An Assessment of the National Institute of Standards and Technology Center for Neutron Research: Fiscal Year 2009

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

Susan Coppersmith, University of Wisconsin,
Sebastian Doniach, Stanford University,
R.G. Hamish Robertson, University of Washington, and
Alton Romig, Jr., Sandia National Laboratories.

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

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Summary

The National Institute of Standards and Technology [NIST] Center for Neutron Research (NCNR) is a national user facility whose mission is to ensure the availability of neutron measurement capabilities in order to meet the needs of U.S. researchers from industry, academia, and government agencies. This mission is aligned with 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.

As requested by the Deputy Director of NIST, the scope of the fiscal year 2009 assessment of the NCNR conducted by the National Research Council's Panel on Neutron Research included the following criteria: (1) the technical merit of the current laboratory programs relative to current state-of-the-art programs worldwide; (2) the adequacy of the laboratory budget, facilities, equipment, and human resources, as they affect the quality of the laboratory technical programs; and (3) the degree to which the laboratory programs in measurement science and standards achieve their stated objectives and desired impact.

The NCNR has been an extremely reliable and comprehensive neutron scattering facility and will continue to be a vital resource for meeting the broad spectrum of users' scientific objectives and needs for neutron scattering in the future. During the past year the NCNR has continued to sustain a high level of creativity, productivity, and quality in science and research in service to industry, academic, and government agency users. Half of U.S. neutron scatterers used the facility during the past year, demonstrating the scientific role that the NCNR plays in the country. The publication record of the NCNR facility attests to the high quality and quantity of research in diverse areas of fundamental neutron science, condensed-matter physics, and engineering. Resurgence in the collaborative partnership of the NCNR with the Polymers Division of the NIST Materials Science and Engineering Laboratory is visible and likely to enhance further the scientific output and impact in the soft-condensed-matter field. As indicated by the NCNR User Group, users are highly satisfied by the quality of the instruments, the support personnel, the access mechanism, and the facility as a whole.

An excellent example of the scientific prowess of the facility in the past year was the work on novel Fe-based superconductors. This work was an exemplar of the strengths of the facility, which include rapid access, permitting crucial measurements to be carried out; the right combination of instruments; scientific leadership in the field; and a culture that seized the opportunity to be at the forefront of this sensational research development and enabled a major breakthrough in the field.

The NCNR Expansion Project is well underway and will be critical for continuing the vitality and effectiveness of the facility. Through upgrades, reconfigurations, and the construction of novel instruments, the Expansion Project will ensure a comprehensive, competitive, and best-in-class suite of instruments for users in the future. To run the new suite of instruments and sample environments, and to continue providing excellent support to the increased number of users who will come to the facility to make use of these instruments, it will be crucial to increase the number of personnel in order to exploit fully the capabilities of the expanded facility. As the Oak Ridge National Laboratory's (ORNL's) Spallation Neutron Source becomes fully operational and ORNL's High Flux Isotope Reactor (HFIR) goes into full user-program mode, the NCNR will continue to be a vital resource for meeting the broad spectrum of user needs for and scientific objectives related to neutron scattering. In many cases,

the NCNR will be the facility of choice owing to its comprehensive capabilities, unique instruments, and the scientific leadership of its personnel.

A report by the Office of Science and Technology Policy Interagency Working Group on Neutron Science provides a summary of the capabilities of the major neutron scattering facilities in the United States and indicates that there are significant differences in the instrument distribution by class among the U.S. facilities.[1] The report also suggests that the number of neutron scattering instruments available in the United States in the future will be less than half that available in Western Europe and less than that available in Japan. On a per capita basis, the United States has half the neutron scattering capacity of either Western Europe or Japan—and this shortfall is unlikely to change for the foreseeable future. The NIST NCNR Web site (http://www.ncnr.nist.gov/nsources.html) provides links to the Web sites for each of the world's major neutron scattering facilities, where detailed information is provided for each facility. The NIST Web site also provides access to detailed descriptions of the instrumentation at the NCNR (http://www.ncnr.nist.gov/instruments/) and of the NCNR Expansion Project and instrumentation (http://www.ncnr.nist.gov/expansion/expansion.html). Descriptions of the NCNR's organization, facilities, and activities are provided in the NCNR 2008 annual report.[2]

A significant component of the excellence of the NCNR is the Center for High Resolution Neutron Scattering (CHRNS) Program. Covering approximately 30 percent of the current beam lines, the CHRNS is the heart of the NCNR User Program and sets the standard of scientific productivity for other U.S. facilities. As described to the panel, each year the CHRNS supports about 500 users, many of them graduate students, and yields about 100 publications, about half of the high-impact publications of the NCNR. Developing the next generation of neutron scattering scientists and engineers is a vital part of the CHRNS and the NCNR. To continue to serve and grow the neutron scattering community and to maintain the excellent scientific productivity carried out at the facility, it is critical that the spirit of open access, while meeting all security requirements, be maintained.

