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

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

Committee on NIST Technical Programs

Laboratory Assessments Board

Division on Engineering and Physical Sciences

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

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Acknowledgment of Reviewers

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

Robert J. Cava, Princeton University,
Paul A. Fleury, Yale University,
Tonya L. Kuhl, University of California, Davis,
E. Ward Plummer, Louisiana State University,
John Root, University of Saskatchewan,
Thomas P. Russell, University of Massachusetts, Amherst,
Ram Seshadri, University of California, Santa Barbara, and
David A. Weitz. Harvard University.

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

Contents

Summary

At the request of the Director of the National Institute of Standards and Technology (NIST), in 2015 the National Research Council[1] formed the Panel on Review of the Center for Neutron Research at the National Institute of Standards and Technology and formulated the following statement of task for the panel:

> The National Research Council shall appoint a panel to assess the scientific and technical work performed by the National Institute of Standards and Technology (NIST) Center for Neutron Research. This panel will review technical reports and technical program descriptions prepared by NIST staff and will visit the facilities at 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 prepare a report summarizing its assessment findings.

The Director of NIST requested that the panel focus its assessment on the following factors:

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

[1] Effective July 1, 2015, the institution is called the National Academies of Sciences, Engineering, and Medicine. References in this report to the National Research Council are used in an historical context identifying programs prior to July 1.

This report presents general observations and recommendations about the NIST Center for Neutron Research (NCNR), based on the assessment foci of the 2015 review. These observations complement those presented in prior reports,[2] whose foci differ.

GENERAL OBSERVATIONS

With the construction of its new guide hall complete and the availability of the new source for producing cold neutrons, the NCNR is well positioned to investigate some of the most important and impactful problems in condensed matter, including superconductivity and magnetism; energy (batteries, fuel cells, and methane storage); biomedical sciences; pharmacy; and geology. The new guide hall sample laboratory will be state of the art, enabling researchers to take advantage of the most exciting developments in sample preparation processes and techniques. Infrastructural developments at the NCNR include new instruments, such as the chromatic analysis neutron reflectometer (CANDOR) and the very small angle neutron scattering (vSANS) instrument designed to improve capabilities in the spatial and temporal properties of materials, as well as the relocation and upgrade of current instruments, such as the neutron spin echo (NSE) spectrometer. The new cold neutron imaging station enables new neutron imaging experiments of elements in samples of virtually any geometrical configuration, including engine parts. The instrumentation development plans involving the ^{3}He wide-angle polarizers, multiaxis crystal spectrometer (MACS II), and CANDOR are imaginative.

The management of the NCNR has effectively planned for the future and has continued to make wise investments. It is anticipated that the strategic plan, which is expected to be completed in the coming months, will formalize the entire planning and operational process, helping to ensure that the long-term goals and objectives of the center are met.

KEY FINDINGS AND RECOMMENDATIONS

The new guide hall is now complete, and new instruments that enhance measurement capabilities are either complete or are at different stages of completion. Moreover, new sample preparation and sample environment capabilities are continually being established. These developments significantly enhance the ability of the NCNR to remain at the leading edge in neutron research in the coming decades. However, some specific actions in the near- and long-term future will be required.

Recommendation 1: The NCNR should develop and document a plan for instrument development, which should include plans for the two remaining end stations in the new guide hall. In addition, the NCNR should hold a workshop in 2017 to get feedback from users regarding the plan. Input from the user community should also be used to update the NCNR strategic plan, expected to be completed by the end of 2016.

It is commendable that NCNR management is identifying creative ways to procure a budget for cold source developments, instrument upgrades, and new instruments from different sources, such as universities, the National Nuclear Security Administration, the National Science Foundation (NSF), and—primarily—from NIST. Nevertheless, this approach is fragmented.

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[2] See the National Research Council reports *Assessment of the National Institute of Standards and Technology Center for Neutron Research—Fiscal Year 2011* and *Assessment of the National Institute of Standards and Technology Center for Neutron Research—Fiscal Year 2013*, published by the National Academies Press, Washington, D.C., in 2011 and 2013, respectively.

Recommendation 2: The NCNR should document a plan that describes the sources of financial support, with specific objectives for budgets and strategies, and sources that would ensure that the plans for future instruments are realized.

The research at the NCNR is at the cutting edge, as evidenced by high-quality publication in the very best journals in the world in different fields, and also by the number of citations. Additional opportunities could be realized if there were a stronger integration between theory and experimentation in some areas. The success is particularly notable in cases where theory and experiment are well integrated.

Recommendation 3: The NCNR should develop a strategy to achieve more substantial interactions with researchers around the world to develop integrated teams capable of addressing forefront neutron problems. Potential strategies should include expanding the sabbatical program.

An important objective of the mission of NIST is to transition fundamental scientific knowledge to practical technology. Within NCNR, the nSOFT program plays a central role in meeting this objective. The evolution of the nSOFT program and its progress are commendable. Deep ties have been developed with companies, and the impact on industrial processes is becoming evident. In this regard, the transfer of awareness and practical applications of neutrons to U.S. industry is now evident. The goals and objectives of the program have evolved during the past 2 years.

