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Panel on Neutron Research

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## PANEL ON NEUTRON RESEARCH

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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 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:

Stuart G. Bush, Rohm and Haas Corporation,
David Chandler, University of California, Berkeley,
Seb Doniach, Stanford University,
Zachary Fisk, University of California, Irvine, and
Lyle H. Schwartz, Air Force Office of Scientific Research (retired).

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 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 committee and the institution.

# Contents

# Summary

The NIST Center for Neutron Research (NCNR) continues to be well run. It consistently and reliably provides a high flux of neutrons to an evolving suite of high-quality instruments. There is a substantial and well-satisfied external user community. The in-house science and technology is robust. The new organizational structure—the NCNR director now reports directly to the Director of the National Institute of Standards and Technology (NIST)—demonstrates NIST recognition of the strength of the facility and allows a more efficient means for the facility to interact synergistically with the broad NIST complex. Ground will soon be broken for a substantial expansion of the guide hall, complemented by the construction of a new set of instruments. With this expansion and by continuing to serve the broad neutron scattering community, the NCNR is likely to remain an important neutron source and knowledge base for years to come.

As the NCNR proceeds with the expansion of the guide hall, it should continue to

- Develop consortia with industrial, academic, and government laboratories to leverage new instrument development and construction.
- Interface with the user community for identification and selection of new instruments.
- Recruit instrument scientists and engineers to construct, operate, and maintain new instruments.
- Work to maintain the necessary scientific openness of the facility within the constraints of increasing security demands.

The NCNR should also

- Aggressively pursue its small grants program to enhance sample environment capabilities and to improve data analysis programs.
- Continue to add instruments to the user suite, including thermal neutron spectrometers.
- Aggressively pursue a replacement for the National Institutes of Health/National Center for Research Resources (NIH/NCRR) grant in biological materials.
- Develop a center for soft matter and biological physics to complement NCNR capabilities.

# Charge to the Panel and Description of the Assessment Process

At the request of NIST, the National Academies, through its 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 eight,[1] as well as the adequacy of the laboratories' resources. In 2007 NIST requested that four of its laboratories be assessed: the NCNR, the Information Technology Laboratory, the Chemical Science and Technology Laboratory, and the Electronics and Electrical Engineering Laboratory. Each laboratory was assessed by a separate panel of experts, and the findings of each panel are summarized in separate reports. This report summarizes the findings of the Panel on Neutron Research.

NIST requested that the panel consider the following criteria as part of its assessment:

1. The degree to which the Laboratory programs in measurement science, standards, and technology address national priorities.
2. The degree to which the Laboratory programs in measurement science, standards, and technology are well-motivated with regard to the following questions:
   a. What is the program trying to accomplish?
   b. What is innovative or different, as compared to efforts at other institutions, about the program's approach that will lead to success?
   c. Is success well defined?
   d. What will be the impact of success?
   e. How will success be disseminated to end users?
   f. How much will success cost, and how long will it take?
3. The technical merit of the Laboratory programs relative to the current state of the art worldwide.
4. Insofar as they affect the quality of the technical programs, the adequacy of the Laboratories' facilities, equipment, and human resources.

To accomplish the assessment, the NRC appointed a panel of seven volunteers whose expertise matched that of the work performed by NCNR staff. The panel members visited the NCNR facility 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, when they conducted interactive sessions with NCNR managers and with leaders of NCNR user groups; the panel also met at this time in a closed session to deliberate its findings and to define the contents of this assessment report.

[1]The eight NIST laboratories are the Building and Fire Research Laboratory, 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.

The panel's approach to the assessment relied upon 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 standards and measurements activities and the technological research presented by the NCNR; it was not possible to review the NCNR programs and projects exhaustively. The panel's goal was to identify and report salient examples of accomplishments and opportunities for further improvement with respect to the technical merit of the NCNR work, its perceived relevance to NIST's own definition of its mission in support of national priorities, and apparent specific elements of the NCNR's resource infrastructure that is intended to support the technical work. These highlighted examples, for each NCNR division, are intended to collectively 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; while the panel applied a largely qualitative rather than 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.

This report is organized in four sections: general assessment comments, facilities and personnel, NCNR as a user facility, and science and technology at NCNR. The comments in this report are intended not to exhaustively address each program within NCNR but to identify key issues, salient programs, and the projects relevant to those issues. Detailed information on NCNR activities and programs can be found on its Web site, www.ncnr.nist.gov, or in published documents. NCNR's annual report in particular highlights scientific research at the Center, lists publications, provides current research titles, and gives information on instrumentation and other developments.