In light of the stellar reliability of the facility and service with respect to neutron scattering needs in the country, the potential for a prolonged and unplanned shutdown of the facility in the event of a safety shim arm failure gives rise to major concern. No spares are available at the facility, and the lead time for replacements is 8 months. Such a failure and an associated long, unplanned shutdown would be extremely detrimental to the neutron scattering capabilities in the U.S. contingency plans. Spares must be put in place as soon as possible to obviate this potential problem.

The panel makes the following recommendations with respect to enhancing the effectiveness of the NCNR in the pursuit of its goals.

1. Sustain NCNR operation and reactor maintenance efforts during the NCNR Expansion Project by carrying out the following:
   - Mitigate the potential for a long, unplanned shutdown of the facility by planning for contingencies with respect to safety shim arms;

[1] Office of Science and Technology Policy Interagency Working Group on Neutron Science, *Report on the Status and Needs of Major Neutron Scattering Facilities and Instruments in the United States*, June 2002. Available at http://permanent.access.gpo.gov/lps23422/neutron.pdf. Accessed August 2009.

[2] National Institute of Standards and Technology, *Accomplishments and Opportunities: 2008 NIST Center for Neutron Research,* NIST Special Publication 1089. Available at http://www.ncnr.nist.gov/AnnualReport/FY2008/AR2008.pdf. Accessed August 2009.

- Schedule all of the planned reactor upgrades, including the upgrade of the reactor control instrumentation, and the installation of the second cold neutron source to allow users to plan effectively;
- Engage in dialogue with the NCNR Users Group concerning access to facilities during the construction phase and upgrades; and
- Continue actively attending to maintenance of the scientific openness of the facility within the constraints of increasing security demands.

2. Enhance the soft-condensed-matter efforts of the facility in the following ways:
   - Continue the development of new technical capabilities that will allow the NCNR to maintain leadership in key research areas that complement those of other facilities, such as the Spallation Neutron Source and the High Flux Isotope Reactor;
   - Continue the development of the soft-matter consortium between the NCNR, the Polymers Division in the NIST Materials Science and Engineering Laboratory, and the University of Delaware;
   - Increase network building with bioscientists at other institutions; strengthen NCNR interactions with the Center for Advanced Research in Biotechnology, involving NIST and the University of Maryland, pursuant to this goal; and more actively engage the broad biological community;
   - Make it a clear objective of NCNR management to pursue aggressively the ongoing recruitment effort for a scientific leader in experimental soft-condensed matter; and
   - Broaden the theory effort in the fields of statistical physics and biophysics; include in this effort a strong partnership with the Polymers Division.

3. Continue improvements to the NCNR User Program, including the following:
   - Renew the CHRNS partnership with the National Science Foundation, which is the cornerstone of the User Program, outreach, and educational program of the NCNR;
   - Commit to increasing research in biology and medicine at the NCNR through coordinated engagement of the broad community;
   - Plan for substantially expanded outreach (for example, workshops and extended scientific programs) when the planned new office building becomes available; and
   - Maintain the regular rotation schedule of new members onto the Beam Time Allocation Committee.

1

The Charge to the Panel and the Assessment Process

At the request of the National Institute of Standards and Technology (NIST), the National Research Council (NRC) has since 1959 annually assembled panels of experts from academia, industry, medicine, and other scientific and engineering environments to assess the quality and effectiveness of the NIST measurements and standards laboratories, of which there are now nine,[1] as well as the adequacy of the laboratories' resources. In 2009, NIST requested that five of its laboratories be assessed: the NIST Center for Neutron Research (NCNR), the Center for Nanoscale Science and Technology, the Information Technology Laboratory, the Chemical Science and Technology Laboratory, and the Electronics and Electrical Engineering Laboratory. Each of these was assessed by a separate panel of experts; the findings of the respective panels are summarized in separate reports. This report summarizes the findings of the Panel on Neutron Research.

For the fiscal year (FY) 2009 assessment, NIST requested that the panel consider the following criteria as part of its assessment:

1. The technical merit of the current laboratory programs relative to current state-of-the-art programs worldwide;
2. The adequacy of the laboratory budget, facilities, equipment, and human resources, as they affect the quality of the laboratory's technical programs; and
3. The degree to which the laboratory programs in measurement science and standards achieve their stated objectives and desired impact.

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 10 volunteers whose expertise matches that of the work performed by the NCNR staff.[2] The panel members visited the NCNR facility at Gaithersburg, Maryland, for a day and a half, during which time they attended presentations, tours, demonstrations, and interactive sessions with NCNR staff. Subsequently, the panel members assembled for another day, during which they conducted interactive sessions with NCNR managers and with leaders of NCNR user groups and met in a closed session to deliberate on the panel's findings and to define the contents of this assessment report.

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[1] The nine NIST laboratories are the Building and Fire Research Laboratory, the Center for Nanoscale Science and Technology, the Chemical Science and Technology Laboratory, the Electronics and Electrical Engineering Laboratory, the Information Technology Laboratory, the Manufacturing Engineering Laboratory, the Materials Science and Engineering Laboratory, the NIST Center for Neutron Research, and the Physics Laboratory.

[2] See http://www.ncnr.nist.gov/ for more information on NCNR programs. Accessed May 1, 2009.

