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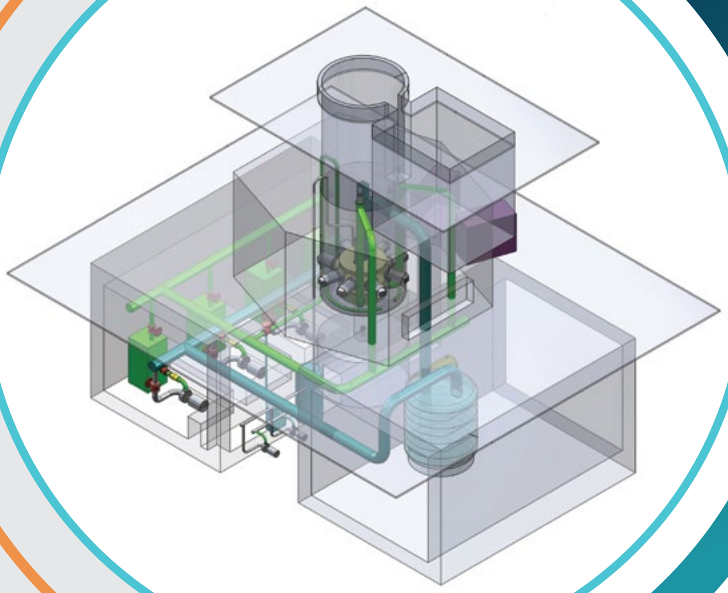
NEUTRONS FOR THE FUTURE

Rockville, MD
October 18-20, 2023



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Abstract

Producing neutrons in quantities sufficient for most applications is challenging and requires centralized facilities that develop and deploy cutting-edge instrumentation for the Nation's scientific and engineering communities. For over 50 years, the NIST Center for Neutron Research (NCNR) has been at the forefront of neutron science, serving the Nation's need for these essential measurement capabilities. However, as the current reactor ages, planning has begun for a replacement facility. This 2023 workshop titled "Neutrons for the Future," attended by over 200 participants from across the US, produced critical insights into the future of neutron measurement science and, therefore, the requirements for a future NIST Neutron Source (NNS). The conceptual design of the NNS, accompanying facilities, equipment, and staffing, will be directed by key findings and priorities identified in this workshop.

Keywords

Neutron Source; Reactor; Neutron Science; Neutron Scattering; Nuclear Methods; Soft Matter; Biosciences; Condensed Matter; Nuclear Physics.

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Foreword

In response to the Chips and Science Act of 2022, a workshop entitled “Neutrons for the Future” was held in Rockville, MD from October 18–20, 2023. This workshop brought together many of the leading researchers from the U.S. neutron scattering user community to discuss plans for a New Neutron Source (NNS). Over 200 attendees from across the Nation were divided into 12 panels to discuss the future needs of the user community and their respective scientific sub-fields as well as to develop a plan to minimize disruptions to the user community during the transition.

The workshop opened with four plenary talks: *Neutrons for the Nation*, which summarized the current state of neutron research in the U.S.; *Assessing the Economic Impact of U.S. Neutron Scattering Facilities*; *NIST Neutron Source Preconceptual Design*; and *A Replacement Reactor for NIST and the Nation*. The remaining two days of the workshop were dedicated to panel breakout sessions, which culminated in written reports from each panel.

Nine science panels were formed to address the areas of Biosciences, Hard Condensed Matter Dynamics, Hard Condensed Matter Structure, Energy and Environment, Engineering, Neutron Physics and Neutrino Physics, Nuclear Methods and Radiochemistry, Soft Matter Dynamics, and Soft Matter Structure. These panels were given the following charges:

1. Identify the scientific and technical drivers for future neutron-based research. Include the expected impact of neutron measurements on science and technology and their ability to address emerging national priorities.

2. Assess the ability of the current plans for the reactor and cold source(s) to provide industrial, academic, and government researchers with the necessary tools and infrastructure to address the identified national priorities.

3. Identify the characteristics of the instrumentation and facilities (including, e.g., sample environments) needed to address the identified national priorities. Identify any technological and instrument developments that are required in the early stages of construction to effectively address national scientific and technological priorities.

Three other panels were formed:

1. The Source Characteristics panel was charged with identifying the ability of the current plans for the reactor and cold source(s) to provide industrial, academic, and government researchers with the necessary tools and infrastructure to address national priorities.

2. The Accompanying Facilities panel was charged with identifying the characteristics of the facilities (including labs, sample environments, IT, shops etc.) required to provide industrial, academic, and government researchers with the necessary tools and infrastructure to impact science and technology; and identifying any technological and instrument developments required in the early stages of the project to address to effectively address emerging national priorities.

3. The Transition Process panel was charged with describing the considerations and steps required to minimize disruptions to the user community during the transition from the current facility to a future one.

The Executive Summary below provides a brief overview of the conclusions drawn from this workshop. This is followed by the 12 panel reports described above.

Acknowledgements

This workshop was planned and organized by the following committee:

Program Co-chairs
Stephen Wilson – University of California, Santa Barbara
Mike Hore – Case Western Reserve University

Organizing Committee
Rob Briber – University of Maryland
Lisa Press – University of Maryland
Peter Gehring – NIST Center for Neutron Research
Dan Neumann – NIST Center for Neutron Research
Pappannan Thiyagarajan – NIST Center for Neutron Research
Jim Rhyne – NIST Center for Neutron Research
Joe Dura – NIST Center for Neutron Research

In addition, this workshop was made possible by the work of many dedicated NCNR staff members who facilitated breakout sessions, compiled session reports, and coordinated local logistics.

Executive Summary

Neutrons are unique, nondestructive probes that greatly enhance our understanding of a huge range of physical phenomena. They offer structural, dynamical, and compositional information about materials, making techniques that use neutrons—such as neutron scattering, interferometry, and activation analysis—integral to many advanced technologies that benefit society. The isotopic sensitivity of neutrons makes them exceptionally well-suited for studying materials composed of light elements like hydrogen and lithium. This sensitivity is particularly valuable for understanding the behavior of novel pharmaceuticals including vaccines and monoclonal antibodies, energy-related technologies such as lithium-ion batteries, and it has driven advances in additive manufacturing. Neutrons sensitivity to light elements is also crucial for applications in hydrogen storage, carbon dioxide sequestration, and enhancing U.S. energy independence. In addition, the neutron magnetic moment makes it the ideal tool with which to explore magnetic phenomena, as neutron techniques are essential for developing quantum materials for new computational paradigms, high-temperature superconductors, new thermoelectric materials, and innovative methods of storing electronic information. These materials will play a vital role in our national security as new “post-quantum” cryptographic techniques emerge. Being charge neutral particles, neutrons can penetrate the walls of furnaces or magnets, thereby allowing for *in operando* or *in situ* observations of complex materials or devices, such as hydrogen fuel cells. Nearly all U.S. industries use or engage in activities requiring documentary standards, data, and materials developed by the National Institute of Standards and Technology (NIST). Neutron techniques are indispensable for certifying standard reference materials (SRMs), which are foundational metrology standards used in areas such as medicine, nutritional analysis, and instrument calibration. Collectively, neutron techniques are essential for creating many of the technologies that permeate everyday life and for developing the advanced technologies of the future.

It is widely acknowledged that well-instrumented neutron research facilities are a key element of the nation’s scientific infrastructure and essential to U.S. competitiveness. Despite this consensus, a key finding from a 2018 American Physical Society report entitled *Neutrons for the Nation*, states “*The United States has lost important capability in neutron R&D in the last two decades and is no longer the world leader. The United States cannot afford to lose its remaining capacity and capability without significant detriment to the quality and quantity of science, engineering, and even medical and manufacturing processes that rely on neutron sources*.” Other nations see the need for advanced neutron facilities. Europe is devoting more than 3B€ to build a new neutron facility called the European Spallation Source. China has also recognized the important role that neutron facilities play in a nation’s scientific and technological ecosystem, commissioning three new neutron facilities in the last decade or so.

The construction of a new neutron source hosted at NIST under the supervision of the Department of Commerce presents an opportunity to establish the premier neutron science center in the world. The New Neutron Source (NNS) at NIST should maximize the brilliance and flux of its neutron beams to enable high-throughput experiments and keep pace with increasing U.S. demand for access to neutron techniques. Emerging directions in science and technology will require facilities that can offer researchers multiple capabilities, including high-efficiency polarized neutron beams, dedicated beam lines for magnetic measurements, multimodal measurement capabilities (e.g., simultaneous X-ray and neutron measurements), advanced sample environments (e.g., high pressure, high magnetic field, extreme temperature, high rates of fluid flow), and optical/electron microscopy. These capabilities should be supported by dedicated general chemistry and sample preparation laboratories, collaboration spaces, and a guest house for visiting researchers. Recognizing the importance of SRMs to U.S. industry, the NNS should include facilities for instrumental and prompt gamma activation analysis. Additionally, neutron depth profiling, thermal column irradiation, and medical isotope R&D facilities are integral to SRM production. Industrial partners would benefit from automated and mail-in sample measurement services for routine characterizations. An adjacent isotope labeling facility would offer further support for these activities while broadening the classes of material systems that could be investigated, uniquely positioning the NNS as a one-of-a-kind neutron science center. Simultaneously, the NNS should continue to support fundamental neutron and neutrino physics experiments by providing, for example, ultracold neutron sources, low-background experimental areas for detecting neutrinos, and environmentally isolated interferometry capabilities.

Constructing the NNS presents many opportunities to incorporate recent developments in machine learning (ML) and artificial intelligence (AI). As new instruments are designed and commissioned at the NNS, AI and ML should be incorporated as optional technologies to guide the efficient exploration of parameter spaces and optimize the collection of data subject to the characteristics of a material, system, or device. This will result in better use of the neutrons as well as increase access to the facility and availability of instruments. Because high-throughput and multimodal measurements at the NNS will generate significant amounts of data, necessitating sophisticated analysis techniques for interpretation, the NNS should provide high-performance computing facilities with appropriate data storage for its users and staff.