# General Assessment

The NCNR management defined the mission of the laboratory as follows:

> The mission of the NIST Center for Neutron Research is to assure the availability of neutron measurement capabilities to meet the needs of U.S. researchers from industry, university, and other Government agencies. Toward this end, the NCNR operates the NIST Research Reactor cost effectively while assuring the safety of the staff and general public; develops neutron measurement techniques, develops new applications of these techniques, and applies them to science and engineering problems of national interest; and serves the needs of researchers from industry, university, and government by operating the research facilities of the Center as a national facility.

NCNR continues to be a well-run facility. It consistently and reliably provides a high flux of neutrons to an evolving suite of high-quality instruments. There is a substantial and well-satisfied external user community. The new organization structure (the NCNR director now reports directly to the NIST director) demonstrates NIST's recognition of the strength of the facility and allows a more efficient means for the facility to interact synergistically with the broad NIST complex. An enhanced coupling of NCNR to NIST organizational units is apparent since the last review. The substantial expansion of the guide hall, complemented by the construction of a new set of instruments, was partially a result of the strong endorsement of NCNR by the Office of Science and Technology Policy's Interagency Working Group on Neutron Science.[2] As detailed by that group, the United States has been neutron poor in the recent past. With the Spallation Neutron Source (SNS) coming on line and the NCNR expansion, this situation is markedly improving. By continuing to serve the broad neutron scattering community, NCNR is likely to remain an important neutron source and knowledge base for years to come.

The SNS is coming on line now with only three instruments (two reflectometers and one back-scattering instrument) and will take years to be fully operational at 1.4 MW. It is imperative that the user community continue to grow and be served by the existing facilities in order to take advantage of the SNS at full operation. In addition, the impending loss of neutron sources Brookhaven National Laboratory and the Internal Pulsed Neutron Source at Argonne National Laboratory will only be offset by the SNS. The United States is neutron poor and needs all the facilities operating well to serve the U.S. science community. NCNR and the expansion are important for maintaining the research capacity and for providing neutrons to the broad scientific community.

[2]Interagency Working Group on Neutron Science, Office of Science and Technology Policy, 2002, *Report on the Status and Needs of Major Neutron Scattering Facilities and Instruments in the United States*.

# Facilities and Personnel

The NCNR operates 24 beam instruments that cover a broad range of energies, resolutions, and capabilities. The NCNR expansion project will increase the cold neutron user facilities by 30 percent to help meet the needs of the growing neutron scattering community. The expansion will add a new cold source, guide, and guide hall and will also allow optimization of the existing instruments across the aggregate flight paths. This optimization includes separation of high magnetic field instruments to minimize cross talk with magnetically sensitive instruments and experiments. To operate the five new funded instruments will require hiring additional staff and a significant increase in operating funds. Continuation of strong staff support to users will be important for maintaining the quality of the science program and output of the NCNR. Partnerships with industry and the formation of consortia will allow the number of instruments to be increased through leveraging (there is currently funding for 5 but space for 10) and should be aggressively pursued. NCNR management is well aware of the impact of the SNS on the neutron program and is choosing instrumentation in the expansion project that will complement the new source. Nevertheless it is important that each instrument is developed with a clear understanding of its existing user community at present and its expected growth. Sustained and robust interaction with the user community is essential for maximizing the number of instruments and their suitability for meeting the needs of various constituents. Current staff levels are unlikely to be sufficient to meet the needs of the user program and also support the design and construction of the new suite of instruments. It is therefore essential that NCNR staff be expanded to design, build, and support these new instruments and maintain the high level of service to the user community. Moreover, in addition to recruiting design and construction engineers for the new beam lines and instruments, NCNR must aggressively recruit instrument scientists to interface with the user community as well as optimize the science capabilities of the new tools.

There has long been an issue of the sufficiency of the numbers of scientists and engineers who are trained and have expertise in neutron scattering science and instrumentation. A contributing factor is that most neutron sources are not at universities but at national laboratories. In order to address this issue, NCNR has been actively pursuing an outreach program that is designed to provide education in the neutron scattering arena. This includes the yearly summer school at the Center for High Resolution Neutron Scattering (CHRNS) for graduate students and postdocs; there is also a summer undergraduate research fellowship administered by NIST.

The new expansion of the experimental facilities, the increased security systems, and important ongoing maintenance are all competing for the extant in-house pool of skilled engineers. While funding for increasing the engineering staff does not appear to be a serious difficulty, competing successfully against the many other industry, government, and university groups now aggressively hiring engineers with nuclear experience will be increasingly difficult. At the present time several additional engineers are needed to meet the projected workload.