Recommendations 4: The NCNR should (a) develop and document a complete strategic plan for nSOFT with elements that include the metrics for success (for example, financial, number of companies, patents, publications, new products), a profile of the type of company that would benefit from becoming a member of nSOFT, a financial model, and personnel commitment; (b) work with the companies to articulate success stories illustrating how neutron research has had an impact; (c) clarify the current approach to technology transfer activities; and (d) revisit the current status of intellectual property.

In 2030 the user needs for access to neutron scattering facilities in the United States will not be met. Moreover, the reactor licensing limit of 2029 imposes an additional challenge.

Recommendation 5: The NCNR should expand current initiative planning for a next-generation reactor. This planning may even include consideration of an additional reactor.

Reactor fuel costs continue to rise at a significant rate. A reduction of access to neutron-scattering capabilities would have a negative impact on the neutron-scattering community in the United States. This would have serious implications for the overall progress of science and technology in some fields.

Recommendation 6: The NCNR should procure resources to afford fuel costs in order to continue to operate at current levels.

1

Introduction

At the request of NIST, the National Research Council[1] has, since 1959, annually assembled panels of experts from academia, industry, medicine, and other scientific and engineering environments to assess the quality and effectiveness of the NIST measurements and standards laboratories, of which there are now seven,[2] as well as the adequacy of the laboratories' resources.

At the request of the Director of NIST, in 2015 the National Academies formed the Panel on Review of the Center for Neutron Research at the National Institute of Standards and Technology and established the following statement of task for the panel:

> The National Research Council shall appoint a panel to assess the scientific and technical work performed by the National Institute of Standards and Technology (NIST) Center for Neutron Research. This panel will review technical reports and technical program descriptions prepared by NIST staff and will visit the facilities at 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 prepare a report summarizing its assessment findings.

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[1] Effective July 1, 2015, the institution is called the National Academies of Sciences, Engineering, and Medicine. References in this report to the National Research Council are used in an historical context identifying programs prior to July 1.

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

[3] See the National Research Council reports *Assessment of the National Institute of Standards and Technology Center for Neutron Research—Fiscal Year 2011* and *Assessment of the National Institute of Standards and Technology Center for Neutron Research—Fiscal Year 2013*, published by the National Academies Press, Washington, D.C., in 2011 and 2013, respectively.

- How well does the organization's scientific expertise support the organization's technical programs and the organization's ability to achieve its stated objectives?

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

In order to accomplish the assessment, the NRC assembled a panel of six volunteers whose expertise matches that of the work performed by the NCNR staff.[4]

On July 7-9, 2015, the panel assembled for two and a half days at the NIST facility, during which it received welcoming remarks from the NIST Director, heard overview presentations by NCNR management and presentations by researchers at the NCNR, and attended an interactive session with NCNR management.

The panel's approach to the assessment relied on the experience, technical knowledge, and expertise of its members. The panel reviewed selected examples of the technical research performed at the NCNR; because of time constraints, it was not possible to review the NCNR programs and projects exhaustively. The examples reviewed by the panel were selected by the NCNR. The panel's goal was to identify and report salient examples of accomplishments, challenges, and opportunities for improvement with respect to the factors suggested by the Director of NIST. These examples are intended collectively to portray an overall impression of the center, while preserving useful suggestions specific to the projects and programs that the panel examined. The panel applied a largely qualitative rather than a quantitative approach to the assessment.

Given the necessarily nonexhaustive nature of the review, the omission in this report of any particular NCNR project should not be interpreted as a negative reflection on the omitted project.

[4] See http://www.ncnr.nist.gov/ for information on the NIST Center for Neutron Research organization and programs, accessed July 24, 2015.

2

Immediate and Long-Term Competitiveness of the NCNR

Approximately 15 years ago, investments were initiated to upgrade and to build new and advanced neutron scattering facilities around the world. Europe, Asia, and Australia have come to account for approximately 75 to 85 percent of the neutron-scattering capabilities worldwide. The increasingly widespread availability of well-characterized and intense neutron sources has been responsible for new insights into the science of neutrons and related improvements in neutron optics and instrumentation. Improvements of the resolution of experimental observables, enhancements in the efficiency of data collection, and new developments in the theoretical analysis of experimental neutron scattering and imaging data have followed. Consequently, applications that include imaging and trace element analysis have become more viable than in prior years. Concurrently, new sample environments that simultaneously accommodate experimental probes, such as x rays, of samples that may be undergoing external perturbations, such as magnetic fields and dynamic or static mechanical stresses, have enabled unprecedented insights into the properties of condensed matter. Neutron scattering has an important impact on diverse fields such as engineering, condensed-matter physics, medicine, pharmacy, biology, chemistry, and geology. Neutron scattering has important technological implications for areas such as oil recovery, the processing of paints and personal healthcare products, energy (fuel cells, batteries, thermoelectrics, solar cells), and manufacturing.