Looking to the future, the U.S. stands to benefit significantly from the construction of a new, reactor-based neutron source at NIST to meet the growing demand for neutron instrumentation. However, the success of the NNS will critically depend on the recruitment and retention of a substantial number of instrument scientists, health physicists, and other supporting staff. The construction of the NNS will help to cultivate a new workforce having expertise in the design, construction, and operation of neutron instruments. Additionally, the establishment of the NNS at NIST will support the work of numerous government, industrial, and academic researchers, yielding broad and far-reaching societal benefits. To minimize disruptions to the U.S. neutron user community and maintain appropriate staffing and expertise levels, the NNS should ideally be constructed on NIST’s Gaithersburg campus in a new facility, separate from the current location of the NIST Center for Neutron Research. Overlapping operations during the initial phases will help to minimize disruptions and outages.

1. Soft Condensed Matter Structure

1.1. Panel

Chairs:
Xiaodan Gu – *University of Southern Mississippi*
Lynn Walker – *University of Minnesota*

Panel Members:
Xi Chen – *Oak Ridge National Laboratory*
Michael Hore – *Case Western Reserve University*
Tonya Kuhl – *University of California, Davis*
Whitney Loo – *University of Wisconsin*
Jeffrey Richards – *Northwestern University*
Simon Rogers – *University of Illinois at Urbana-Champaign*
Arun Yethiraj – *University of Wisconsin*

Scribe:

Peter Beaucage – *National Institute of Standards and Technology*

1.2. Glossary of Terms

1 nm: one nanometer equals one billionth of a meter, or 10 Angstroms.

Contrast variation: the practice of substituting elements in a specific region of a molecule with a different isotope to either enhance or reduce the neutron sensitivity to that region.

Deuteration: the process of selectively replacing hydrogen in a material with deuterium to alter how the material, or parts of the material, are visible to neutrons.

Electrolytes: materials with mobile ions, such that they conduct electricity.

Isotope sensitivity: the (different) sensitivity of an element's isotopes to neutron scattering. This difference can be exploited in a neutron scattering measurement.

Isotopes: one or more forms of a chemical element that has the same atomic number, but a different number of neutrons in its nucleus. Isotopes of a particular element typically have similar physical properties but can have very different neutron scattering properties that can be exploited.

Non-destructive: a measurement technique is non-destructive if the material being tested is unaltered by the measurement technique. Neutron scattering is a non-destructive technique.

Polymers: a large molecule formed by linking many smaller molecules through covalent bonds.

Soft Matter: materials held together by weak interactions, such that the materials are easily deformed by external forces and thermal fluctuations.

Time and spatial resolution: a measure of how short of a time or how small of a distance can be accurately resolved in a measurement.

1.3. Summary

Neutron science coupled with isotopic substitutions at specific locations within molecules can enable the precise determination of the structure and composition of soft materials at and far from equilibrium. These advances will make NIST the premier neutron facility in the world and catalyze the innovation and commercialization of key technologies that society needs. These include sustainability, advanced medicines, improving energy efficiency, and innovation in electronics.

Soft matter must be engineered to address the critical needs of modern society. Soft matter materials are composed of light elements and held together by weak forces often comparable in magnitude to thermal energy at room temperature. The properties of functional soft matter emerge from their physical and chemical complexity with a hierarchy of length scales spanning angstroms to the macroscale. The structure and chemical flexibility of soft matter makes it an ideal engineering solution with outstanding properties in many emerging technologies.

Neutron techniques are non-destructive, sensitive to isotope variation, and able to characterize the structure of soft matter over a wide range of length and time scales. These tremendous advantages separate neutron techniques from others and make them vital to advancing soft matter research and development. Within the next twenty to forty years, new neutron sources will allow the structural changes of single molecules (polymers, proteins, and beyond) to be probed *in operando*, accounting for the complex interplay between equilibrium properties and processing conditions. This newly gained understanding will expand the abilities of scientists and engineers to develop materials for applications critical to societal needs.

Scientists and engineers engaged in neutron science will emerge as leaders in industry and academia who will power the materials revolution required for technological development. Simultaneously, the new advancements in measurement science and technique development enabled by new reactor sources and capabilities will ensure the preservation of a vibrant and active neutron community into the 22nd century and beyond.

1.3.1. Materials for energy generation and efficiency

Neutron science will inform the design of multicomponent soft materials being developed to meet the demands of thermal management and energy efficiency technologies. For example, the structure of advanced polymeric composite coatings can be manipulated to reduce the energy required for thermal management. These coatings must maintain their properties under harsh conditions while retaining the capacity to be recycled or repurposed at the end of life. To achieve these goals, their properties must be characterized in relevant environments and during reprocessing. The ability of neutron science to reveal nanoscale structure in complex sample geometries, and the use of contrast variation via isotopic substitution to highlight specific structural features will revolutionize our ability to design materials. Neutrons will thus lead the way in elucidating and tracking the evolution of nanoscale structure and chemistry as materials fail, pointing the way to longer lasting technologies.

Polymers and polymer-based composites are two of the key materials systems underlying energy storage systems such as batteries, fuel cells, and redox flow batteries. With the technological imperative to advance these energy storage systems, new polymers and polymer-based composite materials must be developed. Some examples include: single-ion-conducting polymer electrolytes, non-fluorinated proton-conducting membranes, polyzwitterionic polymer electrolytes, polymer-superionic ceramic composite electrolytes, and solid-state cathodes with polymer electrolyte binders. All these new materials are structurally more complex on length scales ranging from angstroms to nanometers (ions and ion-clusters), to the mesoscale (microphase separation, ion channels), and finally to the macroscale (device level).

With the emergence of new polymer-based energy storage materials, we must advance our fundamental understanding of structure-property relationships and the structural evolution of these materials during assembly, processing, and operation. Neutron scattering is uniquely able to advance our knowledge. Neutrons are sensitive to light elements, unlike x rays, which means that the structure of polymers can be probed even in an inorganic-rich materials system where the polymer weight percentage is low (in a practical cathode, the polymer loading can be as low as 5 wt%). Neutrons can also penetrate heavy elements, which means that *in operando* measurements are possible during cell cycling through the aluminum coin-cell cans or pouches (or other metal housings). Combined with a high neutron flux and a wide range of scattering angles to provide access to different length scales, the scientific community will use neutrons to understand extremely complex structures in polymer materials and track the structural evolution during processing and operation. These advances will expedite materials discovery and eventually benefit the economy and sustainability of the nation.

1.3.2. Soft and Bio-Electronics

Neutron science will be at the center of the electronic materials revolution. The demand for advanced electronics in the United States is steadily increasing, and this demand extends across a broad spectrum of applications. These applications encompass various areas such as soft robotics, bioelectronics for novel treatments for disabled patients, neuromorphic computing for innovative methods of interacting with data, and the enhancement of human-machine interfaces. These areas hold significant importance for the future of the U.S. economy, as an expanding economic sector relies on advanced sensing, high-efficiency electronics, and the internet of things. Neutrons offer the ability to characterize functional materials with atomistic resolution and provide unique diagnostic capabilities for devices in operation, thereby assisting in the engineering of new electronic materials to enhance device performance. This capability holds the promise of transforming both materials and energy-efficient manufacturing methods, bolstering the U.S.'s position in the global technology landscape.

One important area for functional electronic materials is closely linked to innovations in sustainable energy, especially in the context of semiconducting polymers. These materials play a crucial role in harnessing renewable energy from sunlight, either through photovoltaic processes to convert sunlight directly to electricity or photocatalytic processes to generate hydrogen fuel using artificial synthesis. Currently, the stability of such devices does not meet the requirements for commercialization. Therefore, *in operando* studies of device's failure mechanism are crucial. Neutron-based studies will be essential for advancing human-machine interfaces. Neutrons are non-destructive, making them highly adept at probing the microstructure under relevant biological conditions. A unique feature of neutrons is their unparalleled capacity to aid in the design of soft, biocompatible semiconductive materials. In the field of bioelectronics, neutrons offer a valuable means to investigate the morphological changes in bioelectronic devices and to analyze the ion distribution as it relates to alterations in electronic properties. Conducting such *in operando* studies with other morphological characterization methods is impractical primarily due to the need to operate the device while immersed in electrolytes. A new reactor with high brightness and a smaller beam size (mm range) could enable grazing incidence neutron scattering measurements that would effectively explore the interface between functional electronics and liquids. Lastly, as the need to store ever-expanding volumes of information continues to evolve, transitioning beyond established magnetic techniques toward information storage using soft matter becomes increasingly important. Neutrons offer an unmatched ability to examine the spatial distribution of elements when combined with selective isotopic labeling, further emphasizing their significance in this context.

1.3.3. Microelectronics and semiconductor manufacturing

Neutron science will enable the development of extreme ultraviolet (EUV) lithography technologies including the novel resist materials essential for maintaining U.S. leadership in semiconductor manufacturing, a goal of the CHIPS and Science Act. In EUV lithography, imaging materials are exposed to high-energy photons with a wavelength of 13.5 nm. Current EUV tools are capable of 24 nm full pitch, and next-generation tools, ‘hyper’ NA EUV, may be able to deliver exposure contrast at 8 nm full pitch. While there have been significant advances in EUV tools, the development of novel resist materials has lagged and the most widely used resist materials for EUV are the chemically amplified resists originally developed for photolithography. Unfortunately, these materials do not perform well at the small length-scales of EUV lithography leading to patterns of low quality and high roughness.

Neutron-based techniques will be crucial for resolving the nanoscale structure of resist materials throughout the EUV exposure process. Resist materials are typically comprised of macromolecules containing mostly light elements such as carbon, hydrogen, and oxygen intermixed with heavy metal-oxides, making neutron-based probes well-suited for materials characterization. Through isotopic-labeling, the molecular-level heterogeneities at the nanoscale throughout the resist layer can be resolved via neutron scattering. Since EUV patterns at the molecular level, nanoscopic concentration fluctuations can lead to large structural fluctuations and unacceptable pattern roughness. Critical-dimension small-angle neutron scattering (CD-SANS) is uniquely suitable for resolving the nanoscale structure of patterns after EUV exposures in three dimensions to uncover the structural evolution of pattern formation. The development of new lithography and patterning technologies aided by neutron techniques are necessary for the United States to compete with international semiconductor manufacturers.