The reactor is well maintained and skillfully operated and was available for research during 2006 on 266 of a possible 267 days (99 percent availability). Budget

allocations for routine operations have been adequate, with a 3-4 percent increase in 2006 over 2005. Reserve stockpiles of heavy water and reactor fuel of the type for which it was designed are sufficient for a complete change-out of the heavy water inventory, and enough fresh fuel has been manufactured for several years of operations. Planning for coolant systems modifications and rerouting necessitated by the expansion of the guide hall/experimental area is well in hand. It is based on allowing as much time as possible for making final decisions on the specifications of the new instruments to be located there.

# NCNR as a User Facility

The NCNR is a national center for research that provides the advanced measurement capability of thermal and cold neutrons to researchers from industry, universities, and government agencies. It plays a key role in fulfilling the NIST mission, to promote U.S. innovation and industrial competitiveness by advancing measurement science, standards, and technology and the American Competitiveness Initiative by providing a facility and a wide and evolving array of neutron instruments that enable fundamental scientific discovery and the development of new technologies.

A broad and vibrant user community makes use of the instrument suite at NCNR. Oversubscription of the available instruments and insufficient staff to support NCNR users continue to be a concern. The number of proposals submitted has almost doubled over the past 5 years, and the instruments were oversubscribed by a factor of 2.2, on average, in 2006. The expansion and the reliability enhancement projects are crucial for maintaining NCNR's vigor and scientific output.

The NCNR user program has grown steadily and served approximately 850 physical users during 2006. A recent survey conducted by the NCNR User Group Executive Committee in March 2007 demonstrated that the users are well served. Typical responses rated the training, instruments, and facilities as good to excellent. Importantly, NCNR staff have consistently been evaluated as excellent by the majority of users according to user surveys in 2004 and 2007. The chair of the committee that allocates beam time mentioned to the panel that a strength and driver of the user program has been the strong staff support and the well-organized, critical, and external review process of user proposals. He noted that the research community believes the proposal process is reasonable and fair. A novel concept to further strengthen the scientific output of the facility is the ongoing development of a science group whose leaders range across a spectrum of strong NCNR scientists and whose overarching goals are to produce high-impact science, develop new partnerships and proposals for new funding, guide development of instruments, and conduct outreach to grow and support the burgeoning neutron scattering community.

In the 2007 user survey, the need for additional specialty sample environments was mentioned a number of times. In response, NCNR announced (on www.grants.gov) it is giving small grants to develop and build sample environments. The small grants program initiated by the NCNR facility is an excellent and innovative method of leveraging expertise in the user community to provide enhanced sample environment development and capabilities. If successful, this program could be expanded to address stated needs for improved data analysis programs.

The NSF-supported CHRNS program is a positive example of synergistic activity between government agencies. New ways must be found to support the NCNR expansion project and maintain its robust scientific output. Such collaborative interactions are also indispensable for supporting new users.

NCNR's policy that allocates some fraction of the available beam time for an increasing number of instruments to the general user pool is laudable and should be extended. In particular, the thermal neutron instruments should be added to this suite.

Technical staff should be hired so that the scientific staff have time for the users as well as for their own scientific undertakings.

Since the last NCNR review, the committee has observed an enhanced responsiveness of other NIST divisions to collaborations with NCNR. Last year, 5 percent of the NCNR participants were from NIST (non-NCNR). Some of the collaborating divisions are Analytical Chemistry, Ionizing Radiation, Biochemical Science, and divisions within the Electronics and Electrical Engineering Laboratory. The Polymer Division continues its strong involvement with NCNR.

All nuclear reactors have had to increase the strength and reliability of their security systems in the face of possible harmful intrusion attempts. NCNR has responded by investing in many new systems and components. However, as a facility with a strong commitment to providing excellent facilities and services to its industry-, government-, and university-based users, it can only successfully meet their needs by operating with a substantial degree of openness. A reasonable and stable balance between highly secure and very open operations must be found to avoid creating a sterile fortress. While steady improvements in the scientific capabilities of the facility are justifiable, endless additions to the security systems could severely interfere with the facility's ability to achieve its mission, and care must be exercised to avoid such an unfortunate outcome.

# Science and Technology at the NCNR

NCNR admirably balances attention to development, construction, and maintenance with support of a broad range of scientific and technical investigations. Much of the successful balance is due to carefully constructed cooperation with the many beam users who bring samples for short visits. From this visiting population and its own research staff, the NCNR management chooses the best kinds of target stations to serve scientific needs. Particularly because the SNS will be filling many needs, the NCNR has thoughtfully chosen to build detectors and to develop facilities specifically for the many investigations that will not be optimally served by the SNS. In so doing, the facility has earned high priority for support within NIST.

