has been proposed with capacity for 50 instruments, and this new design will contribute to significantly increasing both the capacity and the capability of the instrument suite. The outcomes of the CHIPS and Science Act of 2022 are strongly applauded by this panel because they support the necessary wide availability of neutrons. The new reactor design and implementation is, in part, in response to this new challenge. The panel commends NCNR on this new design and strongly encourages further development.

Safety

At the October 2022 meeting of the NCNR Safety Assessment Committee (SAC), the assessment team described conversations with many personnel, presentations by team leaders and management, and several reports and documents and concluded that there is a unified front in pursuing the restart of NCNR and a genuine investment in the mission. The breadth and depth of this effort was impressive. The SAC report noted that the chief reactor operational concerns are sustainment and retention. This assessment agrees with those conclusions and has encountered a similar attitude among the operational staff. The operations staff appear to have bought into the safety culture improvements and are incorporating it into their daily work. A challenge remains in maintaining the commitment to sustaining this high level of professionalism in reactor operations when budgetary pressures from the ramp-up in scientific activities begin to compete with flat budgetary resources. High operational performance is linked to a sustained financial commitment to operations. See Chapter 4 for details.

One of the outcomes of the accident that led to the reactor shutdown is that the already strong safety culture at NCNR, demonstrated by a strong safety record over the decades, has been strengthened. The NCNR safety organization now directly reports to the NCNR director. The overall safety and security procedures at NCNR encompass not only the operation of the facilities, but also the users and researchers that come to NCNR to conduct work. As the safety culture is strengthened, it is important that newly implemented safety and security procedures not unnecessarily impede the scientific progress of the

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facility and the researchers. Development of the new procedures would be best accomplished as a collaborative effort between the personnel responsible for safety and those responsible for accomplishing the mission.

Recommendation 2-3: The National Institute of Standards and Technology Center for Neutron Research leadership should ensure that the new procedures implemented for the safe operation of the facility also serve to support the achievement of its mission.

Instrumentation

NCNR supports a complementary suite of scattering instruments able to investigate a wide range of structural and dynamic length and time scales particularly suited to soft matter science. These include the ultra-high-resolution, small-angle neutron scattering (USANS), very-small-angle neutron scattering (VSANS), small-angle neutron scattering (SANS) with two 30-meter SANS, MAGIK (multi-angle grazing incidence K-vector) reflectometer, Polarized Beam Reflectometer, horizontal reflectometer (to be sunset), the new Chromatic Analysis Neutron Diffractometer or Reflectometer (CANDOR), Neutron Spin Echo Spectrometer (NSE), and High-Flux Backscattering Spectrometer instruments.

In total, the NCNR instrument suite has 30 instruments, which can be broken down as follows:

- 17 neutron scattering instruments operated by NCNR;
- 11 imaging, analytical chemistry, and neutron physics instruments operated by the NIST Physical Measurement Laboratory and Material Measurement Laboratory (MML);
- The nSoft SANS instrument operated collaboratively by MML and NCNR; and
- A test station.

This section assesses the quality of those instruments and their value to users of NCNR.

During the past 2 years, as the reactor has been offline, NCNR staff have worked to enhance the operational capabilities of the instrument suite, and it has upgraded some instruments and added others. For example, the staff has worked to maintain the world-leading status of the Multi-Axis Crystal Spectrometer (MACS) and VSANS instruments. The VSANS, commissioned within the past 5 years, has world-class flexibility in instrument configuration allowing for faster data acquisition times over a wide range in length scales. And the operation of MACS has been brought up to modern standards and incorporated into the NCNR standard control system. This will enable faster measurements and more reliable and repeatable operation. The addition of event-mode data collection—as part of the Center for High Resolution Neutron Scattering (CHRNS) Non-Equilibrium Neutron Scattering initiative—will enable MACS to continue production of world-leading, innovative science, and it should continue to be competitive with the best cold neutron spectrometers and deliver world-leading science for years to come.

A new neutron spin echo instrument, the NSE II, is being installed and is scheduled to be commissioned in 2023 or 2024. This project, which is well advanced, will make the NSE instrument world-class in its ability to study molecular dynamics.

Another new instrument, CANDOR, offers unique capabilities and will enable significant enhancements in measurement speed for the study of surfaces and interfaces. The instrument team made use of the unplanned outage to make modifications to enhance the sensitivity of the instrument. This instrument, when outfitted with a full complement of detector banks, will be world-leading for the study of surface and interfacial kinetics.

The planned upgrade of the primary spectrometer of the Spin Polarized Inelastic Neutron Spectrometer (SPINS) cold triple-axis spectrometer is well under way, with procurements made for the neutron optics. This upgrade will bring SPINS up to world-class performance and lay the foundation for a future upgrade of the secondary spectrometer using a multi-analyzer system. The secondary spectrometer upgrade, once funded, will enable SPINS, renamed Polarized Large Angle Resolution Spectrometer, to become a world-leading instrument.

The Double Axis Residual Stress Texture Single Crystal instrument at BT-8,² which is an engineering diffractometer for stress and texture analysis, underwent significant enhancements, which are nearing completion during the unexpected outage. These upgrades include the integration of a new monochromator and detector, an improved sample positioning assembly, and the incorporation of devices for uniaxial, shear, and multiaxial stress with a digital image correlation setup. These advances are expected to deliver an improvement of more than 10 times from the detector and approximately 2 times at monochromator in detection efficiency for cubic systems, signifying a significant advance for this instrument. The improved monochromator is innovative for multiple-peak texture measurements.

The BT-8 diffractometer at NCNR is comparable to Kowari at the Australian Nuclear Science and Technology Organization and Salsa at the ILL. All of them use a bent silicon, double-focusing monochromator at a neutron guide position, a sample stage, and a two-dimensional detector with higher resolution in the diffraction-sensitive direction. Incoming fluxes at a typical gauge volume have yet to be benchmarked at BT-8. The implementation for multiple-wavelength measurements is innovative, although limited by peak overlap. The sample environments, especially the load frames on BT-8, are innovative and in line with the best capabilities in the world. In particular, the multiple stress-tensor deformation applications during texture measurements as well as simultaneous measurements of macroscopic surface strain development using digital image correlation will attract various collaborations from academic and industrial users.

There are also several other ways in which NCNR has delivered new instruments, upgrades, and supporting software to maintain its world leading position. Of particular note,

- SANS neutron guide upgrades will increase the neutron flux by approximately two times, improving the rate of data collection and measurement quality.
- Sample automation and autonomous sampling will significantly improve throughput.
- Upgrading instruments to include time resolution with neutron data collection will open new fields of study.
- Applications of a large goniometer for 20 kg samples and a base table for 200 kg samples allow the users flexibility of sample volume and dimensions for various applications.

While the enhancements described above should enable the various instruments to remain among the best in the world at what they do, the same cannot be said of the BT-4, the SPINS spectrometer, and the BT-1 powder diffractometer. For instance, according to the metrics of performance, the SPINS spectrometer is ranked seventh in the world. The BT-1 diffractometer is 30 years old, and while it still provides very valuable information, the experiments take a great deal of time and special expertise to carry out. Furthermore, the BT-4 thermal triple axis instrument is 40 years old. In order to make NCNR relevant and be able to compete with the best spectrometers and diffractometers at other neutron facilities, it is extremely important to upgrade BT-4 and BT-1 to make them relevant again.

More generally, while NCNR investments in soft condensed matter physics are adequate, the investments in hard condensed matter physics are not. Given the lack of cold neutron spectrometers in the United States, MACS alone is clearly not adequate to satisfy the demand of the community, particularly because the second target station at the spallation neutron source is still many years away. The installation of a dedicated cold-guide for the upgraded SPINS, along with an improved front end of the spectrometer, is good news. However, the budget allocated for improvement of the backend of the spectrometer is inadequate. Having a half-upgraded instrument will not help the community advance the science enabled by the instrument. A properly upgraded SPINS will attract and serve a large hard condensed matter physics community for decades to come. It is not prudent to rely entirely on National Science Foundation

² BT stands for beam tube. But the instruments are referred to as "BT" and that is the nomenclature used in this report.

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(NSF) Major Research Instrumentation (MRI) grants or similar programs for improvement of the SPINS instrument because these programs are subject to review by panels who may not understand the importance of neutron spectroscopy and the composition of which could change from one competition cycle to the next. To provide reliable and competitive cold neutron spectrometers to the community, it will be necessary to include the improvement of the instrument as a core part of the budget for the NCNR suite of instruments. Otherwise, the hard condensed matter physics program at NCNR will be much less competitive and may not be the top choice for the user community. Having one cold spectrometer at NCNR is clearly not sufficient, particularly when SPINS has the potential to be one of the best cold neutron spectrometers in the United States.

Finding 2-1: Instruments such as BT-1 and BT-4 are workhorses, and their normal operation will be important for users around the country, particularly during the period of SNS upgrade.

Finding 2-2: The performance and adequacy of spectrometers and diffractometers, which are used by the hard condensed matter community, will likely not meet the future needs of the community in the United States unless some key investments are made.

Conclusion 2-1: It is extremely important for NCNR management to find resources and prioritize the upgrade of the SPINS instrument in the future cold source guide hall to provide a properly and fully upgraded instrument to the hard condensed matter science community. Relying on NSF MRI grants and other agency programs may prove to be unreliable funding sources.