1.3.4. Advanced medicines

Neutron science will address challenges associated with an aging population that desires an improved quality of life, personalized medicine, and increasingly improved treatments for disease. Accordingly, there is a significant drive within the soft-matter research community to understand the structure of biological molecules in complex environments. The recognition of lipid nanoparticles as drug delivery vehicles has revolutionized targeted delivery of biopharmaceuticals. Understanding how these molecules (RNA, DNA, proteins) change conformation during packaging and delivery will be central to therapy development. Neutrons are the only way one can assess the details of biomolecule structure during delivery. The recurring theme of being able to tag isotopes selectively on complex molecules to permit detailed *in situ* characterization of structure in crowded environments is something that can only be done with neutrons due to their isotope sensitivity, the enhanced time and spatial resolution available at a new reactor, and the non-destructive nature of neutrons as a material probe.

Self-assembled structures (micelles, vesicles, etc.) are central to formulated products. Consumer products make up a significant fraction of the economy, and consumers are demanding sustainable, reliable, and inexpensive products, which requires constant materials innovation. During the processing of self-assembled materials, scientists are often blind to the changes that take place in the macromolecular structure. Neutrons are the only way to assess the details of internal structure of self-assembled materials, which define their function.

Neutron science will also provide a detailed understanding of interfaces in materials that occur between regions of different properties such as phase or composition. All applications in soft matter require the control and tuning of interfaces at equilibrium and kinetically trapped states to imbue desired material properties and functionality. A prime example is biological membranes; a nanoscopic thin film that fluctuates on the nanosecond timescale and remodels on the microsecond timescale to carry out all the complexities of life from reproduction to energy generation. Neutron scattering techniques are the only non-perturbing, non-destructive method that can provide atomic-scale resolution on interfacial systems under operational conditions. This unique capability will be crucial for transitioning from 20th-century approaches to ensuring human sustainability on Earth and beyond.

1.3.5. Sustainability

Neutron science will allow for the creation of sustainable polymeric materials by providing the capability to engineer macromolecules with atomistic precision. The unique capabilities of neutron-based techniques are crucial to the development of future sustainable polymeric materials that will have controlled depolymerization and repolymerization pathways.

The complete recycling of traditional polymeric materials is a challenge, as contemporary recycling methods predominantly rely on mechanical processes for simplicity and cost-effectiveness. Regrettably, this mechanical recycling often generates environmental pollutants, commonly known as "microplastics," with the potential to harm various organisms, including humans. Such is the scale of this issue that microplastic contaminants have been detected even at the peaks of the Earth's tallest mountains and in our food sources.

Neutrons can provide insights into novel synthetic procedures for producing advanced polymers or pathways for the chemical recycling and/or upcycling of common polymers. Widespread chemical upcycling not only represents a major technological breakthrough, potentially enabling the conversion of plastic waste into valuable medical resources, but it also presents a promising economic prospect for American industry. Future neutron investigations are poised to enhance our comprehension of the limitations inherent in existing cutting-edge technologies while laying the groundwork for the design and implementation of genuinely sustainable polymers.

Sustainability in soft matter is much broader than simply recycling or upcycling the materials and entails the creation of materials capable of being reprocessed without loss of mechanical strength. A prime example of this is in food packaging, particularly for fruits and vegetable produce, where polymer-based materials must create a breathing, responsive barrier for these living products. Current technologies based on rigid chemical crosslinks will be replaced by dynamic bonds with specified lifetimes. Neutron-scattering measurements, enabled by a new continuous high-brightness reactor at NIST, will be essential for developing such materials that will find use in next generation agricultural methods, food, water security, and packaging. These are key national security concerns that will become more pressing as the Earth's climate continues to change.

1.3.6. Computation and Computational Techniques

Neutron science will play an important role in benchmarking next-generation computational and theoretical methods. In the future, computational and theoretical methods for soft matter will likely implement high-level quantum-based techniques. The computational methods will go beyond Born-Oppenheimer surfaces and include both nuclear and electronic quantum effects. This is completely uncharted territory compared to the status quo, which relies on classical force fields, and the computational methods will have to be benchmarked and validated. Neutron science will play the key role as both structure and dynamics can be non-invasively measured for single molecules, on an atomic scale.

1.3.7. Need capabilities: automation, high-throughput, sample environments, isotopic labeling.

A new neutron reactor at NIST would provide higher flux to perform a much larger number of high-resolution experiments, thereby increasing our ability to address grand challenges and drive innovation. Broadening access to critical neutron tools, optimizing economic output per neutron, and increasing data reusability all demand automated, high-throughput measurements.

High-throughput modalities based on advancement in robotics will be further augmented by artificial intelligence and machine learning. This includes setting experimental parameters that can more efficiently probe the temporal and structural length scales of interest in soft materials. Automated high-throughput experimentation will also provide significant benefits by guiding new material formulation that can be made and tested on-the-fly after initial experiments have established a baseline.

New plug-and-play modular sample environments can be used to more efficiently exchange samples to reduce downtime and prepare new compositions with distinct structures informed by artificial intelligence models. This essential level of automation acknowledges how precious neutrons are, and will significantly increase beam efficiency, allowing their full power to be realized in the determination of soft material structure.

The power of neutron scattering is tremendously augmented by the ability to label regions of soft matter materials selectively with isotopic specificity. A deuteration and isotope facility would significantly increase the labeling capacity in the United States, which severely lags that of our international competitors.

2. Soft Condensed Matter Dynamics

2.1. Panel

Chairs:
Matthew E. Helgeson – *University of California, Santa Barbara*
Gerald J. Schneider – *Louisiana State University, Baton Rouge*

Panel Members:
Jacinta Conrad – *University of Houston*
Victoria Garcia-Sakai – *Rutherford Appleton Laboratory*
Jonathan Nickels – *University of Cincinnati*
Ryan Poling-Skutvik – *University of Rhode Island*
Jeremy Smith – *Oak Ridge National Laboratory*
Alexei Sokolov – *University of Tennessee*
Norman J. Wagner – *University of Delaware*
Yang Zhang – *University of Michigan*

Scribe:
Elizabeth Kelley – *National Institute of Standards and Technology*

2.2. Glossary of terms

Aging: Processes governed by slow (often intermittent) evolution of a material as it relaxes toward equilibrium.

Dynamics: Processes driven and characterized by fluctuations around a locally (meta)stable state of a material or system.

Electrolysis: a chemical change in an electrolyte, produced by an electric current.

Hierarchical: Structural and dynamical features that exist across multiple length and time scales and exhibit strong coupling across these scales.

Kinetics: Processes by which a material or system evolves along a trajectory through state or structure space.

Multimodal: Use of concurrent probes on a given sample, important as it is nearly impossible to measure a sample a second time under identical conditions. Multimodal can refer to either simultaneous measurements or sequential within the same experiment. Examples include dynamics and structure (QENS and diffraction), NMR and QENS, vibrational spectroscopy and Raman, MD and QENS.

2.3. Summary

Soft materials are materials comprised molecules and structures—including polymers, biomolecules, surfactants, and particulates—that are easily altered by thermal and mechanical forces. They are widely used in many technologies, from packaging to energy storage to medical devices and products. A differentiating feature of soft matter is the diversity of problems arising from the broad range of material classes involved, and the broad ranges of length and timescales that give rise to the important properties and processes. Designing soft materials with desired properties requires predictive understanding of the mechanisms controlling their structure and dynamics. *Dynamics*, i.e., molecular motions, rearrangements, and transport, are the critical phenomenon controlling major properties and function of soft materials, yet our understanding of soft matter dynamics, their cooperativity, and heterogeneity is very limited.

Neutrons provide unique opportunities to study soft matter dynamics due to their sensitivity to light elements (especially hydrogen) that are omnipresent in soft matter. In addition, neutron sensitivity to isotopes provides an opportunity to use labeling to measure the dynamics of targeted molecules or specific parts of molecules and is especially critical in multi-component systems. The wavelengths of neutrons are well-matched with the characteristic length scales in these materials, and the accessible time scales provided by neutron spectroscopy are a perfect match for dynamic phenomena on molecular and mesoscales and those from molecular simulations. Moreover, neutrons are non-destructive, even for sensitive samples, e.g., biological systems. Neutron measurements are therefore the key to coupling between dynamic time- and length-scales that determine the linear (equilibrium) and non-linear (out-of-equilibrium) macroscopic properties of materials and thus their functional performance.

Soft matter dynamics include multiple, often hierarchical, processes that strongly overlapping in their characteristic time scales. Studies of these dynamics require broadband spectroscopy. Neutron spectroscopy (NSE, QENS, INS) covers timescales from femtoseconds to microseconds, while SANS experiments can study processes/structural changes from the millisecond to longer times. At very short times scales molecular vibrations, rotations, and local rearrangements can be identified. Unlike many other techniques limited by specific selection rules, neutrons can provide a comprehensive view on these processes. Good overlap in accessible time and length scale with atomistic MD simulations enables neutrons to provide a powerful benchmark for computational modeling. Neutrons are also unique in their ability to derive fundamental thermodynamic quantities based on the determination of the vibrational density of states.

Slower motions can be measured by time-resolved small-angle (SANS) and wide-angle (WANS) neutron scattering, enabling the determination of motions of milliseconds and slower, and on the sub-nm to the micrometer range. These determine non-equilibrium processes created by external perturbations such as mechanical, electric, or magnetic fields, and aging phenomena. A typical example encountered in the plastics industry is various processes occurring while polymers are flow-processed, and their connection to material properties and their lifetimes. These phenomena are critical for most materials technologies, from additive manufacturing to production of turbines for wind power.

The non-destructive investigation of soft materials by cold neutrons enables unique measurements of dynamics without affecting the studied molecules and structures. Continuing the expansion of accessible time and length-scales will enable studies of more complex processes and phenomena. Though these processes have already been discovered with other techniques, only the combined length- and timescale resolution together with isotopic sensitivity provided by neutron spectroscopy can unravel microscopic details of underlying processes and phenomena. Advanced neutron scattering capabilities will enable development of predictive models and theory, advanced simulations including artificial intelligence and machine learning tools. Along with the anticipated continuing advances in computational technologies, these experiments will enable a unique view on materials and biomolecular processes that will revolutionize the pace of materials design.