Since the 1990s, the NCNR has been among the world's leading facilities for the study of neutrons and their applications. With the very recent completion of the new source for producing cold neutrons and the guide hall, the NCNR is well positioned to investigate some of the most important and impactful problems in condensed matter, including superconductivity and magnetism, energy (batteries, fuel cells, and methane storage), biomedical sciences, pharmaceuticals, and oil recovery. Infrastructural developments at the NCNR include new instruments such as the vSANS technique, designed to improve capabilities in the spatial and temporal properties of materials. The relocation and upgrade of the NSE spectrometer, in collaboration with the Center for High Resolution Neutron Scattering (CHRNS) is also significant. The compensation coils were developed at the Institut Laue-Langevin (ILL). This upgraded instrument will be among the best NSE instruments in the world.

Other developments include the cold neutron imaging station, which is enabling new neutron imaging experiments of elements such as hydrogen in metals or imaging samples of virtually any geometrical configuration, including engine parts. The instrumentation development plans are imaginative. Current and planned instruments (the ^{3}He wide-angle polarizers, MACS II, and CANDOR) represent potential game-changing advances. The new guide hall sample laboratory will be state of the art, enabling researchers to take advantage of the most exciting developments in sample preparation processes and techniques. The continued improvements of sample environments, flow cells, and strain devices create an excellent environment in which to make important scientific discoveries that would otherwise be difficult to achieve.

The output of the NCNR remains consistently high. During the past year, the NCNR has served the research needs of more than 2,270 individuals from 241 academic institutions and government laboratories with 28 instruments. The NCNR's record of operating about 250 days per year compares favorably with neutron facilities around the world. A comparison of days of operation per year across worldwide neuron centers is reported in the previous assessment report.[1] With more than 700 proposals per year, the request for beam time (2,967 days) is 2.1 times that of available time, reflecting an important demand for the use of neutrons to study the properties of condensed matter. The new capabilities enable the NCNR to solve industrially relevant problems. Achievements include improved understanding of lipid bilayers and lipid–protein interactions, superconductivity and magnetism, and polymer nanocomposites. Some of these advances are unique and were possible only because of the recently developed capabilities at the NCNR.

Through effective management practices and collaborations the NCNR, one of only two neutron user programs in the United States is well positioned to play an essential role in the development of new science and enable potentially important technological advances. The high level of competence of NCNR staff and their effective collaborations with users are largely responsible for scientific publications in high-quality international journals. The high productivity level in relation to its instrument capabilities is well exemplified by the following example: Worldwide, more than 100 publications per year, in different fields, from the life sciences, materials sciences, and physics, rely on neutron reflectivity experiments. The NCNR operates only 3 of the 25 reflectometers in the world, yet it accounts for approximately 33 percent of the publications. NIST's collaborative program with NSF, CHRNS, has an important impact on the discovery of new science and the training of young scientists. The CHRNS instruments are used by university, government, and industrial researchers in materials science, chemistry, biology, and condensed-matter physics to investigate materials such as polymers, metals, ceramics, magnetic materials, porous media, fluids and gels, and biological molecules. An extensive list of CHRNS publications is presented on the NIST website.[2]

According to leaders of the NCNR user groups and to user surveys, the user program is highly effective in that it identifies the most meritorious proposals for beam time received by the NCNR; the outcomes are manifested in the quality of the publications, almost all of which are in respected, refereed archival journals. NCNR management has established an effective mechanism to solicit feedback from users that informs its decisions. Based on user surveys and other feedback, the NCNR facility is satisfying the needs of the user community..

With the completion of the new guide hall, the advanced sample environment capabilities, and effective management, coupled with input from the user community, the NCNR is poised to make important scientific and technological advances.

[1] National Research Council, *An Assessment of the National Institute of Standards and Technology Center for Neutron Research—Fiscal Year 2013*, The National Academies Press, Washington, D.C.

[2] NIST Center for Neutron Research, "CHRNS Instrument Publication Lists," https://www.ncnr.nist.gov/programs/CHRNS/publists.html, last modified January 13, 2015.

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Scientific and Technological Problems Investigated at the NCNR

SOFT MATERIALS

Neutron scattering plays a pivotal role in how scientists and engineers understand and design the molecular structure, dynamics, physical properties, and processing of soft materials. This class of condensed matter subsumes an enormous variety of products, including plastics, composites, almost all forms of biological tissue, and complex combinations of organic and inorganic compounds formulated into personal care products. The NCNR provides the nation and the international community with the neutron-scattering facilities, associated measurement techniques, and fundamental knowledge necessary to advance our understanding of how soft materials are spatially configured and how they respond temporally to forces at length scales ranging from 1 to 10,000 nm. This effort draws on an extensive suite of instruments currently in operation or under development, including five small-angle neutron scattering (SANS) machines, four reflectometers, a backscattering instrument, a spin-echo spectrometer, a disk chopper spectrometer (DCS), and an imaging station. This section highlights selected recent advancements in experimental techniques and scientific discoveries at the NCNR through neutron scattering on soft materials.