Recommendation 2-4: To support the hard condensed matter science community, the National Institute of Standards and Technology Center for Neutron Research (NCNR) should

- Upgrade the BT-1 power diffractometer and BT-4 instruments to make them relevant again.
- Fully upgrade the Spin Polarized Inelastic Neutron Spectrometer (SPINS), including the backend of the instrument, to provide a fully upgraded instrument. To accomplish this, NCNR should make the SPINS upgrade a central part of its hard condensed matter science portfolio and fund it accordingly. NCNR should not rely on funding vehicles like the National Science Foundation Major Research Instrumentation grants to accomplish this.

The issue of instrumentation personnel is also of concern. The NCNR instruments are currently operated in a collaborative manner, having, on average, one instrument scientist on each. However, owing to the rising demand for sustained world-class scientific research and support for external users, including industrial partners in structural material manufacturing, it has become crucial that additional scientific personnel be hired to support the neutron instruments. Such an expansion will be crucial to fulfill research obligations and effectively support the expanding user base resulting from the rising demand noted above, which in turn will reinforce NCNR's position as a prominent hub for materials research and collaboration. NCNR recognizes the need for additional scientific staff to meet the growing demand, enhance support for external users, and achieve its objectives more effectively.

Scientific Use

The unplanned outage has meant that there was no direct scientific use of the neutron instruments throughout the period of this review. NCNR staff have made use of the shutdown to bring forward work that will enhance scientific use once the facility restarts.

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FAIR Data Management

One of the staff's tasks during the shutdown was aimed at making NCNR data findable, accessible, interoperable, and reusable (known as FAIR). Under this project funded by CHRNS, Open Researcher and Contributor ID (ORCID) persistent digital identifiers have been fully integrated into NCNR's information management system and the New Instrument Control Environment (NICE) so that digital object identifiers are automatically generated for NICE experiments. Sample metadata are entered into NICE, and a database of metadata is automatically populated. Metadata from preexisting data files have been extracted and published. A search page and programming interface for searching metadata has been added. A process metadata pipeline plan was drafted for MACS integration with NICE. And data processing manifest exports have been established for all CHRNS experiments.

Sample Environment

The Liquid Insertion Pressure System for SANS is designed for the in situ study of biomolecule solutions under high pressure. It enables SANS data collection on liquid samples—biological macromolecules and other liquids—at pressures up to 350 Mpa, with simultaneous temperature control within the range -20° to $+65^{\circ}$ C. Ongoing developments at NCNR include a new insertion base and improved cooling capabilities. This equipment is a complete renewal of the previous hydrostatic pressure cell system that had been running on outdated hardware and will enable a much wider range of problems to be studied in areas of food science, industrial processing, and fundamental colloid science.

Autonomous Formulation Laboratory

The Autonomous Formulation Laboratory is a joint program among the <u>nSoft</u> consortium, NCNR, and NIST's MML, which is focused on accelerating materials discovery and formulation optimization through artificial intelligence and machine learning-directed, multimodal scattering experiments. The core of the Autonomous Formulation Laboratory platform is an open-source, NCNRdeveloped platform to prepare liquid mixtures via pipetting, transfer those mixtures to a measurement cell, perform a SANS (or small-angle X-ray scattering or other method) experiment, and provide the data to an artificial intelligence guidance server.

REFERENCE

NASEM (National Academies of Sciences, Engineering, and Medicine). 2021. An Assessment of the Center for Neutron Research at the National Institute of Standards and Technology: Fiscal Year 2021. Washington, DC: The National Academies Press. https://doi.org/10.17226/26418.

3 Assessment of the Portfolio of Scientific and Technical Projects and Expertise

This chapter addresses the second issue in the statement of task (see Chapter 1), assessing the portfolio of scientific and technical expertise within the National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR). That portion of the statement of task asked two sets of questions: (1) Does the organization have world-class expertise in reactor operations and the development and utilization of advanced neutron instrumentation? If not, in what areas should it be improved? (2) How well does the organization's scientific and technical expertise support the research programs and the organization's ability to achieve its stated objectives?

The answer to each question is generally yes; some facilities are world class and world leading, owing to recent investments and improvements. However, many key instruments are old and inefficient and need to be upgraded with advanced instrumentation and software or, in some cases, replaced. Challenges associated with the use of the NCNR instruments to investigate condensed matter phenomena are highlighted.

OVERVIEW

The quality of the experimental research at NCNR continues to be of high intellectual value, cutting edge, and world leading in diverse areas. The scientific and technical staff are among the most experienced and very best in the world; this is evident from the experience of panel members who have familiarity with facilities around the world and from interviews with the leadership of the user group. It is also evident from the scientific reputations of the instrument scientists. Of course, the quality of the outcomes that a user can achieve depends not only on the quality of the scientific and technical staff but also on the quality and efficiency of the instruments being used. As noted in Chapter 2, some of the instruments at NCNR are world-leading owing to recent upgrades, whereas others will require improvements if they are to provide reliable, high-resolution data at competitive rates. It should be noted, as discussed earlier, that the older instruments still provide reliable data, although the collection process is slow and time-consuming and requires deep expertise on the part of the NCNR instrument scientists. This is a potential liability in the long run, if critical upgrades are not accomplished in a reasonable time years, not a decade. If upgrades are not accomplished in a timely manner, the scientific output of these instruments will curtail rapidly. Because of the number of old instruments, and their overall productivities, this will negatively impact the overall productivity of NCNR. This would negatively impact the quality of neutron research in the United States.

During the unplanned shutdown since February 2021, NCNR staff have devoted valuable time toward working with users to provide support for data analysis, exploiting techniques such as machine learning. These efforts have contributed to a deeper understanding of experimental outcomes. The panel is impressed with the expertise of the reactor operators and the scientific and technical support staff. The collaborative design of experiments and sample environments between users and beam scientists led to important new advances, as discussed later in this chapter. While the NCNR facility is understaffed in some areas, causing a stressful situation, the dedication of NCNR staff is impressive, as always. It must

also be noted that the NCNR researchers did a commendable job mentoring the postdoctoral researchers, including helping them to get access to neutrons in other facilities around the world while NCNR has been shut down. This has contributed to the overall productivity of NCNR's research.

The collaborative efforts between users and beam scientists were highly productive, enabling new advances. In nuclear physics, for example, the research remained focused on meaningful—and important—foundational problems. Experiments on porous inorganic materials, with applications ranging from heat transfer to absorption, were devoted to questions that revolve around structure and dynamics; highly cited publications in high-impact-factor journals, including *Science*, resulted from these efforts.

Another noteworthy area where the research outcomes are notable is electrochemical batteries. Electrochemical batteries play a key role in the energy transition; they are not only important for electric vehicles, but also for grid applications, enabling the increased integration of renewables. Neutron scattering measurements have provided new insights toward improving the performance and safety of batteries. Specifically, the improved neutron depth profiling instrument and sample environment enhancements provided unprecedented information about lithium-ion transport processes, which are otherwise very difficult to obtain. The improved sensitivity and speed of data measurement enabled unique in operando monitoring of the movement of lithium ions in batteries. This work will contribute to higher-capacity battery systems, increased safety, and longer lifetimes of installed batteries. Additionally, the imaging combining neutrons and X rays is among the very best and enables comparatively rapid measurements of the spatial compositional distributions of material components. Machine learning algorithms were exploited to accomplish these outcomes. The proposed cold neutron station will enable unprecedented in situ information about correlations between bulk transport and nano-structural (compositional) changes that affect performance, lifetimes, and failure. The research in other areas of hard condensed matter, with collaborative NIST staff support, continues to be first rate.

The soft condensed matter efforts continue to be highly productive, with important scientific and technological impact. There is a suite of instruments that have either recently undergone upgrades or are scheduled for upgrades, as discussed below. The nSOFT consortium continues to be highly successful because of the unique suite of instruments that provide new and complimentary information. The newly upgraded very-small-angle neutron scattering (VSANS) instrument, for example, enables measurements over wider spatial and temporal scales. The panel continues to be pleased with the scientific support and innovation in this area. In the following sections, additional details of activities and accomplishments in the areas mentioned above are presented.

Fundamental Neutron Physics

The basic neutron physics program at NCNR has a rich history dating back to the early 1990s, when a pioneering neutron interferometry capability was implemented. Neutron physics experiments are carried out by the Neutron Physics Group, which is part of the Radiation Physics Division of the NIST Physical Measurement Laboratory (PML). While not formally part of NCNR, the Neutron Physics Group nevertheless operates eight beam lines beam instruments at NCNR and is fully committed to the goal of delivering world class science using the unique cold neutron beam facilities.

Many of the experiments discussed in this report are still addressing important questions in nuclear physics, particle physics, and astrophysics, such as the neutron lifetime (a key parameter in Big Bang nucleosynthesis), whether the radiative decay of a neutron can be observed (a prediction of quantum electrodynamics), whether time reversal violation can be observed in neutron decay (a possible window into the matter-antimatter asymmetry in the universe), and whether the precession of the spin of a transversely polarized neutron through liquid helium can be observed (a measure of the weak force between two nucleons). The work is often published in *Science, Nature*, and *Physical Review Letters*, the major high-impact journals.

All experiments require meticulous attention to detail, a distinctive characteristic of the work of the Neutron Physics Group. Students and postdocs in the program spend large amounts of time at NCNR

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and become intimately familiar with what is required to execute experiments at a world-class level. The training is invaluable, and many go on to faculty and research positions, at NIST or elsewhere, staying in the neutron field and contributing to the next generation of leaders in neutron research. Recent successes include the following:

- Pendellösung interferometry measurements that set new limits on the existence of so-called "fifth forces" and set new bounds on the neutron charge radius,
- The first image of a physically isolated electric field using neutrons,
- Achievement of neutron helical wavefronts carrying quantized orbital angular momentum values,
- A confirmation that residual gas in the neutron lifetime proton trap is not causing an overestimate of the lifetime in a beam measurement,
- Development of the capability to measure an absolute neutron flux at the 0.1 percent level,
- A new precision result from Electron-Antineutrino Correlation experiments (aCORN³) for the value of the antineutrino–electron correlation "little a,"
- A precision measurement of the antineutrino spectrum at High-Flux Isotope Reactor, setting new limits on sterile antineutrinos and confirming that the anomaly seen by others at around 6 MeV is definitely present.