2.4. Key Grand Challenges

2.4.1. Sustainable materials economy

A sustainable economy will require the development of tailor-made high-performance, upcyclable, low-carbon materials for manufacturing based upon biomass and new chemistries. This will involve large-scale additive manufacturing for future technologies in Energy Earthshot and similar applications. Primary materials are composites made from feedstock materials requiring rational design for processing capability, superior materials properties, and low production energy and cost. An innovation challenge is to harness the power of billions of years of evolution to design biomaterial composites that are significantly improved relative to materials currently in use. Examples of promising biomaterials are cellulose nanofiber-polymer nanocomposites, which have shown tremendous growth as promising material for high-performance sustainable AM (Additive Manufacturing) material design (Fig 1).

There has been very little work to obtain the fundamental understanding needed to rationally design high-performance materials for a circular (bio)economy. Neutrons, when combined with High-Performance Computing (HPC) techniques such as computer simulation and artificial intelligence (AI), will provide the required deep fundamental science understanding of dynamics, structure, and morphology of biomaterials with specific physical and chemical properties optimized for applications progressing towards a high quality decarbonized additive manufacturing industry. Neutrons are central to elucidate polymer conformations, interactions, thermodynamics and self-assembly and thus worldwide can be expected to play a critical role in deriving a foundational predictive understanding of these high-performance (bio) materials. Structure and dynamics, particularly at interfaces, determine mechanical properties and will need to be elucidated using the full range of reactor-based structural and dynamical neutron techniques. The unique contrast variation capability of neutrons will allow high-throughput experiments to exquisitely determine individual component structure, and dynamics at all length scales relevant to materials design will be able to be realized.

Figure 1. Illustration of cellulose nanofibers (green) embedded in a polymer matrix. Understanding the dynamics of these nanofibers together with the matrix motions is critical for designing optimized, sustainable, high-performance, thermoplastic biomaterial-polymer composites.
(Credit: Oak Ridge National Laboratory)

Of fundamental interest is the prospect of new theories for polymer systems with features associated with sustainable chemistries. Existing models fail to incorporate features such as chemical and structural heterogeneity associated with diverse, circular feedstocks (distribution of monomers, branching, polydispersity, additives/contaminants, etc.). For example, chemically specific, or reactive interactions can be engineered that alter conformational structure and dynamics. Also, the development of heterogeneous systems with novel interfaces, such as between membrane and material surfaces will require detailed dynamical exploration.

Accelerating the sustainable materials development cycle using neutrons will require the ability to screen the dynamics of large libraries of materials and solvents. This requires high-throughput measurements, necessitating advanced source and instrument design compared to existing instruments. Specifically, researchers will require expanded access to instruments (and suites of instruments: NSE, backscattering) capable of accessing a wide range of relevant length (1 Å to 10^7Å) and time (1 fs to 100 s) scales without gaps. To efficiently screen large chemical libraries and design spaces this also necessitates synergy with High Performance Computing (HPC) simulation/ Artificial Intelligence (AI) for sample planning, real-time experiment steering, force-field benchmarking, and interpretation of experiments.

The societal impact of these neutron capabilities will contribute to the development of predictive theories and models of material design, accelerating our progress to a sustainable manufacturing economy.

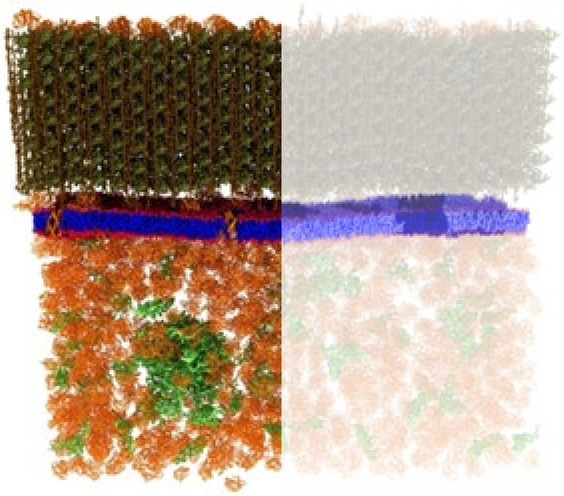


Figure 2. Biorefineries and fermentation processes play a key role in the emerging circular carbon economy. Neutron scattering and the ability to tune scattering length density enable detailed studies of the organisms involved. This image highlights the case of a B. subtilis bacterial cell in which all molecules present neutron contrast (left) and in which all cellular components except the cell membrane have been matched out (right). (https://doi.org/10.1371/journal.pbio.2002214)

2.4.2. Enabling the energy transition

The world faces existential challenges in the transition from fossil energy to renewable sources and accompanying efficient energy use. To address these challenges, we must enhance the performance and efficiency of next-generation energy production, conversion, and storage technologies. A fundamental aspect for many of these technologies are based on the transport of ions, protons, and small molecules through complex soft materials. Key areas of interest include ions in conventional and flow batteries, protons in fuel cells and electrolyzers, and separation of gases, particularly for carbon capture.

The scientific problems at the heart of this endeavor are multifaceted, but all depend on fundamental understanding of transport through, and dynamics of, soft materials. First, hydrogen production methods demand an understanding of molecular-scale processes encompassing high and low-temperature electrolysis, and innovative strategies involving biomass as a feedstock. Understanding the mechanisms controlling ion transport, especially multivalent ions, is critical for designing solid-state batteries, and for development of long-term energy storage systems. Second, for the development of materials optimized for efficient carbon capture and storage, a deep comprehension of the mechanism(s) controlling CO_2 transport through solvents/matrix is essential. Third, the production of biofuels and bioproducts from biomass necessitates a grasp of the principles behind lignocellulosic biomass deconstruction and fractionation. Importantly, in many of these contexts, we lack a comprehensive understanding of the fundamental mechanisms governing the transport of small entities (molecules, ions) and their coupling to the dynamics of matrix materials, including nanostructured and glassy materials, and polymer membranes/gels.

Neutrons are uniquely positioned to study dynamics and transport phenomena in soft materials. The accessible time/energy and spatial ranges provide good bridge between molecular/atomic scale phenomena and macroscopic properties of the studied materials. Neutrons are especially efficient in analysis of proton transport due to the high scattering cross section of the hydrogen atom.

To fully harness the potential of neutron science in advancing the energy transition, several needs must be addressed. First, the design of specialized sample environments and cells, along with instrument configurations for *in operando* (e.g., battery, fuel cell) measurements, is crucial. Second, there is a need for increased neutron flux and brilliance, coupled with improved detector signal-to-noise ratios to achieve spatiotemporal measurements with higher precision and sensitivity. Third, polarization instrumentation and analysis techniques are vital for separating coherent and incoherent scattering, allowing for the isolation and study of self- and collective dynamics. Fourth, smaller q-values (0.01 $Å^{-1}$ to 0.5 $Å^{-1}$) are required to access the relevant length scales for ion and charge transport, including scale of specific matrix nanostructures, ionic channels, etc. All timescales from 1 fs to hundreds of seconds need to become available closing the current gap between 1 µs to 1 ms.

The anticipated benefits of advancing neutron science for the energy transition are far-reaching. Industry standards to continue to develop more efficient energy production, storage, and conversion technologies, along with the discovery of novel routes, resulting in reduced energy use and reduced environmental impact. Society will benefit from the transition to cleaner and more sustainable energy sources, with reduced greenhouse gas emissions and a decreased reliance on finite fossil fuel resources. Additionally, innovations in hydrogen production, carbon capture, and biofuel production will contribute to a more sustainable and resilient energy infrastructure, ultimately improving the quality of life for people worldwide.

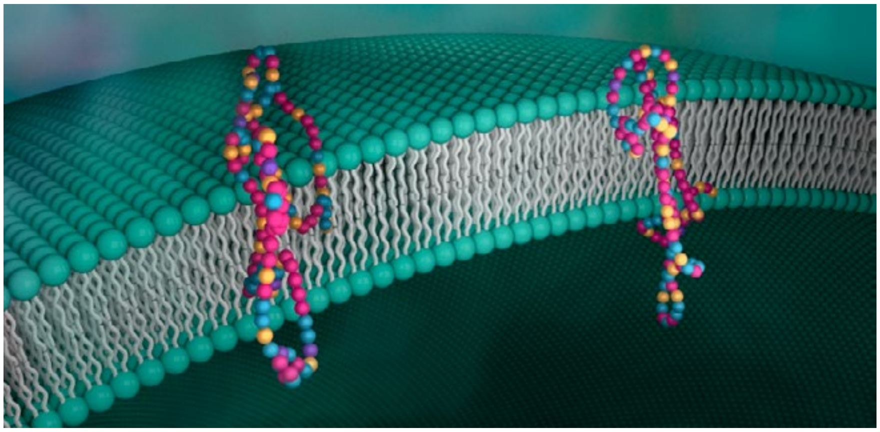


Figure 3. Novel synthetic materials excel compared to natural membranes and can withstand harsh environments. Such materials will have superior properties, long lifetimes, and unprecedented advantages. The molecular mechanism to design such materials are being developed by the help of neutrons (Credit: ORNL/Jill Hemman)