The approach of the panel to the assessment relied on the experience, technical knowledge, and expertise of its members, whose backgrounds were carefully matched to the technical areas of NCNR activities. The panel reviewed selected examples of the technological research presented by the NCNR; because of time constraints, it was not possible to review the NCNR programs and projects exhaustively. The examples reviewed by the panel were selected by the NCNR. The panel's goal was to identify and report salient examples of accomplishments and opportunities for further improvement with respect to the following: the technical merit of the NCNR work, its perceived relevance to NIST's own definition of its mission in support of national priorities, and specific elements of the NCNR's resource infrastructure that are intended to support the technical work. These highlighted examples are intended collectively to portray an overall impression of the laboratory, while preserving useful suggestions specific to projects and programs that the panel considered to be of special note within the set of those examined. The assessment is currently scheduled to be repeated annually, which will allow, over time, exposure to the broad spectrum of NCNR activity. While the panel applied a largely qualitative rather than a quantitative approach to the assessment, it is possible that future assessments will be informed by further consideration of various analytical methods that can be applied.

The comments in this report are not intended to address each program within the NCNR exhaustively. Instead, this report identifies key issues and focuses on representative programs and projects relevant to those issues. Given the necessarily nonexhaustive nature of the review process, the omission of any particular NCNR program or project should not be interpreted as a negative reflection on the omitted program or project.

2

General Assessment of the NIST Center for Neutron Research

As it has for more than a decade, the NIST Center for Neutron Research is fulfilling its mission extremely well—that mission is to ensure the availability of neutron measurement capabilities in order to meet the needs of U.S. researchers from industry, academia, and government agencies. For years, including the long period of "neutron drought" in the United States brought about by the closing of the High Flux Beam Reactor (HFBR), the prolonged shutdown of the High Flux Isotope Reactor (HFIR), and earlier problems with the Lujan Facility at the Los Alamos National Laboratory, the NCNR has helped maintain the strength and competitiveness of neutron scattering research in this country. It has done so through a combination of good management, a culture of excellence, new instrumentation, and continuing improvements to the beam lines.

The NCNR's reactor has continued to perform very reliably, with 253 days of availability out of a possible 255 days in the past year. By almost all of the Office of Science and Technology Policy's performance metrics (e.g., reliability of operation, number of operational days per year, number of instruments, number of users, number of publications, and publications in high-impact journals), the NCNR continues to be the second most scientifically productive neutron facility in the world (comparable to ISIS in England), after the Institut Laue-Langevin (ILL) in France. (The ILL has more than twice as many instruments as the NCNR and consequently has an accepted proposal rate approximately twice that of the NCNR). This is likely to continue at least until the Spallation Neutron Source (SNS) and the Japan Proton Accelerator Research Complex gain full momentum. Even then, with planned upgrades and improvements the NCNR will continue to be a competitive facility for the foreseeable future.

The new suite of instruments planned for the expansion includes enhancements to the neutron guides (by optimizing them for specific instruments) and a new cold source and will help to ensure the NCNR's competitiveness. If expected increases in NIST's funding in the immediate future materialize, a concomitant personnel increase should be made at the NCNR to meet the needs of this transition. This becomes important when considering this country's need for neutron scattering research in years to come, given the recent shutdown of the Intense Pulsed Neutron Source and lingering uncertainties about the long-term future of the Los Alamos Neutron Science Center and the HFIR.

A good example of how the NCNR has met the needs of U.S. researchers is the agility with which samples of the new Fe-based high-temperature superconductors were run on the appropriate instruments. When scientists from other laboratories approached NCNR staff with samples of these materials, the scattering studies were performed, results analyzed, and a manuscript submitted to a prestigious journal within a few days. The researchers managed to obtain some of the earliest definitive results on the structural and magnetic phase transitions quickly, resulting in immediate scientific impact and numerous citations that have put NCNR personnel and collaborators in a leadership position in the field.

Discussions of the Panel on Neutron Research with NCNR users and a review of the user survey conducted by the NCNR User Group (NUG) yielded the conclusion that by and large the NCNR user community is satisfied with access to the NCNR facilities, the NCNR proposal system, the facilities themselves, and the assistance provided by NCNR staff, who are described by users as “helpful,” “dedicated,” and “mindful of tending to user needs.” Users reported that, as in practically all such facilities, there are certain areas that could be improved—examples include transmitting data to users in a standard format and improving the types and quantities of ancillary equipment (such as high magnetic fields and millikelvin-temperature refrigerators, high-temperature furnaces, pressure cells, controlled-humidity cells, complementary and simultaneous optical microscopy and optical spectroscopy tools, and nuclear magnetic resonance microscopy). Often the availability of one or more of these items, as compared with the availability of neutron flux alone, makes the crucial difference in carrying out experiments in a competitive field. Another challenge that most facilities face is to ensure uniformity for interchangeable use of such tools on different instruments. The NCNR management and staff are mindful of these challenges, and they have allocated substantial effort to developing user-friendly data-analysis programs, although it is not clear how close they are to meeting the ideal of standardized data-processing routines that can be used for experiments at all facilities with trivial modifications. Their strategy of trying to enlist the user community to submit proposals to develop some of these ancillary items of equipment has met with limited success. This result probably points to the fact that the development of sophisticated specialized equipment is generally left to scientific and engineering professionals such as NIST staff, with the selective involvement and collaboration of user scientists. An example seems to be the Multi Axis Crystal Spectrometer (MACS) inelastic spectrometer designed and developed with much involvement by researchers at the Johns Hopkins University, with funding from that university, NIST, and the National Science Foundation (NSF).