Future plans include performing an interferometric measurement of the gravitational constant, G, which could lead to an outcome with a relative uncertainty of 50 parts per million (ppm) in a year; the development of thermal kinetic inductance detectors that could affect a new series of beta decay studies; and the completion of the ongoing neutron beam lifetime measurement.

Porous Inorganic Materials

There is a broad portfolio of world-class experiments at NCNR investigating the structure and dynamics of host materials and adsorbed molecules, including systems for hydrogen storage; carbon capture; and molecular separation, sieving, or catalysis. This is enabled through a combination of neutron instrumentation that is particularly suited to exploring the structure and dynamics of materials and molecules, particularly when the latter contain hydrogen, in combination with the complementary development of sample environments and in-house scientists and collaborators of strong international standing.

Despite the age and modest technical performance of the powder diffractometer BT-1,⁴ as mentioned earlier, it is an essential research instrument in this area, responsible for several high-impact publications. The share of time on this instrument has increased steadily in this field in recent years and is likely to continue to increase. This poses an inherent challenge.

The High-Flux Backscattering Spectrometer (HFBS) also plays a key role for developing a deeper understanding of diffusional dynamics of molecules in porous inorganic materials, particularly for hydrogenous species. An illustration of the critical insights this instrument can provide in this field is provided by work on CO_2 diffusion in mesoporous hosts modified by adsorbed polyethyleneimine molecules in which the HFBS revealed the influence of polyethyleneimine chain motion on the efficiency of the host as a material for CO_2 adsorption.

³ aCORN converts the angular correlation into a proton time-of-flight asymmetry. This is counted directly, and thus avoids the need for proton spectroscopy (Collett et al. 2017).

⁴ BT stands for beam tube. But the instruments are referred to as "BT" and that is the nomenclature used in this report.

Battery Materials

NCNR has a long-standing program of research activities supporting the development and analysis of battery technology. Neutrons provide an invaluable and unique probe of the location and movement of lithium within batteries. The work performed by the NIST Material Measurement Laboratory (MML) staff at NCNR using neutron depth profiling is unique worldwide, and the recent upgrade of the neutron depth profiling station operated by MML at NCNR with a dedicated neutron guide and endstation has enhanced the sensitivity of lithium quantification and increased the speed of measurement to enable in operando monitoring of the movement of lithium in batteries. This unique tool provides crucial information in support of developing higher capacity battery systems, enabling more reliable operation under extreme conditions, and ensuring longer lifetimes of installed batteries. All these aspects are key to advancing the electrification and de-carbonization of personal transport.

The Neutron Physics Group from the NIST PML operates the two neutron imaging stations at NCNR, with a world-leading program of neutron imaging. While the development of imaging stations at other facilities, for example, the neutron and X-ray tomography station at the Institut Laue-Langevin, have now surpassed NCNR in terms of flux, the expertise in the development and application of neutron imaging that exists at NCNR is second to none.

The thermal beam Neutron Imaging Facility has been in operation as a national user facility since 2006 and recently underwent upgrades, including a new detector and detector optics and the addition of an X-ray tomography station enabling simultaneous X-ray and neutron tomography. This facility supports imaging of battery systems, providing information on the spatial arrangement of battery chemistry on the several micrometer-length scale and enabling examination of the underlying mechanisms behind the effects that cycling, aging, and storage conditions have on battery performance. During the unplanned outage, the team has worked to compare various machine learning methods available in the tomography community. The primary goal has been to enable faster measurements by permitting the reconstruction of tomographs using fewer source images. This work to understand the limits of such algorithms not only allows for more and faster measurements, but also ensures that the results of such measurements are comparable to standard tomographic reconstructions.

The Cold Neutron Imaging station, which is constructed but still under development, will enable new studies of materials through the application of neutron focusing techniques (Wolter optics) providing for neutron microscopy, and through dark field imaging (the INFER Innovations in Measurement Science project) giving access to spatially resolved information on nanometer-scale structure. These methods will enable, in situ, the correlation of bulk transport of chemical components within batteries with nanostructural changes that can lead to battery lifetime decrease and failure.

Engineering Materials Research

NCNR excels in the domain of condensed matter research, which explores the structures and dynamics of materials such as metals, alloys, polymers, and complex fluids. The primary research revolves around investigating residual stresses arising from manufacturing and processing, measuring applied stresses in multiaxial deformation routes, studying preferred orientation phenomena, and identifying phase compositions. The hard matter research in NCNR has been carried out successfully with industrial partners in transportation sectors for their continuous interests in manufacturing and forming lightweight metals.

As noted in Chapter 2, the BT-8 diffractometer, which is used to perform stress and texture analysis, received significant enhancements during the 2021–2023 outage. Recent research results at the BT-8 diffractometer highlighted the instrument setup of octo-strain deformation with visualization of strain development using an advanced high-strength steel, showing the well-prepared instruments for concurrent neutron diffraction texture measurements. It is also interesting to note that the sample environments team plays a very important role in making modifications to the different experimental

Battery Materials

NCNR has a long-standing program of research activities supporting the development and analysis of battery technology. Neutrons provide an invaluable and unique probe of the location and movement of lithium within batteries. The work performed by the NIST Material Measurement Laboratory (MML) staff at NCNR using neutron depth profiling is unique worldwide, and the recent upgrade of the neutron depth profiling station operated by MML at NCNR with a dedicated neutron guide and endstation has enhanced the sensitivity of lithium quantification and increased the speed of measurement to enable in operando monitoring of the movement of lithium in batteries. This unique tool provides crucial information in support of developing higher capacity battery systems, enabling more reliable operation under extreme conditions, and ensuring longer lifetimes of installed batteries. All these aspects are key to advancing the electrification and de-carbonization of personal transport.

The Neutron Physics Group from the NIST PML operates the two neutron imaging stations at NCNR, with a world-leading program of neutron imaging. While the development of imaging stations at other facilities, for example, the neutron and X-ray tomography station at the Institut Laue-Langevin, have now surpassed NCNR in terms of flux, the expertise in the development and application of neutron imaging that exists at NCNR is second to none.

The thermal beam Neutron Imaging Facility has been in operation as a national user facility since 2006 and recently underwent upgrades, including a new detector and detector optics and the addition of an X-ray tomography station enabling simultaneous X-ray and neutron tomography. This facility supports imaging of battery systems, providing information on the spatial arrangement of battery chemistry on the several micrometer-length scale and enabling examination of the underlying mechanisms behind the effects that cycling, aging, and storage conditions have on battery performance. During the unplanned outage, the team has worked to compare various machine learning methods available in the tomography community. The primary goal has been to enable faster measurements by permitting the reconstruction of tomographs using fewer source images. This work to understand the limits of such algorithms not only allows for more and faster measurements, but also ensures that the results of such measurements are comparable to standard tomographic reconstructions.

The Cold Neutron Imaging station, which is constructed but still under development, will enable new studies of materials through the application of neutron focusing techniques (Wolter optics) providing for neutron microscopy, and through dark field imaging (the INFER Innovations in Measurement Science project) giving access to spatially resolved information on nanometer-scale structure. These methods will enable, in situ, the correlation of bulk transport of chemical components within batteries with nanostructural changes that can lead to battery lifetime decrease and failure.

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that the hard condensed matter physics community has not used other instruments, such as small-angle neutron scattering (SANS) and the spin-echo spectrometer at NCNR. The use of these instruments by the hard condensed matter physics community is important for the long-term health of these instruments, particularly when they consume the major part of the NCNR budget.

Conclusion 3-1: Excellent in-house staff and their collaboration with external groups are important for future world-class scientific output at NCNR. Maintaining a pipeline of fresh postdocs and staff and sufficient advanced instrument capacity are essential to maintain the competitiveness of NCNR and its future as a premium user facility.

MANUFACTURING, ROBOTICS, AND ARTIFICIAL INTELLIGENCE-DRIVEN ANALYSIS

NCNR's advances in support of manufacturing, robotics, and artificial intelligence-driven analysis are impressive. In particular, the work being done to enhance the Q-range accessible to experiments and the speed of data acquisition and analysis are especially welcome. There are a number of customers that NCNR collaborates with, including the National Science Foundation (NSF)-funded Center for High Resolution Neutron Scattering (CHRNS), which has been very successful in providing excellent access to NCNR to the academic community via the various beamlines that have been supported and upgraded; nSoft, which is an industrial consortium designed to help industrial members achieve specific goals via an annual paid membership; and the usual NIST collaborative programs and work individually funded by industrial companies.

Three projects stand out as being at the cutting edge, having no match as yet around the world:

- 1. Modification of the neutron reflectometry specifications at the Chromatic Analysis Neutron Diffractometer or Refractometer (CANDOR) beamline where, instead of collecting data for a single film and a single wavelength, the objective is to use up to 54 multiple wavelengths simultaneously and do the analysis on the backend.
- 2. The automatic dispensing equipment, referred to as the autonomous formulation laboratory, which allows the deposition of multiple material compositions and analysis in tandem and can be used with a variety of beamlines; this laboratory has traveled around the world to demonstrate its usefulness to a variety of applications.
- 3. The VSANS extension to lower Q is an excellent use that will make acquisition of information about the volume and size of scatterers quicker and more accurate over a wide range of Q values.