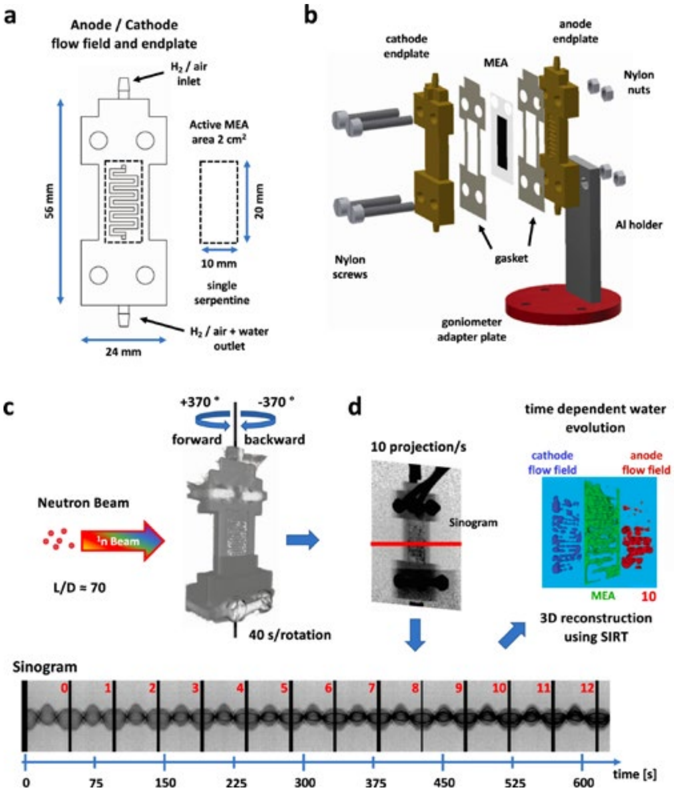


Figure 4. High-speed 4D neutron computed tomography for quantifying water dynamics in polymer electrolyte fuel cells provides a unique view in the inside of processes in materials that determine the energy transition toward a clean and sustainable society. (https://www.nature.com/articles/s41467-022-29313-5)

2.4.3. Advanced materials manufacturing

Innovations in materials manufacturing are pivotal for creating a resilient and sustainable national infrastructure. Next-generation manufacturing must achieve the production of high-performance materials with improved scalability, throughput, energy efficiency, and cost-effectiveness. This endeavor hinges on the discovery and design of advanced processing methods capable of rapidly pushing materials far from equilibrium to unlock optimized structures and properties. These methods often involve manipulating materials through various fields, such as flow, electrical/magnetic/light fields, extreme or rapidly changing pressures and temperatures, and chemically reactive processes. Understanding the intricate interplay between these driving fields and molecular or meso-scale dynamics is crucial to control advanced materials processing. Additionally, predictive models are essential to explain the dramatic changes in dynamics and aging of materials subjected to these processes.

Two primary scientific challenges impede progress in advanced materials manufacturing. The first challenge involves unraveling the complex interplay of driving fields with molecular and meso-scale dynamics, especially how fluctuation-driven processes are modified out of equilibrium. The second challenge is to gain a deeper understanding of the dynamics and aging of materials far from equilibrium to enhance material stability and properties. This entails studying phenomena like glassy dynamics in amorphous solids, complex coarsening, and phase separation processes, as well as intermittent or avalanche-like dynamics.

Neutron science offers a unique set of tools to address these scientific challenges. Neutrons enable non-destructive probing of structure and dynamics within processing equipment and devices. Techniques like quasi-elastic neutron scattering (QENS), inelastic neutron scattering (INS) and neutron spin echo (NSE) cover a broad range of time and length scales, from individual molecules and particles to collective/mesoscale dynamics of molecular assemblies and phase-separated domains.

To make optimal use of neutron science for advanced materials manufacturing and underlying scientific research, several advances in neutron instrument design and operation are necessary:

- **Access to Samples**: Augmented experiments require access to samples not commercially available, including isotopically labeled materials, to take full advantage of the capabilities of neutrons.
- **Increased Neutron Flux:** To enable “one-shot” kinetic measurements, tracking dynamics in response to time-varying fields.
- **Enhanced Beam Brilliance and Coherence:** Supporting spatially resolved and speckle-based measurements, bridging the gap between QENS/NSE and time-resolved small-angle neutron scattering (SANS).
- **Flexible Instruments:** Capable of automatically alternating between low-resolution kinetic monitoring and high-resolution broad-spectrum measurements.
- **Advanced Sample Environments:** Including hardware for beamline integration and software for synchronous and automated sample actuation and data acquisition.
- **Multi-Measurement Methods:** Combining neutron measurements with other techniques for diverse dynamical information.

- **Polarization Instrumentation:** To isolate individualistic and collective dynamics.
- **Measurement automation:** Incorporating data reduction/analysis with machine learning and automated instrument control for efficiently scan vast process parameter spaces.

These advances in neutron science will enable the development of next-generation materials with enhanced properties and scalable manufacturing processes. This encompasses structural and engineering materials including concrete, plastics, and molecular glasses, engineered for superior performance and minimal energy consumption. Moreover, it includes the creation of standardized processing equipment to make a variety of materials by changing the programming of driving fields, thereby realizing adaptable and scalable manufacturing methods to address prompt societal needs as they arise, such as vaccine development, infrastructure investment, and transportation electrification.

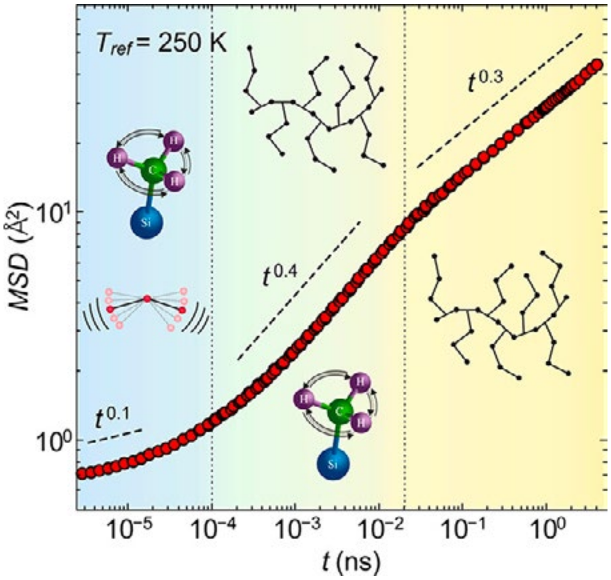


Figure 5. Polymers and proteins are highly flexible complex macromolecules with structures from the molecular scale to the material that we can see with our eyes. Some of the small molecules move very fast and move a million times during the blink of an eye, while others move so much slower than we can observe. Neutrons are one of the most powerful tools to identify a single molecule and to follow these motions over an extremely broad range. The information about the structure and the dynamics enables the discovery of new materials. (10.1021/acs.nanolett.1c01379)

2.4.4. Nature-inspired materials design

Biology has evolved to create precise and adaptable materials with unusual or extreme combinations of properties that are currently unattainable by modern synthetic techniques. Future materials innovation will require an understanding of how biological systems introduce and refine functionality in complex multi-component materials and how to exploit these mechanisms to generate synthetic materials that self-assemble and move to achieve unprecedented performance.

Bioinspired design has the potential to produce materials with unprecedented performance (Figure 6). Realizing this potential requires addressing two essential scientific questions: (1) *How do the molecular-scale motion and dynamics of biomolecules trigger nonlinear/irreversible properties/processes in biological systems?* and (2) *How can these biological mechanisms be translated into synthetic analogues?* Examples of biological motifs that have been identified as exciting potential targets for translation into synthetic materials include:

- **Sequence-defined chemistry:** precision amino acid sequences control the flexibility, self-assembly, and performance of peptides and proteins,

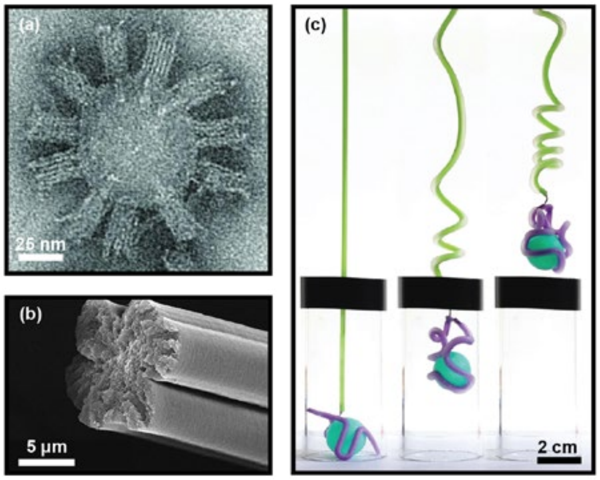


Figure 6. Examples of bioinspired materials capturing micro- to macroscopic function. (a) Synthetic ion channels fabricated from DNA origami exhibit gating responses that mimic the response of the biological ion channel α-hemolysin and can be used to detect single-DNA molecules. (DOI: 10.1126/science.1225624) (b) Amyloid peptides fused with flexible bioproteins form fibers that exhibit mechanical properties (tensile strength and toughness) exceeding those of many natural spider silks (DOI: 10.1021/acsnano.1c02944).

- **Spatiotemporally controlled and sequenced processing:** sequential translation of mRNA into proteins defines a unique energetic pathway resulting in precise structures,
- **Hierarchical 1D/2D/3D/4D assembly:** the dynamic self-assembly pathways of proteins and other biomacromolecules from linear sequence to spatial organization lead to temporally specific and selective functionality,
- **Active processes and materials:** biological species exploit ATP and chemical cycles to power locomotion and dynamic restructuring of their local environment, and
- **Nonlinear processes and function:** the collective nanoscale dynamics underlying signaling pathways generate macroscopic, nonlinear responses to subtle changes in environmental stimuli. **Deuterated materials:** Deuterated materials in amounts that enable experiments to explore the fundamental properties.

Neutrons access structural and dynamical information across a range of scales to enable comprehensive characterization of materials with hierarchical structure and processes. Thus, neutron scattering plays a unique and essential role in resolving how dynamics initiate and transduce processes across length scales, from single molecules (Å-nm) to assemblies (nm-μm) to the macroscale (mm+), to generate lifelike function.

Increases in neutron flux enable smaller sample volumes, such that neutron measurements on precious and expensive biological and bio-inspired substrates are financially feasible. Associated needs include (i) sample environments in which to trigger (bio)chemical activity and kinetically monitor the resulting dynamical response; (ii) multimodal measurements of structural, dynamical, and functional responses in a material; and (iii) capability to deuterate or isotopically label individual molecules or structures to isolate their scattering in a complex multicomponent assembly. Finally, widespread adoption of dynamic techniques requires expanded, reliable, and rapid access to instrumentation across a diverse (and potentially non-expert) user base.