A particularly exciting area of research pursued at the NCNR deals with the structure and dynamics of lipid membranes, which form the boundary of most cellular structures in living tissue. Lipids are a category of molecules known as amphiphiles. One portion of a lipid, known as the "head group," is polar and readily associates with water, while the tail section is a nonpolar, oil-like hydrocarbon that does not mix with aqueous media. These compounds self-assemble into sheetlike bilayer structures just 3 to 4 nm thick with the hydrocarbon tails at the center. In living cells, this bilayer membrane is decorated with a plethora of other structural elements, such as cholesterol and proteins, that mediate chemical and electrical communication inside and outside the cell. Understanding the structure and function of lipid membranes is a central challenge to molecular biology.

Neutron scattering offers unparalleled opportunities to unravel the mysteries associated with lipid bilayers. The NCNR team has provided scientists from around the nation with a robust complement of experimental tools with which to attack these problems. Neutron reflectivity plays a particularly important role. In collaboration with scientists from the National Institutes of Health (NIH), Carnegie Mellon University, the University of Chicago, the University of California, Irvine, and other institutions, NCNR staff members and postdoctoral researchers have explored how integral membrane proteins are embedded in the lipid bilayer and how peripheral membrane proteins attach to the membrane surface. By mathematically inverting the angular-dependent intensity of neutrons reflected from these structures, information regarding the precise location and configuration of such compounds within and around the lipid membranes have been exposed. Augmented by molecular theory, these results are guiding exciting new interpretations of cellular function. These studies provide the basic ingredients to target specific diseases with tailored molecular-level therapies.

Polymers, composites, and self-assembled soft materials such as surfactants inevitably are processed under conditions that require flow and deformation. Neutron scattering offers unique opportunities to explore the basic molecular configurations and molecular-scale deformations that govern the processing conditions required to optimize ultimate material properties. Polyethylene, the largest volume synthetic polymer, is a semicrystalline material that is formed into products such as packaging films and plastic parts at elevated temperatures by melt processing. Viscoelastic fluids, essential to the oil field services industry as drilling fluids, respond to flow in complex ways that reflect the organization of surfactants into nanoscale structures. The NCNR has been a world leader in developing scattering tools that permit the in situ interrogation of molecular structure during flow.

A unique enabling factor is that cold neutrons can penetrate many structural materials such as glass and aluminum, which can be fashioned into tools that can be inserted into a SANS instrument. These rheological devices impose specified flow fields while simultaneously recording the applied forces, providing a direct link between nanoscale structural features and macroscopic viscoelastic properties. The NCNR has developed a host of complementary devices for this purpose. For example, paints are formulated with a complex array of ingredients that include colloidal polymers and inorganic particles that interact in ways that control the flow behavior. When subjected to shear, the associated structures reorganize in a manner that directly influences the formation of coatings. The Dow Chemical Company has used the SANS instrument to determine the state of dispersion in latex paints filled with titanium dioxide particles while shearing the fluid. The resulting knowledge, published in the leading polymer journal *Macromolecules*, enabled the development of theoretical models, providing a critical link for the company's formulation of advanced coatings.

In another project, NCNR scientists teamed up with a research group from the University of Delaware to create a shear flow cell that allows the interrogation of surfactant-based viscoelastic fluids that find applications in myriad products, including cosmetics and drilling fluids. This class of soft materials spontaneously organizes into wormlike micelles, long threadlike moieties that entangle at the nanometer scale, resulting in a soft, gelatinous state. When subjected to shearing flows, these soft solids flow, but not homogeneously. Using a rheological tool designed at the NCNR and operated in conjunction with several SANS instruments, team members were able to unravel how the evolution of a branched micelle structure during shearing resulted in the inhomogeneous flow behavior, and they were able to connect this morphological transition to the applied forces. This discovery holds important consequences for the application of these complex fluids while drilling oil wells.

Another important set of advancements currently being developed at the NCNR is instruments that permit extreme test conditions, including unprecedented temperatures and pressures such as those encountered when drilling deep wells. Other testing devices under development will allow simultaneous application of electric fields to conducting fluids and ionic membranes used in batteries and fuel cells.

Another unique feature afforded by neutron scattering is the ability to label molecules with deuterium, a stable isotope of hydrogen. Because neutrons scatter differently from deuterium, specific structural features can be identified by isotope labeling. Because hydrogen is ubiquitous in soft materials, this technique, enabled by advanced synthetic chemical methods, is an essential tool. NIST scientists are using the NCNR to exploit this approach in order to explore the molecular configurations responsible for the mechanical properties of polyethylene, a $200 billion per year industry worldwide. By swelling semicrystalline polyethylene plastics with deuterium-labeled solvent and monitoring the resulting changes in SANS patterns, scientists were able to establish how portions of the polyethylene molecules connect the crystalline regions of the plastic. This work, conducted in collaboration with the Chevron Phillips Chemical Company, is contributing to the design of tougher and more resilient plastics.

NCNR staff should be applauded for providing an outstanding scientific environment for the diverse range of outside users from universities and industry who make use of the neutron-scattering facilities. The instruments placed at the disposal of the user community play an integral role in the pursuit of fundamental knowledge and the development of advanced and technologically sophisticated soft materials.