Because many of the cutting-edge improvements were instituted just before the reactor shutdown in 2021, not many papers have as yet been published. For the newly proposed reactor, the INFER neutron interferometer—with goals to develop new software, sample environments, and analysis techniques such as machine learning data analysis—is also noteworthy. It is expected that after the reactor is back online there will be many experiments that will be completed and published.

Additionally, for the beamlines that are designed to collect many more spectra than are often currently acquired, it will be important to ensure that NCNR improves its accessibility to computational capability that will allow processing of multiple versions of the machine learning models that will be generated with the goal of more quickly arriving at the best fitted model.

CONDENSED MATTER PHYSICS: SOFT MATTER

In the area of soft matter, the scientific and technical expertise is world-leading and well suited to support the research programs and external user community. NCNR has maintained a world-leading research portfolio in soft matter, particularly in the areas of flow-induced structure, phase behavior, and

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dynamics of self-assembled systems, pharmaceuticals, and membrane biophysics. In addition to a strong academic user community, NCNR continues to be successful in engaging industry to solve commercially relevant problems. This is clearly evident in the continued publications in leading journals, including *Science* and *Nature* (more than 100 per year). The partnership with NSF via CHRNS supporting the operation of these instruments is crucial for the long-term viability and success of the user program.

Protein Interactions

The majority of all Food and Drug Administration–approved small molecule drugs that target membrane proteins are particularly challenging to study because of the atomic compositions and noncrystalline structures in commercial drugs. Molecular interactions become increasingly important to shelf stability, dose, injection, lipid membrane interaction, and efficacy. Neutron scattering is ideally suited to study the structure and dynamics of these systems. NCNR has done a commendable job in engaging industry to help understand the critical problems and where neutron imaging approaches can be helpful. Continued studies on monoclonal antibodies have led to the development of models that can better represent the interaction potential. In addition, the combination of scattering, reflectometry, and neutron spin echo can drive the fundamental understanding of small molecule and membrane interactions. The development of CANDOR and neutron scattering with time resolution, combined with neutron spin echo, will drive the next generation of targeted drug development.

Flow and Rheo-SANS

The mechanical properties of a soft matter system are directly related to the structure across all length scales within the system. Historically, systems were independently characterized where the structure was studied at rest, and researchers speculated about how the structure changed under shear forces. NCNR has established itself as a world leader in the capability to measure soft matter under flow with the implementation of rheo-SANS, 1-2 shear cell, and capillary rheo-SANS. More recently, these techniques have been combined with time-stamp resolution. These techniques have revolutionized the scientific field of rheology with direct application in consumer goods and pharmaceuticals.

Phase Behavior

The phase behavior of complex systems is a primary research focus area for many industrial segments, including consumer goods and pharmaceuticals. While neutrons are particularly suited to study these systems through deuterium isotope contrast matching, mapping out a phase diagram for a system can be time intensive and laborious. NCNR has developed world-leading facilities to efficiently study these systems with the development of temperature-controlled, automated, and artificial intelligence–directed sample environments. This is accomplished in part through the nSoft consortium, highlighting the importance of taking advantage of industrial expertise and capability.

Time Resolution

Soft matter systems are dynamic, even at rest. When perturbed by an external field, these systems will deform or flow. The response is controlled by the internal structure and interactions that constitute the material. Historically, neutron data were collected at equilibrium conditions and averaged over the data-collection time period. This limited the opportunity to study the dynamics of a system. The ability to associate a time stamp with the neutron information has been proven, and NCNR is in the process of expanding this capability across all its sample environments. This is a significant task for the sample environment team but will significantly expand the capability across all areas of soft matter, especially in

the areas of rheology, membrane biophysics, and phase behavior of complex systems. Time-resolved measurements offer a significant improvement across nearly all sample environments. In addition to the added effort in bringing forward this capability, equal effort will need to be taken to educate the user community to integrate this into their experimental plans.

Software

Data reduction and analysis directly complements data collection. Historically, the approach has been extremely fractured, with each facility—and, in many cases, individual research groups—developing their own software without independent verification of accuracy. The NCNR SANS team has led a global effort to develop software, called SasView, which is capable of reducing data universally across all neutron scattering facilities and leads the world in data analysis capability. The hurdle to gaining global alignment and support should not be understated, and this effort is viewed as monumental for the community as a whole. SasView will standardize data reduction, limiting errors and accelerating improvements in data analysis. It also will be a platform for continuing improvements in data analysis as new modeling capability continues to be developed.

Opportunities and Challenges

The most significant challenge for soft matter work is the technician and instrument scientist staffing needed to support the instruments at NCNR, both for startup after the unplanned shutdown and to support the instrument user community. The panel believes that funding needs to be secured urgently and open positions filled to ensure program readiness and instrument proficiency upon reactor startup. The integration of CANDOR, VSANS, and the new Neutron Spin Echo Spectrometer (NSE)-II into the user community is a significant opportunity for NCNR and is a priority with respect to staffing and sustainable access to the user community.

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Budget, Facilities, Instrumentation, and Human Resources

This chapter addresses the third item in the statement of task (see Chapter 1), assessing the adequacy of the budget, facilities, instrumentation, and human resources of the National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR). That portion of the statement of task asked two specific questions: How well do the facilities, instrumentation, and human resources support the NCNR's technical programs and its ability to achieve its stated objectives? and How could they be improved? This addresses this issue by examining, in turn, NCNR's budget, facilities, instrumentation, and human resources, closing with a look at NCNR's reactor management plan and upgrade. There are recommendations for improvements in these areas.

BUDGET

The NCNR baseline budget has remained flat for many years, prior to the reactor event in 2021. In fact, it had been declining when adjusted for annual inflation. The 2021 National Academies' assessment report on NCNR identified the long-term impact of 7 years of flat budgets as causing a 20 percent reduction in the NCNR instrument staff, which resulted in a level considerably below staffing levels typically seen at major international neutron sources (NASEM 2021). This downward trend has gotten worse in the intervening 2 years since the past report. An increase in funds after the reactor event was allocated for the recovery effort, which was primarily directed toward improving reactor operations. High operational performance is linked to a proportionate financial commitment to operations, so sustainment of this support will be critical. Another challenge will be maintaining the commitment to sustaining a high level of professionalism and expertise in reactor operations when budgetary pressures from the coming increase in scientific activities compete with flat budgetary resources. The risk to mission objectives will now come more from a lack of scientific support as budgetary risk may lead to a failure to meet mission and objectives if a corresponding budgetary commitment is not made in scientific staffing resources. Taken all together, this points to a need for increased funding.

Adjustments in appropriations for operations have not kept up with increases in overhead and personnel-related costs since 2018. For instance, the overall result is a shortfall of about \$6 million per year in NCNR Neutron Condensed Matter Science and Research Facility Operation. Given that NCNR's total baseline scientific and technical research services appropriations are in the range of approximately \$50 million to \$60 million, this is a significant decrease. This has resulted in the loss of about 11 permanent staff in the Science and Research Facility Operations groups since the 2018 assessment (NASEM 2018), as well as reductions in capital purchases, bringing on fewer postdocs, and shutting down instruments. This represents a challenging downward spiral that risks the industrial, economic, and commerce-driven mission of the institute.

Conclusion 4-1: A flat budget has been harming NCNR. The base funding for NCNR's scientific and technical research services budget needs to be increased by at least 20 percent to compensate for real inflation-driven losses since 2018.

Recommendation 4-1: The National Institute of Standards and Technology Center for Neutron Research (NCNR) leadership should address its funding challenges. The recommendations and potential from the CHIPS and Science Act of 2022 may be significant. However, the funds have not been appropriated and the timing of new resources remains unclear. NCNR should provide information about the return on investments in neutron characterization and measurement capabilities to science and industry. It should also provide insights into lost opportunities, over the coming years, associated with the limited availability of neutrons. The goal here is to demonstrate the urgent need for additional financial support.

FACILITIES AND INSTRUMENTATION

The Computational Science team is hampered by a lack of access to high-performance computing resources and has been using a home-built, ad hoc cluster of desktop computers with slow interconnections. There are various ongoing individual efforts across the scientific staff to develop artificial intelligence and machine learning methods, enhanced data processing, and advanced data analysis methods. Many of these would benefit from access to high-performance computing resources to enable them to scale up to support the broader user program rather than individual projects. A lack of centralized resources, or of a centrally managed access to such resources, is already limiting the capability and capacity of the scientific computing program and this limitation will become worse in the coming years.

Recommendation 4-2: The National Institute of Standards and Technology Center for Neutron Research should develop a plan for access to, and use of, high-performance computing resources to support initiatives in scientific computing, artificial intelligence, and machine learning and to ensure the ability to scale up to meet the needs of scientist-driven initiatives.

A project to develop a design for a new low enriched uranium (LEU) research reactor is in a preconceptual design stage, with a workshop for community input held in October 2023. This is discussed in more detail in the "Reactor Management Plan and Upgrade" section below.

As set forth in Chapter 2, NCNR hosts a suite of 30 neutron beam instruments, of which 17 are neutron-scattering instruments operated by NCNR; 11 are imaging, analytical chemistry, and neutron physics instruments operated by the NIST Physical Measurement Laboratory (PML) and Material Measurement Laboratory (MML); one is a test station; and one is the nSoft small-angle neutron scattering (SANS) instrument operated collaboratively by MML and NCNR.