The sample of research projects provided to the panel suggests that the science done by NCNR scientists is of high quality, as is their expertise in neutron scattering. The encouragement by NCNR management of the scientific activities of its staff is a commendable complement to its related focus on their service to the user community. The instrument scientists have some discretionary time and generally are able to use it effectively.

For certain experiments, such as powder diffraction, the staff encouraged many users to send their samples, which could be run by the staff more efficiently than if the users traveled to the NCNR to perform the experiments. Small Angle Neutron Scattering (SANS) users have also been encouraged to send samples to staff to run in short measurements in order to assess feasibility.

Of course, while such trends should not be taken to extremes (a cadre of expert users in the community is also essential for the success of the neutron scattering enterprise in the United States), it may be a trend that can be appropriately grown. There seems to be an inclination for some new users, particularly interdisciplinary users, to be somewhat uninterested in developing expertise and sophistication in the techniques of scattering; this makes it imperative to maintain the scientific and technical excellence of the NCNR staff. Nevertheless, in order to generate interest and expertise in the outside scientific community, it continues to be important that NCNR scientists maintain outreach efforts (with an organized presence at major scientific conferences, for example) and increase throughput at the neutron schools that they have been organizing.

The facility seems to be serving the needs of industrial users reasonably well, although it should continue to take a proactive role in educating industrial scientists about the unique advantages that neutrons offer in investigating certain problems. There appears to be substantial industrial involvement in the facility, through participating research teams (PRTs) or direct collaboration with NIST scientists. The Polymers Division in NIST’s Materials Science and

Engineering Laboratory in particular has been responsible for much industrial involvement with NCNR programs, many of which use the NCNR facilities as crucial characterization tools. For example, the NCNR has developed collaborations with companies such as Xerox, IBM, Merck and Company, Corning Incorporated, the Dow Chemical Company, Hitachi, and Intel Corporation. In particular, these industrial users seem eager to take advantage of the SANS instruments and reflectometers. A successful example is the Ultra-Small Angle Neutron Scattering (USANS) instrument, which was fairly undersubscribed until an active campaign to advertise its capabilities resulted in many proposals, many of which are from industry.

3

Science and Technology at the Center

During the past year the NIST Center for Neutron Research has sustained a high level of creativity, productivity, and quality in science and research that primarily take advantage of the neutron-based resources available at the laboratory. Presentations delivered to the Panel on Neutron Research by NCNR scientists and university collaborators covered a wide range of activities, including those in solid-state physics, fundamental neutron physics, polymer science and engineering, biological science, and energy storage. These activities demonstrated a competent staff whose members interact with one another and with a rich complement of outside users. Overall, the work presented illustrates the vital contributions made by the NCNR to the sustenance of fundamental science and the development of technology in the United States and internationally. The following discussion highlights selected recent accomplishments at the NCNR and assesses future opportunities in several areas of investigation.

Overall, a high level of technical merit characterizes the neutron science at NIST, and the NCNR addresses a host of national priorities related to basic science and applied technologies. The continuing development of the neutron source, along with the ongoing improvement of existing instrumentation and acquisition of new measurement devices, plays a pivotal role in satisfying the goals of maintaining high technical merit relative to the state of the art and addressing national priorities relevant to NIST.

Two calls for proposals during 2008 resulted in the submission of 652 proposals, of which 414 were approved and received beam time. In 2008, 321 proposals resulted in more than 2,200 research participants (68 percent from universities), leading to 320 publications; 11 percent of these appeared in high impact factor journals and 59 percent in journals whose impact factor is greater than 2 (journals of respectable caliber).[1] These metrics are comparable to those from the past few years at the NCNR.

The fundamental neutron physics program is thriving. A number of experiments are in development or poised to begin, and many will benefit greatly from the higher flux expected after the guide hall expansion. The NCNR should select a few of these experiments and focus its effort on those over the next year in order to demonstrate full viability prior to the shutdown period. One good choice would be the neutron lifetime measurement experiment.

The technology for polarizing and analyzing neutron spins by means of transmission through polarized ^{3}He continues to find new applications at the NCNR, particularly in situations where super-mirrors are inapplicable or prohibitively expensive. The group that addresses this technology includes nine scientific staff members, who add a rich and valuable complement to the team of (mostly scattering) scientists working at the NCNR.

The neutron activation (NA) metrology program in standards and commerce has good value. The reports of the Analytical Chemistry Division in NIST's Chemical Science and Technology Laboratory on certification of standard reference materials (13 in 2008) are an

[1] Impact factor is a measure of the citations to a journal; it is an indication of a journal's relative importance in its field. High impact factor journals include *Science, Nature, Nature Materials, Proceedings of the National Academy of Sciences,* and *Physical Review Letters.* A journal impact factor, JIF, is calculated by comparing the average number of a journal's citations over a given time period against the number of articles published in that journal during the time period.

additional measure of the productivity of the NCNR, along with journal publications and patents issued. Refurbishment of the thermal column, a stated goal of the management, would allow for even more NA studies to be undertaken.