Because of the very broad range of topics being addressed at NCNR and its members' wish for substance in presentation, the panel heard descriptions of only about half of the research activities conducted at the NCNR. The facility is providing excellent data, for example, on the states of water at low temperature and in the vicinity of macromolecules. It is bringing a better view of proteins in solutions, particularly as distinct from crystal structures, and is revealing new levels of polymer organization that correlate with the toughness of materials. The renowned work on multiferroics, materials that show ferromagnetic and ferroelectric properties, is progressing rapidly.

The NCNR hosts fundamental physics studies of the properties of the neutron, as well as a number of more applied physics measurements, on a total of seven ports. The cold beam lines (NG-6 and -7) are a world-class site for basic physics with the neutron, competitive with the Institut Laue-Langevin (ILL) in Grenoble, France.

The neutron lifetime and a set of parameters describing correlations between the neutron spin and the kinematic parameters of the decay electron, proton, and antineutrino provide the most model-independent source of information on the unitarity of the Cabibbo-Kobayashi-Maskawa matrix, which in turn is an avenue to extensions of the standard model. The Standard Model is now known to be broken with the discovery of neutrino mass and oscillations, and it is important to find other deviations in order to advance to a new, correct, and predictive model. The neutron lifetime has long been a topic of study at NIST, although the most precise measurements (which do not mutually agree) were made at ILL. To resolve this situation, NIST and a group of universities are developing a new measurement based on magnetically trapped ultracold neutrons.

Perhaps the most important neutron physical parameter for the new physics is a possible electric dipole moment (EDM), which would be zero if nature respected the symmetry CP (charge conjugation and parity reversal). This bears directly on the question of why the universe contains matter but essentially no antimatter, because it would reveal a source of CP violation larger than the (inadequate) amount contained within the Standard Model. A large U.S. neutron EDM project is planned for the SNS, but NIST scientists in collaboration with other universities and Argonne National Laboratory are investigating a completely different approach that might be as sensitive and that would have different systematics. A proof-of-principle test is a measurement of the magnetic dipole moment. This creative approach and plan hold promise. This experiment has been approved and is under development at the NCNR.

There is an initiative to develop high-capacity hydrogen storage for fuel cells, small relative to the amount of work being done by industry but critical for the systematic investigation that is possible at the NCNR.

Of concern to the panel and to the staff at NIST was the loss of an NIH/NCRR grant for the study of biological materials. The formal consortium operating the AND/R instrument has ended, and NIST is concerned about losing momentum in this research area. Appropriately, NCNR wants to continue its biological work and is trying to forge new associations. An important opportunity will be lost if the NIH grant cannot be replaced. The ongoing collaboration between NCNR and both the Child Health and Human Development Institute and the Cancer Institute at the NIH is a positive sign for the restoration of funding.

Within the larger purview of soft materials, NCNR should develop more relationships with leaders in the field to enhance and drive science. What is needed is a strong biology and soft matter center to complement the capabilities at NCNR. There are already productive interactions with the Biochemical Science Division at the NIST Chemical Science and Technology Laboratory. With characteristic foresight, NCNR is now interviewing candidates for a scientist who will take a permanent staff position and who will lead the soft matter research. Other mechanisms such as visiting scholars and systematic visits with nearby institutions such as the NIH can be created to allow NCNR to build a center of excellence.

The science and technology to which the panel was exposed are strong. In 2006 there were 35 papers in high-impact journals (*Nature, Physical Review Letters, Science, Proceedings of the National Academy of Sciences,* and the *Journal of the American Chemical Society*). Taking into account the aforementioned soft matter and biological sciences, it can be judged that science is healthy at NCNR.

# Conclusions

The NCNR continues to be well run. It consistently and reliably provides a high flux of neutrons to an evolving suite of high-quality instruments. There is a substantial and well-satisfied external user community. The in-house science and technology is robust. The new organizational structure (the NCNR director now reports directly to the NIST director) demonstrates NIST recognition of the strength of the facility and allows a more efficient means for the facility to interact synergistically with the entire NIST complex. Ground will soon be broken for a substantial expansion of the guide hall, complemented by the construction of a new set of instruments. With this expansion and by continuing to serve the broad neutron scattering community, the NCNR is likely to remain an important neutron source and knowledge base for years to come.