Using neutrons to inspire and implement biological motifs into synthetic materials will lead to control over the nanoscale dynamic mechanisms that generate macroscopic responses, resulting in autonomous, self-healing, and responsive materials with improved reliability, reduced maintenance, scalable production, enhanced safety, and facile integration with living systems.

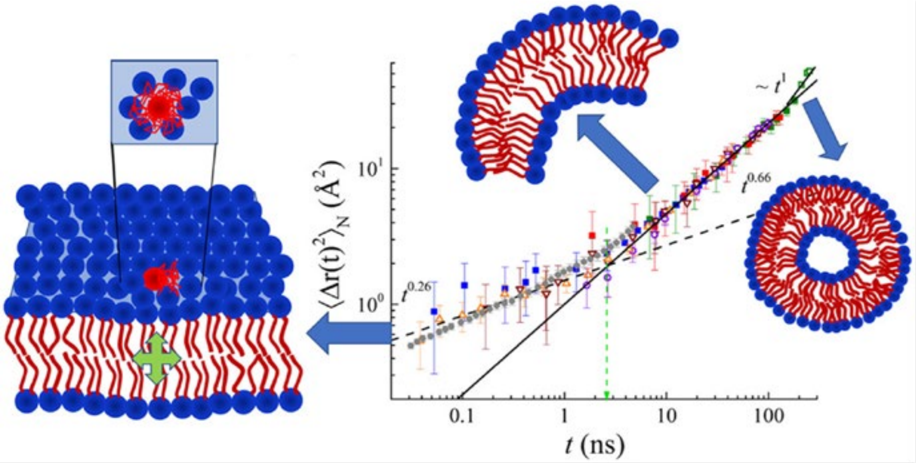


Figure 7. The role of membrane undulations is vital for many biological processes, including membrane protein activity. Experimental data, such as that obtainable from neutron spin-echo spectroscopy, are essential for developing a theoretical description of these collective dynamical processes in more realistic lipid bilayers, such as those containing asymmetric lipids, for which current theories are invalid. [https://pubs.acs.org/doi/full/10.1021/acs.jpclett.8b01008]

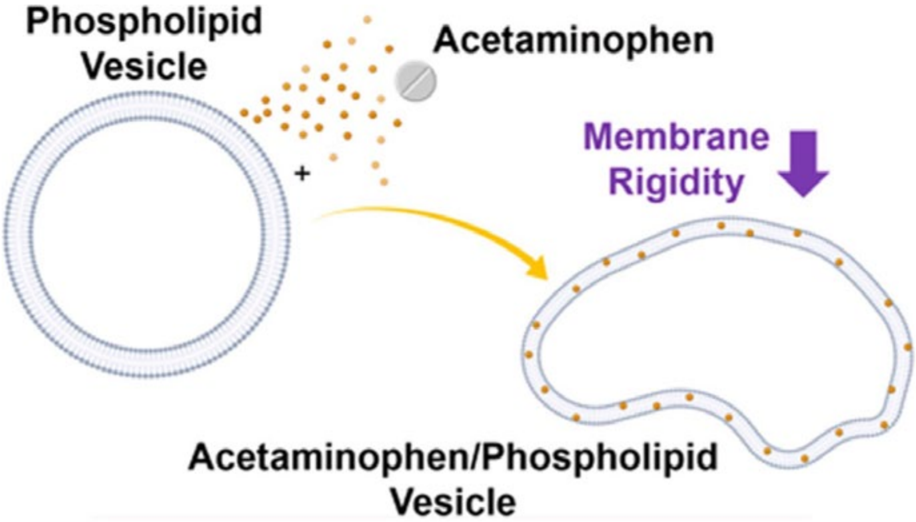


Figure 8. Vaccines are the new frontier in cancer immunotherapy. Personalized vaccines made from neoantigens (cancer-cell peptides mutated from those in healthy cells) are of particular promise. Dynamical fluctuations (shown) of cancer vaccine neoantigens when bound to cell-surface major histocompatibility complex receptors (green) directly determine their T-cell receptor activation and immunogenicity (tumor-destroying ability). https://pubs.acs.org/cms/10.1021/acs.langmuir.1c01458/asset/images/large/la1c01458_0009.jpeg

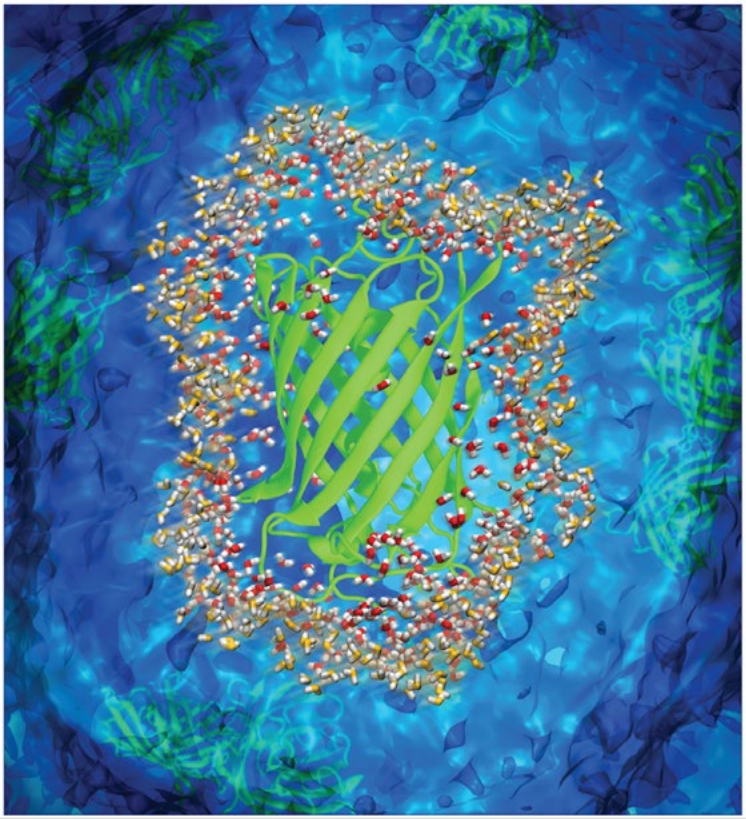


Figure 9. The stability of biologicals within pharmaceutical formulations is intimately tied to protein and solvent interactions. These interactions can be uniquely interrogated using neutron inelastic scattering methods. Techniques such as quasielastic neutron scattering study nanosecond/picosecond motions of water and small molecule additives while methods such as neutron spin echo are ideal to study protein diffusion and stability. Image: https://doi.org/10.1021/jacs.6b08845

2.4.5. Advanced medicine

The future of medicine is marked by a transformative shift towards targeted, personalized therapies and diagnostics. This paradigm change hinges on gaining a more comprehensive understanding of the mechanistic aspects of molecular biophysics and its role in disease. While ‘omics and other medical data have hitherto mostly been interpreted with analytics and non-physical approaches, it has become clear that to optimize utility such biological data need to be translated into 3D structure, dynamics, and mechanics on wide ranges of length- and timescales. Neutron scattering will be pivotal in obtaining the required predictive understanding.

Opportunities in this area include the development of next-generation biopharmaceuticals and macromolecular therapies that can affect biochemical processes underlying various diseases. Importantly, the dynamics and formulation stability of these therapeutics may be as important as their molecular structure. Some notable challenges include:

- **Development of Molecular Therapies:** The quest to develop new and better molecular therapies that are targeted to specific diseases. This includes addressing the behavior of monoclonal antibodies (mABs), disordered proteins (IDPs), oligonucleotides, and related macromolecular complexes. Also, changes of target dynamics on ligand binding determine drug affinity and neoantigen fluctuations in cell-surface receptor binding sites determine cancer vaccine immunogenicity. Correlated motions drive the allosteric changes that determine drug activity in G-protein coupled receptors.

- **Product Formulation and Stability:** Addressing the formulation and stability of biomolecular therapies, particularly mABs, which are at the forefront of therapeutic innovations.

- **Design of Engineered Delivery Vehicles:** Developing engineered delivery vehicles for biomolecules, such as messenger RNA (mRNA) encapsulated in lipid nanoparticles (LNPs) and investigating their interactions in formulation and ultimately *in vivo.*

- **Engineering Interactions:** Studying the interactions between therapeutics and biological interfaces, which include interactions with membranes, membrane-bound species, and tissues.

To tackle these grand challenges effectively, a profound understanding of the structure **and dynamics** of (bio)macromolecular structures is crucial, as they dictate their function and macroscopic properties. This understanding is particularly pertinent for proteins, lipid membranes and synthetic self-assembled entities.

The primary reason neutron scattering plays an indispensable role in addressing these scientific problems is its sensitivity to hydrogen, which constitutes a large proportion of the atoms in these systems. Hydrogen atoms not only mediate hydrogen bridges that are essential for defining 3-D structures, but they also contribute to the complex energy landscape of proteins, their conformational flexibility and biological molecular activity more generally. The strong interaction of the neutron with hydrogen, and differences with deuterium, enables the isolation of dynamical signatures from individual components within complex biological milieus and formulations and aids achieving a description of the dynamical processes.

Neutron science is ideally suited to probe molecular structures and dynamical behavior since they cover the wide relevant length and time scales. Neutrons uniquely probe the structure and dynamics of biomolecular structures, including proteins, lipid membranes, and more. This knowledge is vital for unveiling the molecular mechanisms underlying disease. Neutrons can also distinguish and isolate specific signatures from individual components within complex systems via H/D contrast, which is invaluable for discerning the contributions of different elements to biological function.

Meeting the demands of advancing medicine using neutron scattering will require:

- **Higher beam flux and better collimation:** to enable routine dynamical measurements on lower-dimensional materials, such as supported membranes, to resolve both in-plane and out-of-plane dynamics; to enable handling smaller sample volumes more in line with that available in the medical community.