The area of soft and self-assembling materials represents a wide range of topics, including synthetic and natural polymers and surfactant and colloidal dispersions. Various forms of neutron scattering (e.g., SANS, neutron reflection, and spin echo spectroscopy) are pivotal to understanding the statics and dynamics of these systems; accordingly, the NCNR has maintained strength in these subjects for many years. The NCNR continues to play an important—in some respects a dominant—role in exploring soft materials. Competence within the NCNR staff and an expanded group of outside (mostly university) collaborators have resulted in a group of users whose expertise is state of the art. These activities have been augmented by especially strong collaborations with several universities, notably the University of Delaware, where pioneering in situ rheology/SANS experiments have established connections between the microscopic configuration of surfactants and polymers and the macroscopic stress-strain relationships.

Polymers warrant particular attention. With about 100 research scientists, the Polymers Division at NIST is a premier center for the investigation of macromolecular science and engineering, and it is ideally positioned to partner with the NCNR. The division chief has articulated an exciting future for polymers at NIST that includes a closer partnership with the NCNR and draws a bevy of industrial companies to the collaboration. Examples of recent activities include neutron reflectivity from organic semiconductors, organic photovoltaics, and complex fluids. These activities, including the participation by Polymers Division theorists, augur a promising future for soft-materials research at the NCNR.

The solid-state physics group produced an outstanding research success during the past year. In response to a request to examine a new compound, La(O,F)FeAs, staff members at the NCNR quickly arranged to obtain powder diffraction patterns, and subsequently inelastic scattering data, during a weekend. It became rapidly apparent that they had determined the essential structural properties of a new type of superconducting material. Within several days the work was submitted for publication, and it soon appeared in *Nature*. Since this initial publication, many groups have turned their attention to these Fe-based superconductors, which exhibit critical temperatures as high as 55 K and are characterized by nearly isotropic properties, including a superior mechanical response. Significantly, the Fe-based compounds appear to be similar electronically to the cuprate superconductors, offering a tantalizing opportunity to gain valuable insights into the underlying mechanism of superconductivity. These very exciting developments underscore the health of the solid-state program at NIST. While serving the nation through the user facility, NCNR scientists are nimble and capable of acting quickly when opportunities arise. The neutron scattering facilities play a crucial role in this area, and the quality of the instruments and capabilities of the staff are laudable.

The solid-state group had another very impressive discovery in 2008. In collaboration with Korea University, the group explored dilute ferromagnetic semiconductor superlattices using polarized neutron reflectometry. Conclusive evidence documented both antiferromagnetic and ferromagnetic order, depending on the temperature and magnetic-field strength. This important discovery provides the first evidence of antiferromagnetic coupling in gallium-manganese-arsenic layers separated by gallium-arsenic-beryllium spacers and promises to guide the future development of new devices.

The NCNR should continue to commit to research in biology and medicine. The neutron technologies provided by the NCNR can address certain questions in ways not permitted by other approaches, and such research contributions could become increasingly urgent as biotechnology and medicine grow in their roles in the national economy and the health of the population. While some of the ongoing work is highly relevant and meritorious, the quality is uneven overall, and further insights concerning the questions of interest in contemporary biological science should be sought and developed. Examples of the excellent work include the voltage-gated channel effort, where independent review by the National Institutes of Health (NIH) has resulted in a grant supporting the project to study membrane protein folding in lipid bilayers. Another measure of serious interest is the commitment of effort and materials by outside groups, as in the involvement of scientists at the NIH with the HIV Gag protein project.

There are other areas in which a more informed biological overview could lead to more and better use of the instruments. For example, the large community of computational scientists deriving dynamic features of macromolecular function might consider modeling cases in which large conformational changes attend biological functions and making corresponding dynamic measurements, as in the kinase family. Work on membrane bilayers might include studies of the drug interactions that are a key to cellular entry; it should be possible to generally broaden the range of important membrane surface interactions studied with supported bilayers. A large group of scientists is interested in natively unfolded proteins and could benefit from some of the insights that work with neutrons can provide. Some work on these topics is underway at the NCNR, but there should be more, and there must be more effective outreach in order to exploit the opportunities. Examples of communities that might have more involvement include the growing group that is using x-ray solution scattering at the nation's synchrotron facilities and the community of computational biologists engaged in molecular dynamics modeling.

A barrier to substantially increased biomedical research in the areas addressed at the NCNR is the modest level of awareness of neutron science capabilities by those engaged with interesting areas in biology and biophysics. Previous NRC assessment reports have encouraged the NCNR to address this perceived problem by means of direct hires and/or the development of new partnerships, and efforts have been ongoing to accomplish this important aim. Interactions with the nearby groups at the NIH might be improved by finding ways to let the scientists there know which of their scientific questions might be answered by working with the NCNR. Outreach at meetings of professional societies could be better planned and implemented, and a question-based approach might also be effective in that outreach. The Center for Advanced Research in Biotechnology, involving NIST and the University of Maryland, is a step in the right direction. NIST should continue to undertake such steps to realize the full potential of its excellent facilities.