HARD MATTER

The Hard Matter research program at the NCNR is focused on three important areas: magnetic materials, novel superconductivity, and the structure of thin films and interfaces. The first two of these are predicated on an excellent suite of inelastic neutron-scattering instruments: MACS; a double-focusing triple-axis spectrometer (BT7); a DCS time-of-flight chopper instrument; and the Spin Polarized Inelastic Neutron Spectrometer (SPINS). Additionally, a very successful program of reflectometry studies has been enabled by NCNR's strength in this area. The recent exploitation of sophisticated polarization analysis using polarized ^3He transmission cells has contributed significantly to all programs related to magnetism in materials.

Magnetism is widely regarded as a significant application of neutron scattering, because the neutron possesses a spin magnetic moment and couples well to magnetism in solids. The magnetism program at the NCNR has focused on a range of very topical magnetic materials, including quantum, low-dimensional, and geometrically frustrated magnetism; multiferroic materials; novel magnetic superconductors; and exotic metals close to a magnetic instability. New capabilities on MACS, in particular, have enabled very important and appreciated studies of the quantum $S = 1/2$ Kagomé antiferromagnet, herbertsmithite. This general problem is a cause-célèbre in contemporary condensed-matter physics, and the MACS NCNR results have been an extremely high-profile contribution to the field.

NCNR staff and collaborators have carried out very comprehensive studies on several families of Fe-based superconductors and their magnetic parent compounds, mostly using the BT7 and BT1 powder diffractometer, and these have also been well appreciated internationally. The DCS time-of-flight chopper instrument continues to support a broad-ranging program in hard matter research, mainly related to magnetism and low-energy spin dynamics in new materials.

Recent impressive advances in ^3He polarization analysis cells at the NCNR have led to the development of new polarization analysis capabilities with wide angular coverage on both BT7 and MACS. This technical advance is state of the art and is expected to very soon enhance the impact of the magnetism program at the NCNR generally. Large area polarization cells have been tested with very encouraging results on both BT7 and MACS. This will make spin flip and non-spin flip measurements of a ~3 dimensional $S(Q, \omega)$ relatively routine in the near future, and that would be a significant advance.

The NCNR has longstanding strengths in neutron reflectometry and SANS. In tandem with sophisticated polarization analysis, these capabilities have been exploited to address challenging hard matter problems involving long wavelength and nanoscale magnetism that are of great interest and importance in both basic and applied science. In particular, the recent polarized neutron reflectivity studies performed at the NCNR have beautifully resolved complex interfacial magnetism in oxide thin-film assemblies, which would not have been amenable to study by other techniques.

Inelastic neutron scattering is well known as a powerful probe of lattice dynamics, and measurements of phonon dispersions and densities of state in new materials on BT7 have made important contributions in this area. In particular, recent measurements on new superconducting materials as well as related materials have been used to benchmark theoretical calculations, using density functional theory. The combination of these experimental and theoretical techniques has nicely elucidated the role of electron–phonon interactions in such new materials. This work also clearly illustrates the close interaction between sophisticated theory and neutron scattering and their role in advancing our understanding of ground states in new hard materials.

All of these research programs depend critically on the availability of sophisticated sample environments such that NCNR neutron experiments can be carried out under conditions that most directly reveal the novelty of the states that the new materials display. The NCNR has developed impressive capabilities for neutron scattering at low temperatures and high magnetic fields, and it currently operates the most advanced suite of infrastructure in North America for neutron scattering at low temperatures and high magnetic fields by comparison with its only competitor, the Oak Ridge National Laboratory Spallation Neutron Source (ORNL/SNS). Low temperatures and high magnetic fields are very important to cold neutron spectroscopy. One of the great strengths of the NCNR is that the energy scale of relevance to cold neutrons (> 0.1 meV ~ 1 K) matches the scales accessed with ^{3}He and dilution fridges, which corresponds to the energy scale of magnetic moments in magnetic fields up to 10 T. The NCNR deserves credit for recognizing the importance of sophisticated sample environment to the broad range of materials research programs that it facilitates.

ENERGY-RELATED RESEARCH

Energy-related research is well recognized as a crucial area of research to serve critical current societal needs. Because neutron-related research can have an impact on important problems in this area, such as energy storage and energy production, of both hydrocarbon forms of energy and alternative energy sources, this is a reasonable program for NIST scientists to be involved in.

One technologically important area is the development of alternative fuels for motor vehicles. The NCNR appears to be one of the few places where serious neutron research is being carried out on metal organic framework (MOF) compounds. These have the potential to store large quantities of methane and could enable motor vehicles to be powered by natural gas (e.g., methane) in a cleaner, safer way, if the energy density storage requirements can be met to be competitive with gasoline or compressed natural gas. Work at the NCNR using neutron powder diffraction and inelastic neutron scattering, coupled with density functional methods to calculate electronic structure and energies from first principles, has given insight into the mechanisms of methane adsorption in MOFs and the importance of open metal sites in these compounds and possible modifications of the structures—for example, with linker functionalization—to begin to approach the Department of Energy (DOE) energy storage requirements. Already, researchers at the NCNR, in collaboration with University of Texas, San Antonio, have found a compound with a record high, to date, CH_4 working capacity (257 cm^3(STP)/cm^3). The capacity nevertheless remains approximately 30 percent below DOE targets for methane storage.