- **Sample environment capabilities:** appropriate sample cell design and sample environment equipment to enable control of parameters with high precision and stability, such as humidity or cryogenic temperatures, without compromising signal to noise ratios. High throughput sample environments coupled with concurrent data analysis and ML/AI methods are desired especially for QENS.

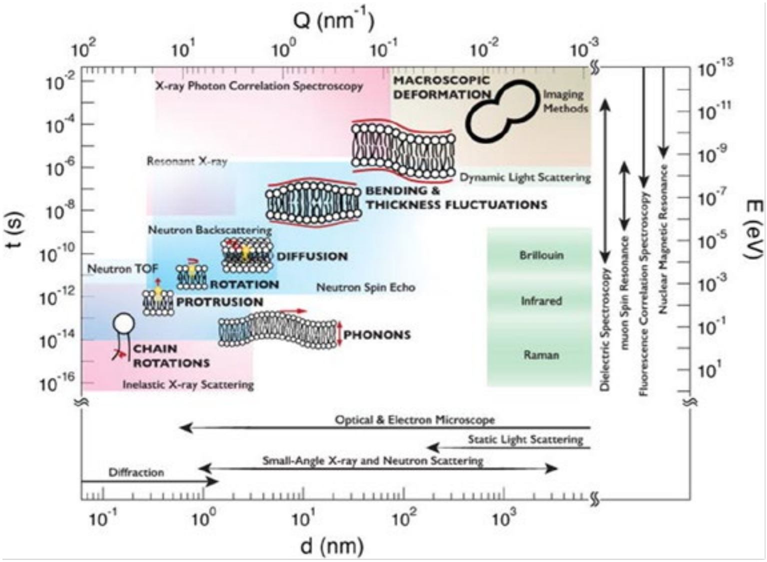
- **Deuteration facility:** to support the selective deuteration of libraries of biomolecules to facilitate the isolation and screening of specific biomolecular and biomolecule-material interactions.

- **On-site characterization and sample preparation infrastructure** and facilities appropriate for biomolecular research, with dedicated laboratory space and equipment, including sample synthesis.

The enhanced understanding of the dynamical properties of biomolecules applied to advanced medicine promises significant benefits for fundamental soft matter science, industry, and human health. These include:

- **Soft Matter Science:** Understanding the nanoscale dynamics of complex macromolecules and macromolecular assemblies in formulation and *in vivo* using the unique capabilities afforded by neutrons will lead to new directions of scientific inquiry and possibly, new rules for the development of therapeutics.
- **Innovative Medicines:** The use of this understanding will promote the development of fundamentally new therapeutics that target specific biomolecular processes, which promises more effective and tailored treatments for a wider range of diseases with fewer side effects.
- **Improved Drug Formulation:** Enhanced capabilities in formulating and stabilizing biopharmaceuticals will greatly improve the safety and efficacy of drug products and dramatically lower the cost of health care (e.g., moving to syringeable formulations as opposed to IV delivery). This also opens up the opportunity to sell therapeutics in markets with limited medical infrastructure.
- **Precise Drug Delivery:** Designing delivery vehicles that can precisely target biological processes and interfaces, optimizing drug delivery, and minimizing side effects.
- **Accelerated Research:** Accelerating the pace of research in the fields of biopharmaceuticals and macromolecular therapies, advancements in healthcare, where a deeper molecular understanding of drug function can also accelerate approval and market availability with significant health and economic benefits.
- **Economic and Societal Advancements:** Although advanced medicines can initially increase drug costs, they contribute significantly to economic growth, job creation, and innovation. The net economic benefits are associated with improved health and well-being of the population.

In total, the use of neutron scattering to interrogate the dynamics of biomacromolecules, and complexes used in medicine holds great promise as a novel route for developing advanced therapeutics that can be tailored to individuals, are more stable in formulation and delivery, and significantly improve human health, with all of the associated economic benefits. While such therapeutics are often initially expensive, their greater efficacy, reduced side effects, greater accessibility in broader markets and enhanced efficiency in delivery and outcome can significantly lower overall health care costs while greatly improving the general health of the population.

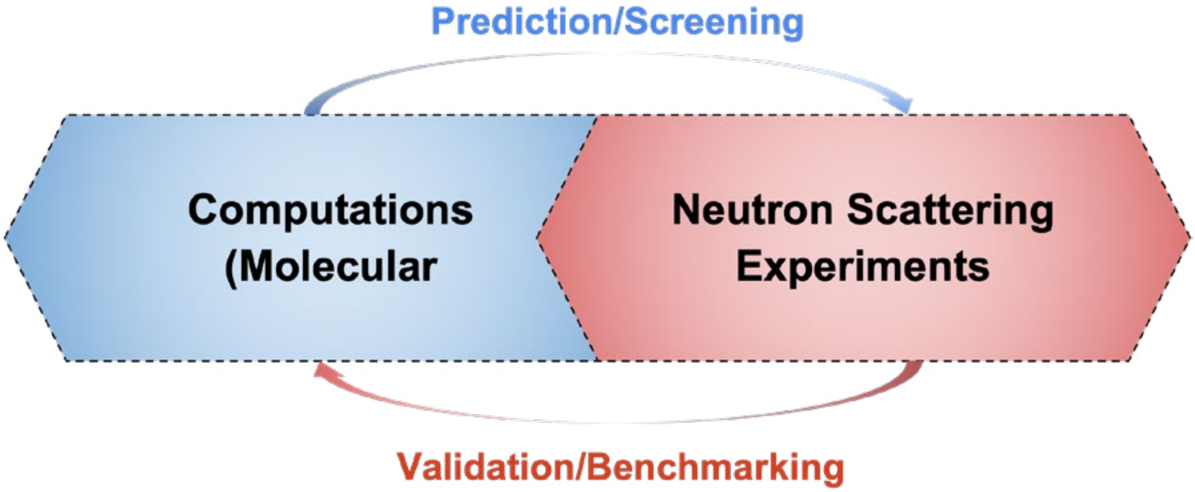


Nagao and Seto, *Biophys. Rev.* **4**, 021306 (2023).

The length (*d*) and timescales (*t*), and the corresponding momentum (*Q*) and energy (*E*) transfers, covering the hierarchy of membrane dynamics. The range of interested length scales in lipid structure study is covered by a variety of scattering and microscopic techniques as shown in the bottom of the figure. The dynamic ranges of the spectroscopic techniques available to measure the different dynamics are also shown, with neutron techniques as light blue, x-ray in magenta, light in green, and fluorescence and optical imaging techniques in orange. Spectroscopic techniques, such as dielectric spectroscopy, muon spin resonance, nuclear magnetic resonance (NMR), and fluorescence correlation spectroscopy, access a broad range of timescales without any specific associated length scales.

Figure 10. Spatiotemporal mapping of the hierarchical dynamical processes that take place in lipid membranes alongside the analytical tools available to probe these membranes. For an animation of the dynamics of the membrane, see https://www.nist.gov/video/cell-membrane-viscosity

2.4.6. Aiding computationally-driven materials design



The emergence of High-Performance Computing (HPC) and Artificial Intelligence (AI) are transformative technologies that are already revolutionizing materials design and development. Current methodologies have made significant strides in predicting and inversely designing material structures through efforts such as the Materials Genome Initiative (https://doi.org/10.1038/s41524-019-0173-4), yet these methods often struggle to predict the dynamics and emergence of continuum-scale properties of materials, especially those exhibited out of equilibrium. Realizing the full power, flexibility and creativity of emerging computational tools requires not just structure, but *dynamics*, benchmarks to train, constrain, and validate emerging computational and AI methods (https://doi.org/10.1021/acs.chemrev.0c01111 and https://doi.org/10.1016/j.jmst.2020.01.067).

A primary challenge in this area is to develop physics-informed and experimentally validated computational models that are able to capture and predict the dynamic properties of soft matter across a broad spectrum of length and time scales. Understanding and predicting the properties of soft materials demand benchmarking against real-world observations. Neutron scattering cover an umbrella of elastic and inelastic techniques that can directly measure the space and time correlation functions at the length and time scale comparable to molecular simulations. These measurements serve as direct and critical benchmarking tools to establish reliable computational models and force fields for a variety of soft materials.

An additional challenge is to identify opportunities for AI/ML-assisted experiments, especially with neutron scattering measurements where the source neutrons are precious relative to other radiation sources. Specifically, there is a need to identify how computations, including AI techniques, can aid real-time planning, operation, analysis, and even interpretation of neutron scattering experiments. Despite the advantages of neutron scattering, it is generally not considered as an easily accessible high-throughput materials characterization tool. This is partly due to the limited access to neutron facilities, but also due to the time needed to plan for experiments as well as the analysis of the experimental data. Computational predictions and screening can help narrow down the search space and identify key samples to be measured experimentally. Computations can also help the analysis and interpretation of the experimental results, which can assist scientists with real-time decision-making.

In the field of molecular modeling, benchmarking and validation against experimental data are crucial to develop and validate standardized force fields and atomistic models. Currently, computational tools are not routinely parameterized against experimental observations of molecular motions, leading to inaccurate reproduction of important equilibrium dynamics in soft materials. This inhibits the potential of such methods to predict important emergent phenomena. To address this shortcoming, accurate determination of many types of molecular motion against which simulation outputs can be compared is necessary.

Neutrons are uniquely well-suited for this task as they provide a unique way to access the large range of time and length scales important for determining the hierarchy of structures and dynamics in soft materials. Neutrons are also particularly well matched to computational outputs, probing an overlapping time and spatial window. In light of these convergent time and length scales, neutron scattering has a central role in providing experimental truth for new computational developments (DOI 10.1088/2399-6528/ac9728).

There is a strong need within the community for standardized observations of structure and dynamics against which computational models can be validated. The establishment of 'NIST Standard' benchmarks of structure and dynamics observation at a range of fixed temperatures and pressures for a set of materials would provide the research community with common benchmark data which models must accurately predict. This would help to improve the accuracy and reliability of molecular models, ultimately leading to better understandings of the behavior of soft materials.