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Facilities and Human Resources

The NIST Center for Neutron Research has been an extremely reliable and comprehensive neutron scattering facility and will continue to be a vital resource for meeting the broad spectrum of users' scientific objectives and needs for neutron scattering in the future. The NCNR reactor's operation has continued to perform outstandingly well, with 253 days of availability out of a possible 255 days in the past year. The beam delivery is almost twice that of any other U.S. facility. With this availability, coupled with the number of competitive instruments, the NCNR provides half of all scattering instrument days in the United States and serves about 800 individual users each year—about twice as many as the other U.S. facilities combined. These ratios are likely to change in the near future as the High Flux Isotope Reactor begins to operate a full user program and the Spallation Neutron Source comes up to full capabilities. With the NCNR Expansion Project and judicious selection of new instruments and upgrades, the NCNR is well positioned to continue to serve a leading role in neutron scattering in the future.

The NCNR's management of reactor operations, maintenance, and equipment updating is consistently carried out with careful attention in order to ensure a high level of availability of the facility to users. The two NCNR operational groups, the Research Facility Operations Division and the Reactor Operations Engineering Division, meet prior to each shutdown to discuss the coordination required for maintenance activities. In addition, another group has been meeting to plan the activities that will take place before, during, and after the long shutdown required for the NCNR expansion. The plans for installation of the new reactor control panel appear well under control, with careful consideration given to minimizing the downtime of the NCNR. All necessary components will be in hand prior to the shutdown to ensure that there are no delays involving delivery of components. Although the HFIR and SNS will be able to accommodate additional users during NCNR downtime, users will, nevertheless, be greatly constrained during this time.

The lean and economical management style of the NCNR Reactor Operations Engineering Division has served the facility and its users well over the years. The safety record throughout that time has been excellent, and safety is a major component of the relicensing process that is nearing completion. With the facility expansion, the installation of a new cold source and guide system, and upgrade projects, two new operators have been hired, and two additional hires are planned. Management is mindful of the need for succession planning to prepare for the retirement of the group leader and reactor lead. It appears that the need expressed in previous NRC assessment reports for additional human resources has been addressed. In addition, a novel and cost-effective solution has been proposed to fix the thermal shield and leak problem.

However, additional financial resources are needed to address other challenges in the area of facility operations successfully. For the most part, major NCNR budget increases have been directed toward user support and instrumentation. While operations have been adequately supported, as evidenced by the excellent reliability, increased costs of reactor fuel have not yet been adjusted for. The potential for a long shutdown in the event of a safety shim arm failure represents a very significant concern. No spares are available at the facility, and the lead time for a replacement is 8 months. Such a failure and an associated long, unplanned shutdown would be extremely detrimental to the neutron scattering capabilities in the United States and would damage the stellar reliability record of the NCNR.

A number of hires have been made to increase staffing at the NCNR in support of the Expansion Project: three engineers have been hired to carry out the mechanical design of new neutron scattering instruments and procurements of various components, and to help with non-expansion-related activities such as maintenance and improvements of existing instruments; one new staff member will work on instrument control software development; and four administrative hires will focus on tasks such as logistics, procurements, fiscal planning, and tracking. An additional engineer will likely be hired in the near term to help with instrument assembly. One area of potential weakness is electrical engineering technical support. If possible, a further hire in this area would strengthen the team assembled. There is also need for funds to hire additional staff to run the suite of new instruments and to provide support to the increased number of users that will come to the facility to make use of these instruments. These hires will be crucial for maintaining the excellence of the user program and the scientific output of the facility.

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The Center as a User Facility

The NIST Center for Neutron Research is a national user facility whose mission is to ensure the availability of neutron measurement capabilities in order to meet the needs of U.S. researchers from industry, academia, and government agencies. The NCNR user community is robust and eager to obtain access to the NCNR facilities, routinely submitting more than 600 proposals per year. In the most recent call for proposals, more than 1,800 days of beam time were requested, corresponding to an average instrument oversubscription of 2.0. The new option to mail in samples for the powder diffractometer is being exercised, providing a good alternative to costly travel and difficult scheduling issues.

As indicated to the panel, in 2008 about 800 users came to the NCNR, and the productivity of the instruments was estimated to be more than 50 users per instrument, a figure on par with European sources. Users from universities make up 68 percent of the total, 8 percent are from other NIST laboratories, 5 percent are from industry, and 14 percent come from other national laboratories. The balance of beam time allocation—two thirds of beam time for the user program and one third for in-house instrument use—has been excellent for meeting the needs of users and maintaining outstanding instrument scientists. The flexibility allows NCNR services to be provided to the broad neutron scattering community; to industrial users, who frequently need fast turnaround times; and to users from other NIST laboratories; it also offers rapid access for high-impact scientific research, as well as a means to bring in new users who do not have previous experience in neutron scattering techniques.