Because of the ability to deuterate and therefore change the contrast of hydrocarbons, neutrons provide a unique and effective tool to image hydrocarbon flow through porous media such as shale or other porous rocks. This is being set up at the imaging facility and is likely to enable high-quality, high-resolution dynamic imaging of hydrocarbon flow in such materials. This is of importance in problems such as secondary and tertiary oil recovery. This facility should also be useful for imaging fuel cells and battery materials under actual working conditions.

FUNDAMENTAL NEUTRON SCIENCE AND APPLICATIONS

The availability of intense, well-characterized cold neutron beams at the NCNR opens the opportunity to perform studies in fundamental neutron science and important applications in imaging and trace element analysis.

Neutron Lifetime

It is remarkable that more than 80 years after the discovery of the neutron, the lifetime of this elementary constituent of matter is still uncertain at the 1 percent level, with a major discrepancy occurring between beam and bottle-type measurements. It is well within the NIST portfolio to resolve this discrepancy and to improve the precision of this fundamental parameter. Plans were presented for a group of several university partners working with NIST staff to perform the necessary measurements in a new location in the guide hall, providing an order of magnitude more intense beam than was used for the previous measurements.

aCORN

Neutrons beta-decay into a proton, an electron, and a neutrino. The standard model of particle physics predicted the angular correlation between the electron and the neutrino. Neutrinos are very hard to detect; however, their directions may be inferred from a measurement of the electron and proton momenta, assuming that the parent neutron is essentially at rest. This measurement is being pursued by a collaboration including external university groups (academic, industrial, and government researchers) working with NIST staff. The apparatus uses a more intense cold neutron beam. This will result in a more definitive measurement with smaller error bars.

Neutron Imaging

Neutrons offer several unique characteristics for imaging. The contrast between rocks and hydrogen-containing fluids opens the possibility of following fluid-penetration through porous rocks as a function of time; the superior penetration ability of neutrons offers the possibility of imaging hydrogen fuel cells in operando, of imaging turbine blades, and following the time development of the curing process in concrete. The NCNR has built a facility to perform simultaneous tomography capabilities using neutrons and x rays, enabling imaging at 10-20 micron resolution. This facility is in high demand, and it will be upgraded using Wolter mirrors. These optical elements, originally developed by the National Aeronautics and Space Administration (NASA), promise to provide magnification capabilities in neutron imaging that may extend the resolution to the 1 micron level.

Prompt Gamma

Neutron activation analysis is a time-honored technique of elemental identification. The Prompt Gamma End Station at the NCNR is used by the NIST Elemental Measurement Science Group to develop standard reference materials used by a wide variety of industries and research institutions. The Prompt Gamma End Station has a new home at the neutron beam guide NGD (neutron-gamma density), where it enjoys a higher cold neutron flux and lower background in its high-resolution gamma-ray detector. This yields lower detection limits for trace elements in the samples of interest.

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NCNR Partnerships

USER PROGRAM

The user program, involving NCNR staff and the user community of academic, industrial, and government laboratory researchers, continues to be successful. The success is, in part, manifested in the large number of high-impact, high-quality scientific publications in diverse technical areas that include condensed-matter physics, materials processing and manufacturing, biology, pharmacy, and geology. Many publications are collaborative, reflective of important contributions from NCNR staff. Such contributions may include input from NCNR staff to users before they submit proposals for beam time. NCNR staff may at times perform proof-of-concept, or feasibility, experiments to ensure the viability of proposed experiments. Additionally, NCNR staff may develop data analysis tools or assist with the analysis of the neutron-scattering data. NCNR staff members have also assisted in the preparation of scientific manuscripts and with the response to referee queries.

The process used to evaluate proposals for neutron experiments continues to be fair and ensures that high-quality proposals are successful. Each proposal is read by three to five reviewers. The reviews are evaluated by the beam time allocation committee (BTAC) before the final decision is reached; this ensures fairness to the authors and that the proposals that are allocated beam time are of high quality. Requests for time to perform experiments exceed available time. Eventually, however, meritorious proposals are allocated beam time.

NCNR management has benefited from this important relationship with the user community. Workshops involving members of the user community have proven to be an effective source of feedback and guidance regarding appropriate investments in new instruments, instrument upgrades, and related facilities necessary to ensure that the research remains at the cutting edge of the field.

Overall, this is a successful program.