Since the inception of the facility, NCNR has maintained an ongoing program of instrument replacement, upgrades, and renewals in order to meet the needs of stakeholders across government, academia, and industry. This program is dependent not only on sufficient capital funding, but also on sufficient base funding for staffing. The current budget and staffing levels will not support continued operation of the full suite of NCNR instruments, and there is a significant risk that valuable and productive instruments will need to be mothballed. This will be a further blow to the neutron-scattering community in the United States and will hamper efforts to recover scientific productivity following the unplanned outage owing to the reactor event in 2021. As was highlighted in the presentations made to the panel, there is no redundancy built into the neutron-scattering instruments, particularly in the United States, where instruments are already oversubscribed when all facilities and systems are operational.

The ultra-high-resolution, small-angle neutron scattering (USANS) instrument, for example, is unstaffed at present. The SANS program is core to NCNR, and a loss of a third of the SANS beamtime will be devastating.

BUDGET, FACILITIES, INSTRUMENTATION, AND HUMAN RESOURCES

As explained in detail in previous chapters, the BT-1⁵ diffractometer is a workhorse instrument that has been exceptionally productive over its 30 years of operation. It has been key to the success of NCNR research in the area of inorganic materials for gas capture and storage. The proposed modernization of BT-1 is key to ensuring that this world-leading research program continues to advance. The strategic investment in this instrument is estimated to cost an additional \$20 million.

An upgrade to the cold source and associated guide system is progressing well and will provide across-the-board improvements to the cold neutron instrument suites, with particularly impressive gains for the Polarized Large Angle Resolution Spectrometer (PoLAR) instrument, which will benefit from a fully redesigned and dedicated guide system. PoLAR is a proposed project (approximately \$15 million) to build a replacement for the aging cold triple-axis instrument. This new triple-axis spectrometer for NG5 would be a cold neutron instrument with a polarized beam capability. The cold source and guide installation will require an 11-month reactor outage, the timing of which will need to be coordinated with the plans for restart following the 2021 reactor event outage.

A project to improve the system known as the rabbit system would restore full functionality of the in-core irradiation system (approximately \$2 million to \$3 million). Eighty percent of NIST-produced standard reference materials are related to chemical composition. The in-core irradiation system supports neutron activation analysis of many of those materials. A fully functional system consists of two irradiation transfer stations. Currently, one of the two has been cannibalized to scavenge parts to support a single operational system. This situation poses a failure risk to NIST's standard reference material work.

Recommendation 4-3: The National Institute of Standards and Technology Center for Neutron Research should continue to fund and execute an adequate suite of capital improvement projects to better exploit the instrument suite.

HUMAN RESOURCES

The 2021 National Academies' assessment report on NCNR concluded that the number of instrument staff was already low compared with major international neutron sources (NASEM 2021). For example, at NCNR the instrument-staff-to-neutron-instrument ratio is 4–4.5:1. At the Australian Nuclear Science and Technology Organisation, the ratio is 5.5–6:1; at the Institut Laue Langevin it is about 7:1; and at the Spallation Neutron Source at Oak Ridge National Laboratory it is 7–8:1. NCNR's low instrument-staff-to-neutron-instrument ratio is reducing capabilities that are essential for a world-class user facility and reducing NCNR's ability to develop and continuously upgrade cutting-edge instruments, something necessary for a very old reactor if one is to increase scientific productivity. Improvements in the efficiency of work and the implementation of better technology have both helped to mitigate this staff shortage in the short term, but they have accomplished about all that could be hoped, and the 2021 report identified a risk to staff morale and the scientific productivity of the facility resulting from this situation (NASEM 2021). This risk is starting to be realized. The impending ramp-up of scientific activities once neutrons are available is presenting a challenge to the scientific staff. Staffing levels have become worse through the loss of key personnel, particularly to support the SANS instruments.

The impact of the long unplanned shutdown on research output is not yet visible in the publication metrics. Rapidly increasing the overall productivity of NCNR will include an urgent reengagement of the user community. Concurrently, there is an urgent need to increase the number of staff, as the reactor restarts, and as the user program rapidly grows. Reassignment of scientific staff to fill the most critical vacancies, such as on the SANS instruments, may mitigate this to some extent. There will, however, be significant impacts to staff morale as scientists are moved away from their areas of expertise and interest. Reassignment will also create capability and capacity gaps elsewhere in the

⁵ BT stands for beam tube. But the instruments are referred to as "BT" and that is the nomenclature used in this report.

instrument suite and is therefore at best a temporary fix. The current instrument staffing level does not allow for sustainable scientific operation with the current level of capability and capacity.

Having opportunities for career growth is a primary concern among reactor operations staff, who feel that holding an operator license limits career mobility when reactor staffing is low because the regulatory staffing requirements of the control room will take priority over individual professional development. NCNR's challenges in offering competitive pay is also an obstacle. The addition of a fifth reactor operator shift will provide for adequate training and career growth among the operations and facility engineering staff. NCNR is working on setting up this fifth shift.

NCNR's Safety Assessment Committee (SAC) report in 2022 reported a "monumental effort" by NCNR staff and a unity of purpose in restarting the NCNR reactor and said that NCNR staff are fully committed to the NCNR mission (NCNR 2022). An example of the staff's dedication to the NCNR mission is how, despite the challenging circumstances, they have supported their researchers through aftercare to such a level that the user community stated that support has not dwindled despite the loss in scientific personnel. This is a remarkable and commendable effort on behalf of the remaining scientific personnel, but it reveals that the existing staff is now at greater risk of burnout, particularly with the anticipated increased workload once neutrons become available.

In its report, the SAC did note challenges. A major concern is the ability to retain NCNR staff. NCNR is not able to compete on the basis of pay. Staff have left for other, better-paying positions in the federal government. Also, candidates interested in employment at NCNR are reported to be withdrawing from consideration after learning what their salary would be and determining that it will not meet their needs. The SAC concluded that a special pay scale would seem to be appropriate to address these concerns (NCNR 2022). Personnel shortages will be challenging in restarting scientific activities at NCNR, fully staffing neutron instruments, and supporting any expansions in work at NCNR.

In 2023, the Government Accountability Office (GAO) released the report *National Institute of Standards and Technology: Improved Workforce Planning Needed to Address Recruitment and Retention Challenges* (GAO 2023). It found that NIST is competing for a specialized candidate pool without being able to offer the salary (up to three times higher than NCNR can offer) and other flexibilities that the private sector offers. Furthermore, NIST is suffering from a tighter recruiting environment because postdoc applications are down. Postdocs are an important recruiting pool for NCNR. The GAO report also talks about succession challenges. NIST's workforce is very specialized, and there is a great deal of knowledge that can only be obtained once one is working there. When people leave, either for other positions or when they retire, it is very hard to replace these people in a timely manner, which creates knowledge and experience gaps. The GAO report concluded that there is a need for long-term planning and concomitant commitment to mitigate these challenges (GAO 2023). While that report addresses NIST as a whole, NCNR's personnel challenges are similar to those of NIST overall.

Conclusion 4-2: A substantial increase in scientific staff to support the neutron instruments is needed. This is essential in order to benefit from a return on the substantial investment in facility and instrument improvements over the years. NCNR will fall behind other facilities around the world without such a staff increase and would risk entering into a death spiral of low morale owing to overwork leading to even lower staffing, and lower morale, etc. At bottom, it will require an increase in NCNR's funding to recruit and retain world-class scientific staff.

Recommendation 4-4: The leadership of the National Institute of Standards and Technology Center for Neutron Research (NCNR) should engage with NIST leadership to secure the funding necessary to hire more world-class scientific staff and retain the necessary reactor operations staff to meet the demands of resuming normal operations, prevent a degradation in NCNR's capabilities owing to understaffing, and to allow for growth in NCNR's work in the future. NCNR should explore special pay rates to help it recruit and retain the best available staff. That will, of course, require an adequate budget. BUDGET, FACILITIES, INSTRUMENTATION, AND HUMAN RESOURCES

In spite of the challenges discussed above, it was noted that a large number of students and postdocs who have worked at NCNR have been hired as assistant professors at many different universities or have gone to industry to take on leadership positions. It is also interesting that, at least for the postdocs with whom the panel interacted, there was an impressive number of female postdocs. The mentoring of young graduate students and postdocs by senior researchers appears to have been working well because, in spite of not having access to neutrons at NCNR, the students are very enthusiastic and excited about their work and prospects and have been supported by NCNR's beamline staff to get beamtime at other facilities around the world. Nevertheless, there is a sense of concern that will only deepen further if the reactor does not restart at high power and neutron beam time resumes quickly.

That said, there is an urgent need to reengage with the neutron user community, which has suffered from lack of access to neutron beamtime during the NCNR outage (see, e.g., Kramer 2021). Since August 2023, the outage of the Spallation Neutron Source at Oak Ridge National Laboratory has been undergoing an outage to install accelerator and target components as part of its Proton Power Upgrade; this outage, which is projected to extend until July 2024, will further restrict access to neutron beamtime in the United States, compounding the effects of outages at NCNR. These factors all need to be carefully considered when deciding on the timing of the cold source outage at NCNR with the goal of restoring and maintaining neutron access for users in the United States.

Another noteworthy accomplishment in terms of workforce development is the SANS overview online course developed by NCNR for teaching University of Delaware students and remote students at 18 other universities that was held in spring 2023. The course will once again be taught in spring 2024, and there are plans to convert the material presented into a textbook, which will be an enormous contribution to helping educate a new cadre of future neutron scattering scientists.