To further increase the number of industrial users, the NCNR staff lowers barriers to instrument access through the collaborative access mechanism and provides robust support during measurements. Another mechanism for increasing the number of industrial users is through collaborative participating research teams. The PRT involving the Neutron Imaging Facility BT2 instrument has fostered excellent industrial participation and has provided crucial information on the operation of membrane fuel cells. To promote additional industrial interactions, an industry-university-government consortium led by the NIST Polymers Division is being developed to operate the new 10 m SANS instrument as part of the Expansion Project.

Current users of the NCNR are highly satisfied with the quality and support of the facility and personnel. The NCNR User Group surveys users approximately every 3 years. The most recent survey, conducted in 2007, included responses from students and postdoctoral researchers, staff members, and external principal investigators. Discussion by the panel with the head of the NUG confirmed that users rate the quality and reliability of instruments and support from the NCNR personnel as “excellent.” The variety of sample environments and ease of proposal submission are also regarded highly by users. Adequacy of office space for visiting scientists and user amenities received relatively lower marks, but these will be improved substantially by the addition of the new office building as part of the facility expansion. The NUG chair noted that more timely and detailed acquisition of users’ impressions from their NCNR facility experience could be obtained by converting the user exit survey to be Web-based. Such a change to a more efficient information collection method would help the facility adjust to perceived needs of the users more quickly.

Other concerns raised by users in the 2007 survey were primarily associated with the availability of specialized sample environments, the need for easy access to their data after leaving the facility (on the World Wide Web, for example), the availability of software and associated tutorials for data analysis, and more time-effective health physics training. In addition, the NUG chair commented that users were apprehensive that the Expansion Project would result in further delays in upgrading the thermal instruments. As noted on the NCNR Web site, a project to modernize the older neutron scattering instruments in the confinement building will be implemented over the next few years (http://www.ncnr.nist.gov/instruments/therminstr.html). Subsequent NRC assessment panels should examine the progress of this plan.

To increase the pool of specialized sample environments, the NCNR initiated a Small Grants Program in 2007. One proposal has been funded from the 2008 call. Although previous NRC panels were enthusiastic and supportive of this creative means of increasing the range of ancillary equipment available, it remains to be determined whether this will be an effective method of increasing the sample environment capabilities of the facility. NCNR management should seek out additional schemes for augmenting the ancillary equipment, because often the availability of one or more of these pieces of equipment, rather than neutron flux alone, makes the crucial difference in carrying out experiments in a competitive field.

A significant advance in SANS analysis software based on the IGOR-Pro software tool was developed in-house by an NCNR staff member. The 2006 paper detailing the software[1] has been cited 60 times, and Web-based video tutorials have greatly facilitated the use of the software, which has also been adopted at other facilities. Similarly, the user-friendly MSLICE data-reduction module is being broadly employed at U.S. and international facilities. Two NCNR personnel also contribute to the analysis software being developed through the Distributed Data Analysis for Neutron Scattering Experiments (DANSE) project. A critical need of users is for well-documented and well-maintained software. NCNR management is to be commended for these contributions to the scattering community.

Another noteworthy development is the greater ease of conducting polarized neutron scattering experiments based on ^{3}He flippers. In 2008 more than 20 separate experiments were conducted. Additional growth and expansion to two additional instruments are planned for 2009. A proposal for a deuteration facility has been submitted to the NIST Innovations in Measurement Science Program; the facility would be located at the Center for Advanced Research in Biotechnology, a joint institute of the University of Maryland and NIST. If funded, deuterium labeling may be an especially attractive means of encouraging more biomedical research at the facility.

A common criticism of similar facilities is the lengthy time required for safety training. The NCNR, whose safety record has been superb, has taken welcomed steps to further streamline this process while increasing the depth of information for users. Facility access remains a growing challenge. To its credit, in contrast to some government installations whose security apparatus impedes contact with the outside, the NCNR is trying to maintain a rational security program in order to allow efficient use of the facility. Two people are employed to facilitate user access. Foreign visitors are required to apply for permission 35 days before arriving at the NCNR; the 35-day period is on a par with or shorter than the lead time required at similar national facilities. The present system seems to meet all security requirements while keeping the spirit needed in a center of learning. However, this area requires ongoing attention.

[1] S.R. Kline, "Reduction and Analysis of SANS and USANS Data Using IGOR Pro," *Journal of Applied Crystallography* 39 (2006): 895-900.

The NCNR Expansion Project will greatly affect users during the shutdown of the facility and through the increased scientific capacity after its completion. Because users will be challenged to obtain sufficient neutron scattering time during the shutdown, NCNR management is thoughtfully working on implementing upgrades, transitioning instruments to new beam lines, and implementing new instruments in ways that reflect attention to minimizing the necessary downtime.

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Center for High Resolution Neutron Scattering Program

The Center for High Resolution Neutron Scattering Program has done an excellent job of meeting and exceeding its objectives. The CHRNS is a National Science Foundation program started in 1990 that currently supports the operation of six spectrometers and associated personnel at the NCNR. Covering roughly 30 percent of the NCNR beam lines, the CHRNS is the heart of the NCNR User Program and sets the standard for other U.S. facilities with respect to productivity. Each year, the CHRNS supports about 500 users, many of them graduate students, and yields about 100 publications. About half of the high-impact publications of the NCNR are from the CHRNS, and more than 25 Ph.D. theses benefited from research conducted on CHRNS instruments.