EDUCATION AND OUTREACH

Educational activities at the NCNR are an important component of the overall program. The most notable component is the highly oversubscribed summer school, sponsored by CHRNS, for graduate students and young scientists. Two such summer schools are offered in alternate years. These focus on neutron spectroscopy and on neutron reflectometry and SANS, respectively, and are more focused than the complementary National School on Neutron and X-ray Scattering offered each year by Argonne National Laboratory and ORNL. The CHRNS summer school features significant hands-on time with the instrumentation and are widely regarded as a success. The CHRNS summer school typically serves 35 graduate students, postdoctoral researchers, and junior faculty each year. About 75 percent of attendees come back as users, so this activity is very important for the future of the neutron-scattering community.

Other commendable activities include a summer internship for a high school teacher (to be expanded in the future), numerous tours for school groups, and participation in the NIST Summer Undergraduate Research Fellowship (SURF). Educational programs are largely supported by NSF.

Outreach activities by NCNR staff include visits to universities and participation in national and international conferences. Periodic workshops organized by the NCNR are an important component of planning for future instrument development at NCNR.

CENTER FOR HIGH RESOLUTION NEUTRON SCATTERING

The partnership between the NCNR and the NSF, CHRNS, has been reestablished. A renewal proposal was funded by NSF, enabling the partnership to continue. This has been a successful center, with more than 500 publications citing support from CHRNS and more than 100 doctoral students who received partial support for their graduate research in the past 5 years. Many of these students have subsequently joined the faculties of universities, and some have won important awards for young researchers, including awards from the American Physical Society, the American Chemical Society, the Society of Rheology, and the Canadian Association of Physicists. Numerous high school students, undergraduates, and high school teachers have benefited from programs supported by CHRNS.

This newly reestablished CHRNS will support a set of instruments with unprecedented capabilities: the 30 m SANS instrument; ultra-SANS, High Flux Backscattering Spectrometers (HFBS), NSE, MACS, vSANS, and the CANDOR reflectometer. Both CANDOR and vSANS will become available in the next few years. CANDOR, which will be available in 2017, will enable data acquisition at a higher rate than any other such instrument currently available in the world. Currently, MACS has the highest monochromatic cold-neutron intensity in the world, which enables the study of magnetic properties of materials with a very large volume of $S(Q,\omega)$. The vSANS instrument will be the first such instrument in the United States to operate in a large range of wavelengths, enabling a study of the morphology of materials at broader length scales. The capabilities of the newly planned NSE spectrometer are among the best in the world.

This reestablished collaboration will enable an unprecedented study of the structure and dynamics of hard and soft matter, including lipid bilayer fluctuations, the morphology of polymer-based systems, magnetism, superconductivity, and the storage of methane and batteries. NCNR staff are to be commended for the plans that they have established for instrument upgrades and their accomplishments to date. Their plans for CANDOR and vSANS are appropriate.

nSOFT

The nSOFT collaboration between the NIST and U.S. industry, to use neutron-based techniques to investigate the properties of soft materials relevant to technological applications, is proving to be a viable program, of value to industry and with a promising future, supporting the mission of NIST. In nSOFT, researchers from U.S. companies work collaboratively with NIST to address problems of technological interest. Members of NIST collaborate with industrial researchers to identify appropriate neutron experiments and other complementary techniques and tools at NIST to address problems. Member companies pay $25,000 per year for this opportunity.

The program has progressed well during the past 2 years, and it now includes six companies. The projects are innovative and responsible for advances in experimental procedures, such as new sample environment capabilities and data analysis procedures. Examples of projects include the processing of paints, oil recovery, manufacturing, and fuel cells. Capabilities that have been developed as a result of the nSOFT collaborations have benefited academic researchers.

There has been a change in the original plans for nSOFT. The initial goal was to attract as many companies as possible to become members of nSOFT. NIST's new goal is to identify companies that would specifically benefit from this collaboration and to work closely with them on wider-range problems, in greater detail, to achieve higher impact.

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Challenges and Opportunities

The management of the NCNR has effectively planned for the future and has continued to make wise investments. With the completion of the new source for producing cold neutrons and the guide hall, the NCNR is well positioned to investigate some of the most important and impactful problems in condensed matter. It is anticipated that the strategic plan, which could be completed in the coming months, will formalize the entire planning and operational process, helping to ensure that the long-term goals and objectives of the center are met.

There are a few challenges, nevertheless. Reactor fuel costs have risen by nearly a factor of 10 over the past dozen years, and while there are efforts to procure funds, it is essential that these efforts be successful. While there is an increase for reactor fuel in the fiscal year (FY) 2016 President's budget, insufficient resources to meet fuel costs would be a devastating blow for neutron science in the United States. Any solutions, such as the implementation of user fees, that might have the effect of reducing the diversity of users or undermine the current merit review criteria, should involve the user community. Without a functioning reactor that is accessible to researchers with meritorious proposals, new scientific and technological opportunities, including energy, pharmacy, and geology, would be lost. Some users would be forced to travel abroad; some other users might no longer be able to perform neutron-scattering experiments.

Additional opportunities are possible by further developing collaborations with the very best researchers in different locations around the world. The current collaborations with researchers near the NCNR have been very fruitful. Nevertheless, NCNR activities would benefit significantly by engaging theorists who would further improve the integration of theory and experiment. Modifying the sabbatical program could help to address these issues.