REACTOR MANAGEMENT PLAN AND UPGRADE

The NCNR reactor is among the oldest operating large research reactors in the world, more than 50 years old. The current U.S. Nuclear Regulatory Commission (NRC) license will expire in 2029, and a new operating license application will be required. The change in the nuclear fuel from highly enriched uranium (HEU) to LEU will not occur before 2030. The NCNR reactor had an excellent safety and reliability record until 2020, delivering a 4-year average of 220 days of operations per year. However, on February 3, 2021, the reactor experienced an automatic unplanned shutdown owing to fission products detected in the confinement building upon normal startup. The source of the problem was traced to an unlatched fuel element.

NCNR rapidly committed to a number of corrective actions, and NIST and the Department of Commerce provided NCNR Reactor Operations and Engineering short-term funding for reactor recovery activities and ongoing funding increases for corrective actions. The base budget was increased by \$5.0 million per year in both 2022 and 2023 from the 2021 level of \$14.2 million per year, and one-off allocations of recovery funds of \$13.4 million and \$11.7 million were made in 2022 and 2023 respectively. There was extensive reorganization and changes in practice for the Reactor Operations and Engineering team, together with new and more extensive training and the introduction of enhanced standards for qualification and proficiency.

A request to restart the reactor was submitted to the NRC on October 1, 2021. This request included the root causes of the reactor event and specified corrective actions. The NRC gave permission to restart the reactor on March 9, 2023, and initial criticality (50 kW) was achieved on March 16, 2023. Operations were started at 1 MW on June 1, 2023, in preparation for operator licensing.

The low-power operations have revealed the presence of fission products in reactor helium sweep gas and indicate that despite extensive clean-up work, there is still probably about 1 g of fissionable

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material near the core. However, fission products seen in effluents are not near regulatory limits, and engineering fixes are being developed to address this.

As this is written, it is expected that the reactor power may be raised beyond 1 MW by late summer 2023, with extensive monitoring of effluent fluxes and tests conducted on the engineering fixes. However, there are insufficient licensed operators to run the reactor 24/7 for any extended period until the current class of additional operators completes licensing examinations. Once complete, the full complement of five four-person shift crews will support reliable 24/7 operations.

Although the NCNR reactor is more than 50 years old, systems incorporate fail-safe design and a proven hierarchy of interlocks and protective features, so the age does not increase the risk to human safety. However, the age does pose a risk to reliability, requiring the replacement of aging components periodically—often at considerable expense. The reactor design could be improved in conjunction with these planned replacements to deliver significantly higher neutron flux. These aging management issues are being appropriately handled through the programs implemented as corrective actions from the recent events. Preconceptual design work has been initiated to address these points. The creation of the reactor aging management division shows a commitment to improving and maintaining the core reactor support facilities.

The plan to convert the NCNR reactor to LEU involves high-density monolithic uraniummolybdenum fuel with 19.75 percent enrichment; the conversion is not expected to occur before 2030. This fuel is expected to have 10–15 percent lower neutron flux than the present HEU fuel and be more expensive. Moreover, the installation of a new cold source is delayed and will require a shutdown of 11 months. However, additional funding will be required for user operations post-conversion to LEU due, in part, to the fuel being more expensive.

Planning is under way for a new reactor. The 2021 NCNR assessment report recommended the following:

The Director of the National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR) should take a leadership role and own this mission with full support of NIST. The Director of NCNR should <u>commission</u> a study to define what the research community needs for the next 50 years in addition to the economic study already commissioned. In parallel and starting as soon as possible, the Director of NIST and the Director of NCNR should be proactive with the Visiting Committee on Advanced Technology, the User Group Executive Committee, the local community, the U.S. Nuclear Regulatory Commission (NRC),) and the appropriate congressional committees to ensure support and to build the case for constructing a new research reactor. (NASEM 2022, p. 17)

Section 10231 of the CHIPS and Science Act of 2022 stated as follows:

The Director shall develop a strategic plan for the future of the NIST Center for Neutron Research after the current neutron reactor is decommissioned, including: (1) a succession plan for the reactor, including a roadmap with timeline and milestones; (2) conceptual design of a new reactor and accompanying facilities, as appropriate; and (3) a plan to minimize disruptions to the user community during the transition.

At the time of the assessment meeting, NCNR was nearing the completion of a preconceptual design report for a new reactor and an economic impact study. A scientific community workshop occurred in October 2023 to gather community input on the design. A final report from this workshop is expected in January 2024.

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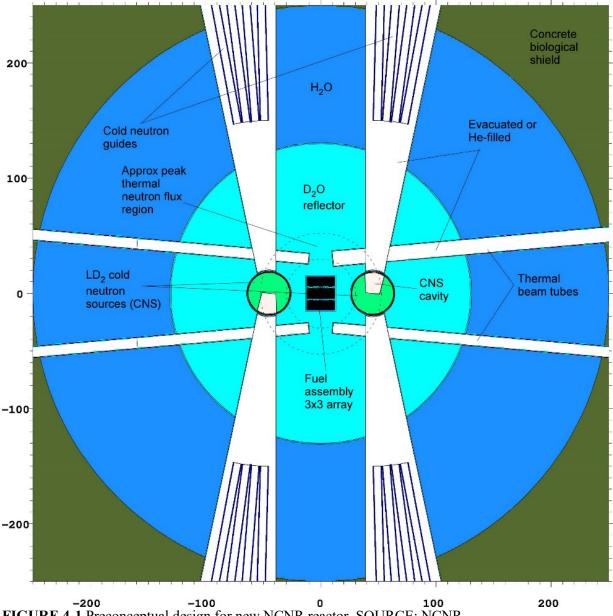


FIGURE 4-1 Preconceptual design for new NCNR reactor. SOURCE: NCNR.

The main elements of the preconceptual design include simple, safe, and affordable reactor operations; providing significantly increased capacity for U.S. neutron research and significantly increased data rates compared to the current suite of instruments, both from improved instrument and optics design and placing cold sources in regions of higher neutron fluxes. The preconceptual design is for a reactor of nominal 20 MW power using LEU in a light-water-cooled compact reactor core. This will be surrounded by a reflector tank containing heavy water. Plans include 2 cold neutron sources, 8 thermal neutron beams, and a capacity for up to 50 instruments. Figure 4-1 shows the elements of the preconceptual design.

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5 Dissemination of Program Outputs

The current publications and engagement activities of National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR) are scientifically focused. An opportunity exists to provide materials to familiarize those who are not already aware of the impact and importance of NCNR's work. Tracing the evolution of the research from current projects to final applications in everyday life would improve the general public's understanding of the impact of NCNR for fundamental research in this area.

This chapter addresses the fourth issue in the statement of task (see Chapter 1), assessing the effectiveness with which NCNR disseminates its program outputs. That portion of the statement of task asked three sets of questions: (1) How well are the NCNR's instrument development activities and research programs driven by stakeholder needs? (2) How effective are the mechanisms by which the NCNR provides access to its instrument suite by a broad subset of the scientific community? Are these mechanisms sufficiently comprehensive? (3) How well does the NCNR monitor the scientific use and impact of its facility? How could this be improved? This chapter answers these questions.

STAKEHOLDER INFLUENCE ON NCNR'S INSTRUMENT DEVELOPMENT ACTIVITIES RESEARCH PROGRAMS

As part of the preliminary planning for a new neutron reactor, a scientific community workshop called "Neutrons for the Future" was held in fall 2023 to gather community input. The workshop included 12 breakout groups that explored drivers for future neutron research, identified the necessary characteristics of instrumentation and facilities, and generated ideas to minimize disruption during any transitions to new instruments or facilities. NCNR will subsequently conduct an assessment of needs for neutron research to support the overall NIST mission.

The panel met with members of the NCNR User's Committee to learn about their experience working with NCNR facilities and staff. The feedback was very positive. NCNR staff was described as very helpful; they worked with users as partners, ensuring that they are able to acquire and analyze high-quality data. The users also commended the staff's aftercare—that is, data analysis and preparation of manuscripts after experiments were performed. They noted that NCNR staff also developed new sample environments to improve the efficiency and versatility of data collection; this was highly appreciated by users. The users also commended the willingness of staff to provide valuable help to them despite the fact that they were short-handed.

MECHANISMS TO PROVIDE ACCESS TO ITS INSTRUMENT SUITE

During the reduction in onsite access owing to the COVID-19 pandemic, NCNR staff performed many experiments on a mail-in basis. This was particularly effective for hard matter experiments and minimized the backlog. However, since the unplanned shutdown following the February 2021 reactor event, even with the resumption in onsite activities, there has been virtually no experimental activity. Meetings with the User Committee, graduate students, and postdocs revealed significant efforts by NCNR staff to assist users in acquiring beamtime at other facilities, including international facilities, during

NCNR's unplanned shutdown. It is apparent that NCNR staff made notable efforts to mitigate the impacts of the interruption in the availability of neutrons.

EDUCATION AND OUTREACH

Most of the education and outreach activities at NCNR are performed under the auspices of the Center for High Resolution Neutron Scattering (CHRNS), a partnership between the National Science Foundation (NSF) and NIST. One of the four main objectives of CHRNS is "to contribute to the development of human resources through educational and outreach efforts." These efforts are recognized as being integral to the success of CHRNS, particularly as a means to grow a diverse facility user base and to recruit enthusiastic, qualified staff.

NCNR's instrument scientists play a crucial role in bringing new faculty and graduate student users up to speed in conducting neutron scattering experiments. A key aspect of this is one-on-one user training by an NCNR instrument scientist before, during, and after the user visits NCNR to perform experiments and collect data. NCNR staff scientists frequently teach courses or give lectures on topics including scattering theory and techniques at universities nearby NCNR and at other schools around the nation and internationally. This personal interaction is vital for expanding the user base to research groups that have not previously done neutron scattering, and it is also important for the new students of established research groups. Fully staffing instrument scientist positions is vital for maintaining capabilities for a positive new user experience.