The suite of CHRNS instruments covers a broad length scale and energy range for dynamical studies. The reliability of the instruments is excellent, consistently over 98 percent. The oversubscription rate of the instruments is 2.2, attesting to the strong user base. Five of the six instruments are state of the art, including the following: the BT5-USANS, a unique, ultra-small-angle neutron scattering instrument; the NG2-HFBS, a state-of-the-art inelastic high flux backscattering spectrometer (HFBS) with the highest count rate and smallest energy resolution in the world; the NG3-30 m SANS, a workhorse instrument and the only polarized SANS in the United States; the NG5-Spin-Echo spectrometer, which will be upgraded with a guide, polarizer, and improved magnetic-field compensation, making it competitive with the new instrument under construction at the Spallation Neutron Source; and the NG5-SPINS, which has the highest magnetic field on a spin-polarized inelastic neutron scattering instrument in the United States. The NG-4 DCS (disk chopper spectrometer) has been a workhorse instrument for the CHRNS, but it will be less competitive with the commissioning of the Cold Neutron Chopper Spectrometer (CNCS) at the SNS. The timely replacement of the DCS with the Multi Axis Crystal Spectrometer (MACS) will add an internationally competitive instrument, 100 times faster than the DCS and 10 times faster than the CNCS at a constant energy plane, with unique sample environment capabilities—11 T magnet and dilution refrigeration to 0.03 K. The CHRNS suite of instruments will, therefore, continue to offer internationally competitive instruments for the broad materials science community.

A key contribution of the CHRNS program is its educational impact on the neutron scattering community. Every educational program produced by the NCNR is solely supported by the CHRNS. In addition, the NSF Research Experiences for Undergraduates and the Summer Undergraduate Research Fellowship programs at NIST are leveraged through the CHRNS to provide undergraduates with summer research opportunities to learn about and use neutrons in the students' research activities. The chair of the NUG commented to the panel that the CHRNS summer schools are oversubscribed by a factor of three. To address this great need for additional educational opportunities, the inelastic and small-angle themed summer schools should be offered every year instead of every other year. This doubling of summer school slots would enable more students to be served in a timely fashion.

Another key outreach activity is the advertisement of neutron scattering at scientific conferences to attract new users. Talks by NCNR personnel offer an effective bridge from researchers investigating the type of scientific questions and problems that neutron scattering can address to researchers in a broad range of fields who currently do not use neutron scattering. A key aspect of interfacing with new users, beyond providing assistance during the measurements, is following up to ensure that no questions remain and that the data are fully analyzed after researchers return to their home institutions. Such educational outreach is as important as providing the summer school and is a great benefit for novice users of the CHRNS instruments.

The development of analysis software by CHRNS-affiliated personnel has also been substantial. Inelastic scattering software (Data Analysis and Visualization Environment, or DAVE) and IGOR-based SANS analysis software continue to be developed and maintained with the support of the CHRNS. Other educational activities have included a coordinated effort to increase the visibility and use of the new USANS instrument. Over the past year, this has led to a doubling in the number of beam time request proposals. The instrument is now oversubscribed by a factor of 1.6, a number that is likely to grow in the near future. The increased workload for CHRNS personnel warrants additional support so that an expanded summer school can be offered and the excellent user program and high-impact science conducted with the CHRNS instruments can be maintained.

In summary, the CHRNS partnership between the NCNR and NSF is commendable. The high-impact and prodigious scientific output from the use of the CHRNS instruments is outstanding. The cost sharing—two thirds from NIST-NCNR and one third from NSF—is highly effective. If CHRNS funding is not continued in subsequent years, the impact on the neutron scattering community in the United States would be extremely negative. State-of-the-art and internationally competitive instruments would have to be removed from the user program if there would no longer be sufficient personnel to operate and maintain the instruments. The United States already lags behind Europe by 50 percent in terms of neutron scattering instruments. The user program would be dealt a further blow if the level of support to carry out experiments, analyze data, provide software, and provide educational opportunities were greatly reduced. The continuation of the CHRNS partnership should be given strong support.

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Conclusions

The NIST Center for Neutron Research is successfully accomplishing its missions, as a national user facility, to ensure the availability of neutron measurement capabilities to meet the needs of U.S. researchers from industry, academia, and government agencies and to develop the next generation of neutron scattering scientists and engineers.

The NCNR continues to provide reliably a high flux of neutrons to an evolving suite of high-quality instruments and sample environments. The array of thermal and cold neutron instruments available at the NCNR enables measurements over a wide range of time, energy, and length scales.

These capabilities of the NCNR play a critical role in advancing science and developing new technologies in the United States and enable NIST to fulfill its role of promoting science, standards, and technology in support of the U.S. economy. The new instruments and upgrades associated with the planned facility expansion will ensure that the NCNR continues to provide users with access to internationally competitive instruments.