An ambitious program of adding new and powerful neutron instrumentation at the NCNR is a crucial part of an overall neutron science infrastructure program needed to address the likelihood that in 2030 the user needs for access to neutron scattering facilities in the United States will not be met. Currently in the United States, there are only reactor-based user programs at NIST and ORNL (high flux isotope reactor, HFIR), and the spallation source-based program at the first target station at SNS. Planning for a second target station at SNS is underway, but even the most aggressive timeline would not result in these new facilities being available for users before approximately 2024. The Chalk River reactor-based neutron source in Canada will close by 2018 at the latest, and that will further constrain access to neutrons in North America. All of these facilities are oversubscribed by factors of between 2 and 5. Additionally, if the NCNR's response to its reactor licensing limit of 2029 involves curtailment of availability of its resources, that could further impact users.

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Key Findings and Recommendations

The new NCNR guide hall is now complete, and new instruments that enhance measurement capabilities are either complete or are at different stages of completion. Moreover, new sample preparation and sample environment capabilities are continually being established. These developments significantly enhance the ability of the NCNR to remain at the leading edge in neutron research in the coming decades. However, some specific actions in the near- and long-term future will be required.

Recommendation 1: The NCNR should develop and document a plan for instrument development, which should include plans for the two remaining end-stations in the new guide hall. In addition, the NCNR should hold a workshop in 2017 to get feedback from users regarding the plan. Input from the user community should also be used to update the NCNR strategic plan, expected to be complete by the end of 2016.

It is commendable that NCNR management is identifying creative ways to procure a budget for cold source developments, instrument upgrades, and new instruments from different sources such as universities, the National Nuclear Security Administration, the National Science Foundation, and—primarily—NIST. Nevertheless, this approach is fragmented.

Recommendation 2: The NCNR should document a plan that describes the sources of financial support, with specific objectives for budgets and strategies, and sources that would ensure that the plans for future instruments are realized.

The research at the NCNR is at the cutting edge, as evidenced by high-quality publications in the very best journals in the world in different fields, and also by the number of citations. Additional opportunities could be realized if there were stronger integration between theory and experimentation in some areas. The success is particularly notable in cases where theory and experiment are well integrated.

Recommendation 3: The NCNR should develop a strategy to achieve more substantial interactions with researchers around the world to develop integrated teams capable of addressing forefront neutron problems. Potential strategies should include expanding the sabbatical program.

A major objective of the mission of NIST is to transition fundamental scientific knowledge to practical technology. Within NCNR, the nSOFT program plays a central role toward meeting this objective. The evolution of the nSOFT program, and its progress, is commendable. Deep ties have been developed with companies, and the impact on industrial processes is becoming evident. In this regard, the transfer of awareness and practical applications of neutrons to U.S. industry is now evident. The goals and objectives of the program have evolved during the past 2 years.

Recommendations 4: The NCNR should (a) develop and document a complete strategic plan for nSOFT with elements that include the metrics for success (for example, financial,

number of companies, patents, publications, new products), a profile of the type of company that would benefit from becoming a member of nSOFT, a financial model, and personnel commitment; (b) work with the companies to articulate success stories illustrating how neutron research has had an impact; (c) clarify the current approach to technology transfer activities; and (d) revisit the current status of intellectual property.

In 2030 the user needs for access to neutron scattering facilities in the United States will not be met. Additionally, the reactor licensing limit of 2029 imposes an additional challenge.

Recommendation 5: The NCNR should expand current initiative planning for a next generation reactor. This planning may even include consideration of an additional reactor.

The reactor fuel costs continue to rise at a significant rate. A reduction of the access to neutron-scattering capabilities would have a negative impact on the neutron-scattering community in the United States. This would have serious implications on the overall progress of science and technology in some fields.

Recommendation 6: The NCNR should procure resources to afford fuel costs in order to continue to operate at current levels.

Acronyms

aCORN	‘a’ correlation in neutron decay
BTAC	beam time allocation committee
CANDOR	chromatic analysis neutron diffractometer or reflectometer
CHRNS	Center for High Resolution Neutron Scattering
DOE	Department of Energy
DCS	disk chopper spectrometer
HFBS	High Flux Backscattering Spectrometers
HFIR	high flux isotope reactor
ILL	Institut Laue-Langevin
MOF	metal organic framework compound
MACS	multi axis crystal spectrometer
NASA	National Aeronautics and Space Administration
NCNR	NIST Center for Neutron Research
NGD	neutron-gamma density
NIH	National Institutes of Health
NIST	National Institute of Standards and Technology
NRC	National Research Council
NSF	National Science Foundation
NSE	neutron spin echo
nSOFT	colloquium of companies that use neutron-based techniques to investigate the properties of soft materials relevant to technological applications
ORNL	Oak Ridge National Laboratory
SANS	small angle neutron scattering
SNS	Spallation Neutron Source at the Oak Ridge National Laboratory
SPINS	Spin Polarized Inelastic Neutron Spectrometer
SURF	Summer Undergraduate Research Fellowship
vSANS	very small angle neutron scattering