Outreach is clearly a priority to NCNR. Community engagement and developing the next generation of scientific expertise is a critical part of NCNR's mission, and NCNR hosts and participates in a commendable number of outreach activities that serve to engage with a wide variety of students, teachers, and researchers that expose students to neutron physics and serve to attract the next generation of neutron scientists. Of particular note is the CHRNS summer school, which has open invitations across both academia and industry to teach about applications of neutron scattering to soft matter. This past summer more than 80 people applied for the summer school, which shows how highly it is regarded by the community. It is the oldest neutron scattering school in the United States, with three-quarters of the participants returning as users. More importantly, more than 40 percent of graduate students who attend use neutron techniques after receiving their PhD. In addition, many graduate students from various universities-including the University of Delaware and the University of Maryland-have worked directly at NCNR. Typically, members of underrepresented groups make up more than 30 percent of the 30-40 participants that attend each year, and, more generally, NCNR has excellent outreach to traditionally underrepresented groups. The length of the school is 1 week, and the attendance is limited to 30-40 students each year to ensure that each student receives individualized attention and is fully engaged. A hallmark of this school is hands-on training.

The panel collected the following numbers that quantify some of NCNR's outreach efforts. A partnership between CHRNS and the Interdisciplinary Materials Research and Education Laboratory at Fayetteville State University involved 11 people. The CHRNS Summer School on Neutron Scattering served 128 students over the past three sessions combined. Various other NCNR workshops, schools, and tutorials have reached more than 450 people. Four graduate students funded by the NSF INTERN program have either participated or will participate in NCNR programs once access to neutron beams is restored at NCNR. Over the past two summers, 33 undergraduates have had research experiences through the Summer Undergraduate Research Fellowship, and approximately 5 high school students annually participate in the Summer High School Internship Program. While several presentations to the panel followed the career path of some past graduate students and postdocs, a more formal tracking program could improve the measure of NCNR's impact and reduce unnecessary attrition of neutron scientific talent.

NCNR also hosts a number of National Research Council postdocs (funded by the National Research Council Research Associateship Programs). Of the graduate students and postdocs with whom

DISSEMINATION OF PROGRAM OUTPUTS

the panel spoke directly, all were positive about the engagement with NCNR staff, specifically citing the community as being broadly welcoming. Many expressed the desire to work at NCNR, NIST, or other federal facilities after their tenure, which is a testament to the staff culture.

CHRNS has routinely provided facility tours to middle school, high school, and college students, reaching hundreds of students each year. Staff typically develop presentations, demonstrations, and other activities that are targeted to diverse groups of visitors and inform them about neutron scattering and its applications. Staff members also routinely travel to schools and organizations to give presentations and participate in other science, technology, engineering, and mathematics (STEM)-related activities such as judging regional science fairs, school career days, and other school-related events. Additionally, an effort is made to routinely seek out and provide to underrepresented student groups tours, demonstrations, and onsite tutorials.

CHRNS has successfully partnered with two important NSF programs serving minority institutions: the Partnerships for Research and Education in Materials Research program "to enable, build, and grow partnerships" and the Centers of Research Excellence in Science and Technology program "to enhance the research capabilities of minority-serving institutions." CHRNS has ongoing Partnerships for Research and Education in Materials Research program activities with Fayetteville State University, and it partners with two recipients of Centers of Research Excellence in Science and Technology grants, Morgan State University and California State University, San Bernardino.

NCNR also actively disseminates research findings, increasing the number of publications in particular with high impacts in the areas of energy materials, catalysis, and battery research, showcasing its commitment to knowledge sharing and collaborations.

MONITORING THE SCIENTIFIC USE AND IMPACT OF THE FACILITY

NCNR tracks the impact of its publications, and many of them are impactful based on the number of citations they attract. In 2022, there were five highly cited publications (i.e., having 21 or more citations each by the time of this assessment in 2023). In 2021, there were five such publications, with two of these having more than 100 citations by the time of this assessment in 2023. In 2020, 11 publications had more than 100 citations each by the time of this assessment in 2023.

However, the materials provided to the panel make no mention of patents of records of invention resulting from work done at NCNR. Accordingly, NCNR would benefit from tracking patents and records of invention. It could also increase the promotion of patenting the new devices and techniques that it develops throughout the course of its activities.

nSOFT is an industrial consortium, unique among neutron-scattering user facilities, designed specifically to engage industry in neutron scattering. Traditional measures of productivity may not capture the impact of the program and the 2018 National Academies' assessment report on NCNR cited a need to develop appropriate metrics to define success (NASEM 2018). The report states that

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. (NASEM 2018, p. 24)

This panel supports the intent of the panel that authored the 2018 assessment report. Professional outside organizations with experience in conducting broader impact surveys may be better suited to the task of obtaining the appropriate data than NCNR staff who are currently performing this function.

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Appendixes

An Assessment of the National Institute of Standards and Technology Center for Neutron Research: Fiscal Year 2023

A Acronyms and Abbreviations

AI	artificial intelligence
CANDOR	Chromatic Analysis Neutron Diffractometer or Reflector
CHRNS	Center for High Resolution Neutron Scattering
FY	fiscal year
GAO	Government Accountability Office
HEU	highly enriched uranium
HFBS	High-Flux Backscattering Spectrometer
ILL	Institut Laue-Langevin
IMS	Innovations in Measurement Science
LEU	low enriched uranium
MACS	multi-axis crystal spectrometer (MACS)-II spectrometer
MAGIK	multi-angle grazing incidence K-vector reflectometer
ML	machine learning
MML	Material Measurement Laboratory
MRI	major research instrumentation
NB	non-base
NCNR	NIST Center for Neutron Research
NICE	new instrument control environment
NIST	National Institute of Standards and Technology
NRC	U.S. Nuclear Regulatory Commission
NSE	neutron spin echo spectrometer
NSF	National Science Foundation
OA	other government agencies
ORCID	open researcher and contributor ID
ORNL	Oak Ridge National Laboratory
PML	Physical Measurement Laboratory
PoLAR	polarized large angle resolution spectrometer
ppm	parts per million
SAC	Safety Assessment Committee

SANS SNS SPINS STEM STRS	small-angle neutron scattering Spallation Neutron Source spin polarized inelastic neutron spectrometer science, technology, engineering, and mathematics scientific and technical research service
USANS	ultra-high-resolution small-angle neutron scattering
VSANS	very-small-angle neutron scattering
WCF	working capital fund

B Biographical Sketches

PETER F. GREEN, Chair, is the chief research officer and the deputy laboratory director for science and technology at the National Renewable Energy Laboratory in Golden, Colorado. He began his professional career at Sandia National Laboratories where he spent 11 years in positions that included senior member of the technical staff and department manager. He subsequently became a professor of chemical engineering and the BF Goodrich Endowed Professor of Materials Engineering at The University of Texas at Austin. In 2005, he became a professor and the chair of the Department of Materials Science and Engineering at the University of Michigan, where he was also the Vincent T. and Gloria M. Gorguze Endowed Professor of Engineering and a professor of chemical engineering, macromolecular science, engineering, and applied physics. During this time, he was the director of the Department of Energy (DOE) Frontier Research Center and the Center for Solar and Thermal Energy Conversion. Dr. Green was the 2006 president of the Materials Research Society (MRS). He is a fellow of the American Physical Society (APS), the Royal Society of Chemistry (United Kingdom), the American Association for the Advancement Science (AAAS), the American Ceramics Society (ACerS), and the MRS. He is a former divisional associate editor for Physical Review Letters and the inaugural editor-in-chief of MRS Communications. Dr. Green is a former member of the National Academies of Sciences, Engineering, and Medicine's Board on Physics and Astronomy and Board on Army Science and Technology. He is a former chair of the National Academies' Solid State Sciences Committee (currently known as the Condensed Matter and Materials Research Committee) and the former chair of the Panel for Neutron Research. Dr. Green is a recipient of the DOE Secretary's Achievement Award, in 2021 and again in 2023. He is a member of the National Academy of Engineering. He earned his BA and MA in physics in 1981 from Hunter College. His MS and PhD are from Cornell University in materials science and engineering.

KEN ANDERSEN is the director of the Institut Laue-Langevin (ILL) in Grenoble, France. Previously, he was the associate laboratory director (ALD) for neutron sciences at Oak Ridge National Laboratory (ORNL). As ALD, Dr. Andersen oversees the operation and management of two neutron facilities: the Spallation Neutron Source (SNS) and the High Flux Isotope Reactor. Each year these facilities support about 3,000 visiting users. Dr. Andersen aims to further broaden ORNL's role in neutron sciences globally, expand ORNL's instrument capabilities, and prepare for a second target station at SNS. Previously, he was the director for the Neutron Technologies Division within the Neutron Sciences Directorate. Between 2010 and 2019, Dr. Andersen was the head of the Neutron Instruments Division at the European Spallation Source (ESS) in Lund, Sweden. He was previously in charge of the Neutron Optics Muon Source in the United Kingdom, as well as having spent a brief period as a postdoc at the KENS neutron facility in Japan. His research interests center around the design and optimization of neutron instruments for both steady-state and pulsed neutron sources. He has a PhD in physics from the University of Keele in the United Kingdom (1994).

PENGCHENG DAI is the Sam and Helen Professor of Physics at Rice University. His research focuses on using neutron scattering as a probe to study strongly correlated electron materials. In his career, he worked on copper, iron, and heavy fermion superconductors; quantum spin liquid; and other magnetic

materials; mostly using neutron scattering to study their bulk magnetic properties. He is a fellow of the APS, the AAAS, and the Neutron Scattering Society of America (NSSA). He won the Sustained Research Prize of NSSA in 2016, and the Kamerlingh Onnes Prize in 2022. He obtained his PhD in condensed matter physics from the University of Missouri in 1993.

AARON P.R. EBERLE is the energy and technology advisor to ExxonMobil Corporate Strategic Planning. Over the past decade, Dr. Eberle has held various assignments across the company within its chemicals, business, and technology organizations. Before joining ExxonMobil, he held a National Academies' postdoc at the National Institute of Standards and Technology (NIST) Center for Neutron Research where he studied colloidal systems with cold neutron instruments. He received his BS and PhD in chemical engineering from the University of Rochester and Virginia Polytechnic Institute and State University, respectively.

ROSARIO A. GERHARDT is a full professor at the School of Materials Science and Engineering at the Georgia Institute of Technology where she has been on the faculty since 1991. She was chosen as the Goizueta Foundation Faculty Chair in 2015. Her primary research for several years has related to the underlying structure of materials to their properties from the atomic level to macroscopic dimensions using X-ray and neutron scattering together with transmission electron microscopy, scanning electron microscopy, and atomic force microscopy to unravel the intricacies of conducting thin films to insulating materials. She has worked with ceramics, ceramics composites, and polymer composites, as well as conducting polymers and metallic alloys, and has expertise on fabrication and characterization of porous materials and percolating composites. She received her DEngSc from Columbia University in 1983. She was a NASA/American Society for Engineering Education faculty fellow at the NASA Marshall Space Flight Center in 1995 and served as a visiting professor at the Center for Nanophase Materials Sciences at ORNL during the 2007–2008 academic year. She is a fellow of the ACerS, was recently elevated to an Institute of Electrical and Electronics Engineers senior member and was recently elected to the World Academy of Ceramics. She delivered the 2017 ACeRS Friedberg Lecture. She has served as a reviewer on many National Science Foundation panels and National Academies' panels, in particular the Research Associateship Program and the Defense Materials and Manufacturing and Infrastructure Program. Dr. Gerhardt has also assisted the Advanced Photon Source at Argonne National Laboratory as well as SNS and the High Flux Isotope Reactor at ORNL as a reviewer.

CHRISTOPHER R. GOULD is an Alumni Distinguished Undergraduate Professor of Physics Emeritus at North Carolina State University. He is a nuclear physicist by training, with interests in cosmology, energy research and policy, science education, and neutron and neutrino physics. He has held visiting appointments at Los Alamos National Laboratory; the Institut für Kernphysik, Frankfurt; the Atomic Energy Institute, Beijing; the University of Petroleum and Minerals, Dhahran; and the Oak Ridge Center for Advanced Studies. Following retirement in 2016, he took a 2-year interagency personnel agreement position with the Office of Science at DOE, serving as the program manager for the nuclear structure and nuclear astrophysics programs in the Office of Nuclear Physics. His current interests focus on energy issues and the role that nuclear reactors may play in backing up intermittency concerns associated with solar and wind electrical power generation. Dr. Gould is a fellow of the APS, a co-recipient of a 2008 presidential award from RTI-International, and a recipient of the 2016 Breakthrough Prize in Fundamental Physics. He holds a BSc from Imperial College, London, and a PhD from the University of Pennsylvania.

ANDREW HARRISON became the director of science at the Extreme Light Infrastructure ERIC in 2022, having been the chief executive officer of Diamond Light Source, the United Kingdom's national synchrotron facility (2014–2022) and the scientific director and then director general of the ILL in Grenoble, France (2006–2014). Prior to that, he held research fellowships and faculty positions at the University of McMaster (1988–1990), the University of Oxford (1990–1992), and the University of

APPENDIX B

Edinburgh (1992–2006), where he led research in solid-state magnetism, largely using neutron scattering techniques. He has chaired EIROForum, the collection of European international infrastructures, including CERN (European Organization for Nuclear Research), European Southern Observatory, and the European Space Agency. He is a UK delegate for the European Strategy Forum on Research Infrastructures Council of the European Commission—when the United Kingdom is allowed to participate—and in 2017, he became the chair of the Association of European-Level Research Infrastructures Facilities, the organization that represents European research infrastructures not in EIROForum. His awards include the Fellowship of the Royal Society of Edinburgh (2002), Most Excellent Order of the British Empire for services to science (2021), Fellow of the Royal Society (2022), and he has honorary positions or degrees at St. John's College, Oxford (2015), the University of Manchester (2017), the University of Edinburgh (2017), and the University of Bath (2019). He has a doctorate and undergraduate degree in chemistry (Oxford 1986 and 1982). He has served on National Academies' reviews at NIST twice before.

ANDREW J. JACKSON is the group leader for instrument scientists and the acting head of the Neutron Instruments division at ESS. In this role, he leads the development, design, commissioning, and operation of the neutron scattering instruments. He has worked at ESS since 2011, starting as an instrument scientist for small angle neutron scattering. Prior to working at ESS, Dr. Jackson held positions as a guest researcher at the NIST Center for Neutron Research, visiting researcher at the Lawrence Berkeley National Laboratory, senior scientist at the University of Delaware, research associate at the University of Maryland, and postdoctoral research fellow at the Australian National University. He has more than 25 years of experience in the development and application of neutron and X-ray scattering methods to problems in soft matter physics, colloid science, and polymer science. Dr. Jackson also holds a position as an associate professor in physical chemistry at Lund University and his current research interest is in the structure and behavior of deep eutectic solvents, and especially self-assembly in these nonaqueous hydrogen bonded solvents. He holds master's and doctoral degrees in chemistry from the University of Oxford.

MEGUMI KAWASAKI is a Jack R. Meredith Faculty Scholar and an associate professor in the School of Mechanical, Industrial, and Manufacturing Engineering at Oregon State University. She previously served as an associate professor at Hanyang University in Seoul, South Korea, where she joined as an assistant professor in 2012. In addition, she held the position of adjunct research associate professor in aerospace and mechanical engineering at the University of Southern California from 2012 to 2017 and currently holds a visiting research associate professor position in materials science at Osaka Metropolitan University since 2013. Dr. Kawasaki's research expertise lies in the processing of bulk nanostructured metals and materials (BNM) using severe plastic deformation techniques, as well as characterizing the microstructural evolution of BNM under extreme conditions such as stress and heat using X-ray and neutron diffraction, as well as synchrotron high-energy X rays. Her research has been recognized internationally, with successful beamline proposals awarded in Japan (Spring 8 and JPARC), Germany (DESY), and the United States (ALS). She serves on the International NanoSPD Steering Committee.

THOMAS K. KROC is an applications physicist III at the Fermi National Accelerator Laboratory (Fermilab). He develops new applications of accelerators and accelerator technologies such as medical device sterilization. He has led the organizing committee for four workshops on medical device sterilization to promote the use of electron beams and X rays held at Fermilab in 2019 through 2022. For 20 years he worked with the Neutron Therapy Facility at Fermilab, which provided external beam radiation therapy for cancer using high-energy neutrons. He assumed leadership of this program from 2008 until its closure in 2013. His educational and professional experience includes accelerator physics, medical physics, experimental high-energy physics, and nuclear engineering. He was the chair of a National Academies' committee that published the report *Radioactive Sources: Applications and*

Alternative Technologies. Dr. Kroc holds a BS in engineering physics from The Ohio State University and a PhD in physics from the University of Illinois at Urbana-Champaign.

ANDREW T. SMOLINSKI is the chief of the Radiation Sources Section at the Armed Forces Radiobiology Research Institute (AFRRI), responsible for facility management of the research reactor and cobalt irradiator facilities. His expertise is in radiation facility management, operations, and engineering, with 24 years of experience working with more than 10 research and power nuclear reactors under the U.S. Nuclear Regulatory Commission (NRC), naval reactors, and DOE regulatory frameworks. Mr. Smolinski performed engineering, research support, and facility management functions for hot cells and research reactors at Idaho National Laboratory to support DOE advanced nuclear fuels and materials. He served as a senior reactor operator-certified shift technical advisor at the Kewaunee Nuclear Power Station and worked for Knolls Atomic Power Laboratory as a test engineer in support of reactor startups for the Naval Nuclear Propulsion Program. He has held NRC SRO licenses from AFRRI and the University of Wisconsin. He serves on the executive committee of the National Organization of Training, Research, and Test Reactors, various standards committees for the American Nuclear Society, and several reactor and radiation safety committees, including AFRRI and the University of Maryland.



An overview of the 30 experimental beam instruments and experiments at the National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR) is provided in Figure B-1.

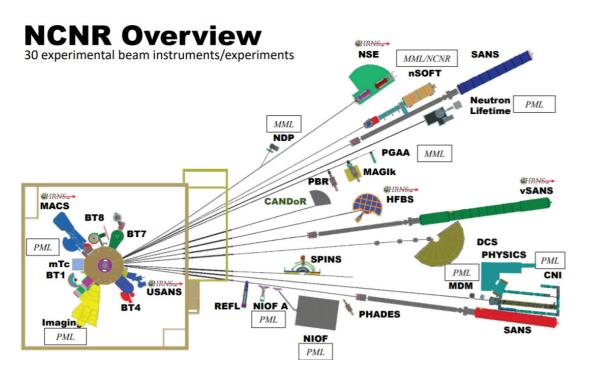


FIGURE B-1 Beamlines and instruments at NCNR. NOTES: The mTc instrument has been removed. An updated figure is not yet available. SOURCE: NCNR.

An Assessment of the National Institute of Standards and Technology Center for Neutron Research: Fiscal Year 2023