To harness the full potential of neutron scattering in aiding computationally driven materials design, several crucial needs must be addressed:

- **Dynamical measurements covering a wide range of time scales:** A combination of neutron scattering techniques like Quasi-Elastic Neutron Scattering (QENS), Inelastic Neutron Scattering (INS), and Neutron Spin Echo (NSE) must be employed to gather dynamic information over the broadest possible range of length and time scales. This wealth of data will provide critical insights into materials' behavior under various conditions.
- **Reference sample libraries:** The development and curation of reference sample libraries are essential. These libraries will serve as a foundational resource for researchers, enabling them to compare computational predictions with real-world observations, ultimately refining their models. These reference samples include isotopically labelled materials to enable advanced simulations.
- **Increased measurement resolution:** Achieving an excellent Signal-to-Noise Ratio (SNR) is paramount. High measurement resolution is needed to ensure the precision required for generating reference datasets. Improved SNR will lead to more accurate and reliable data, bolstering the quality of benchmarking.
- **Software Workflows:** The development of software workflows that directly connect computational simulations with neutron scattering data is crucial. Tools like SASSENA (https://doi.org/10.1016/j.cpc.2012.02.010), MDANSE (Molecular Dynamics Analysis of Neutron Scattering Experiments) (https://doi.org/10.1021/acs.jcim.6b00571) and LiquidLib (https://doi.org/10.1016/j.cpc.2018.03.005) bridge the gap between simulations and experiments, facilitating seamless integration.

The integration of neutron scattering based standards into computationally driven materials design workflows holds immense promise to converge more accurate outputs for material design. Through understanding of critical dynamical processes within materials industry stands to benefit from accelerated materials discovery and optimization, leading to enhanced product development, reduced costs, and improved sustainability. Society more broadly will benefit from innovations in areas such as renewable energy, healthcare, and transportation, all underpinned by advanced materials with tailored properties.

In sum, the potential for neutron scattering to ground computationally driven materials design presents a compelling opportunity to advance a grand challenge in materials science, and usher in an era of unprecedented materials innovation with profound implications for industry and society.

3. Bioscience

3.1. Panel

Chairs:
Frank Heinrich – *Carnegie Mellon University*
Hugh O'Neill – *Oak Ridge National Laboratory*

Panel Members:
Maria Monica Castellanos – *AstraZeneca*
Nicholas J. Clark – *Amgen Inc.*
Kushol Gupta – *University of Pennsylvania*
John Hackett – *Florida International University*
Shuo Qian – *Oak Ridge National Laboratory*
Nairiti Sinha – *The Pennsylvania State University*
Olivier Soubias – *National Institutes of Health*
Susan Tsutakawa – *Lawrence Berkeley National Laboratory*

Scribe:

David P. Hoogerheide – *National Institute of Standards and Technology*

3.2. Glossary of terms

Antibodies: Y-shaped proteins that are produced by your immune system to protect you from harmful foreign bodies. Antibodies are also called immunoglobulins.

Biocomposites: Materials composed of biological components (such as fibers, resins, or other natural materials) combined with a matrix (often synthetic polymers) to create a new material with enhanced properties.

Deuterium Labeling: The process of replacing the hydrogen atoms in a material with an isotope of hydrogen, deuterium, to alter the neutron scattering properties of the material.

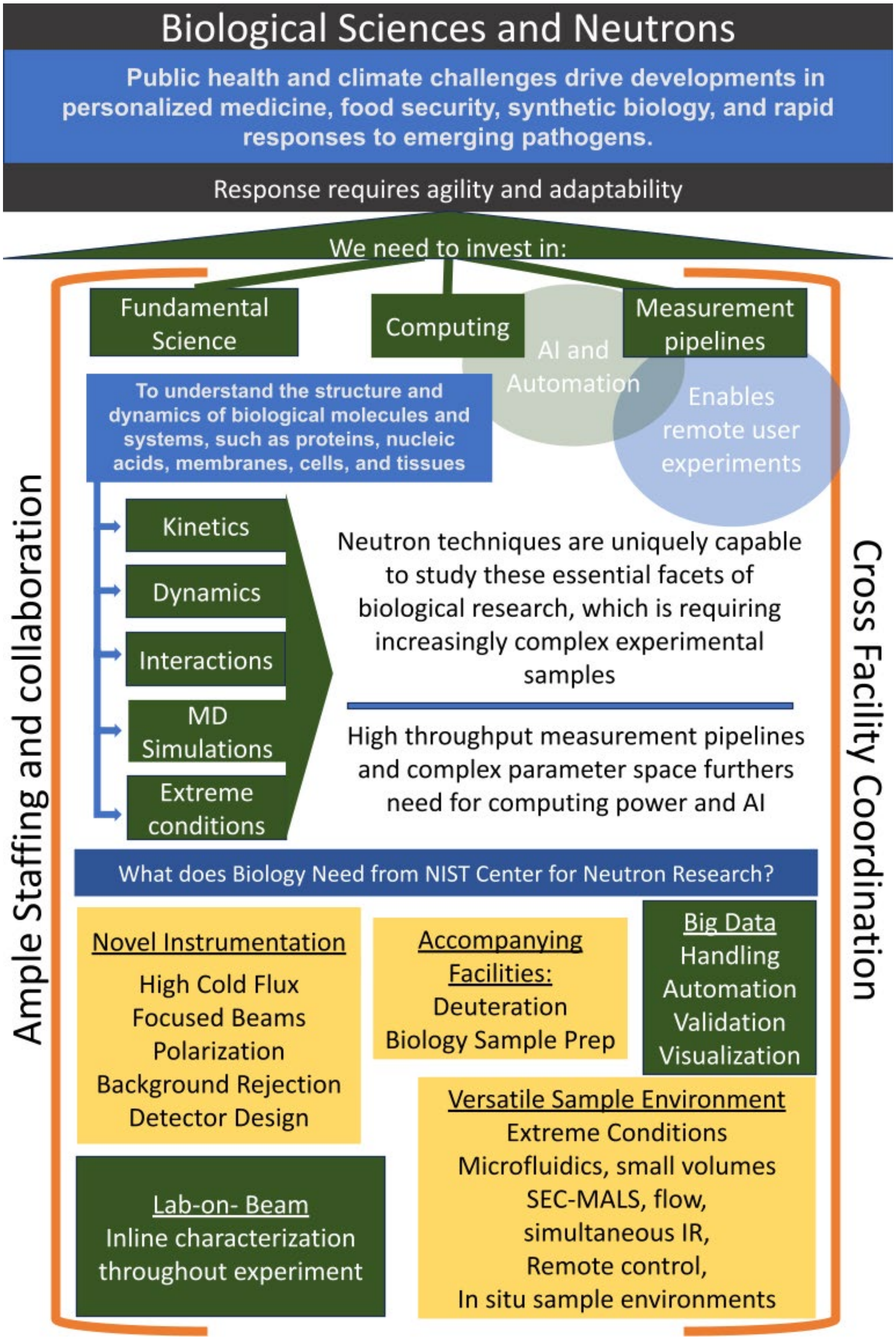
Isotopes: One of two or more atoms with the same atomic number but with different numbers of neutrons. Isotopes generally have similar material properties but can have different neutron scattering properties.

Multispecific Therapies: Therapies that utilize multiple bioactive materials to enhance the activity and effectiveness of the therapy.

3.3. Summary

Over the past few decades, continuous investments in facilities, instrumentation, and methodology have positioned biological neutron scattering as a powerful tool to tackle current and future scientific challenges aligned with U.S. national research priorities. Neutron scattering has become integral to the biomedical sciences, biotechnology, and fundamental research. To sustain and enhance its relevance, the panel underscores the necessity for biological neutron scattering to bolster its readiness for national emergencies, adapt to evolving manufacturing and technological landscapes, leverage revolutionary developments in artificial intelligence, and conduct groundbreaking research that unveils new opportunities for neutron users. We advocate for strategic investments in lab-on-beam instrumentation, which would integrate neutron scattering with complementary sample characterization and enhance the flexibility of our research operations. We propose investing in automated, high-throughput beamlines that cater to the biotechnology sector and align with emerging artificial intelligence and machine learning approaches. We recommend advancing fundamental research and method development in neutron measurements of kinetic processes and molecular dynamics, thereby enabling future research directions. Targeted investments in advanced instrumentation, facility support, and research methodologies at the NCNR and in collaboration with other scattering facilities will ensure the continued development and adaptability of biological neutron scattering, fortifying its vital role across various research domains and national initiatives.

Graphic Abstract



Biological Sciences and Neutrons

Public health and climate challenges drive developments in personalized medicine, food security, synthetic biology, and rapid responses to emerging pathogens.

Response requires agility and adaptability

We need to invest in:

Fundamental Science

Computing

Measurement pipelines

AI and Automation

Enables remote user experiments

To understand the structure and dynamics of biological molecules and systems, such as proteins, nucleic acids, membranes, cells, and tissues

- Kinetics
- Dynamics
- Interactions
- MD Simulations
- Extreme conditions

Neutron techniques are uniquely capable to study these essential facets of biological research, which is requiring increasingly complex experimental samples

High throughput measurement pipelines and complex parameter space furthers need for computing power and AI

Ample Staffing and collaboration

Cross Facility Coordination

What does Biology Need from NIST Center for Neutron Research?

Novel Instrumentation
High Cold Flux
Focused Beams
Polarization
Background Rejection
Detector Design

Accompanying Facilities:
Deuteration
Biology Sample Prep

Big Data
Handling
Automation
Validation
Visualization

Versatile Sample Environment
Extreme Conditions
Microfluidics, small volumes
SEC-MALS, flow,
simultaneous IR,
Remote control,
In situ sample environments

Lab-on- Beam
Inline characterization throughout experiment

Credit: Megan Mitchell

3.4. Current Status of Biological Neutron Scattering

3.4.1. Neutrons in Biology

Neutrons are discriminating, non-destructive, and deeply penetrating, and therefore, an ideal probe for applications in biosciences, probing a wide range of length and time scales using a combination of elastic and inelastic scattering techniques. It allows *in situ*, time-resolved (seconds to minutes) studies under native conditions. Several properties of neutrons and their interaction with biological matter led to a widespread application, as identified by this panel and previously [1-3]:

- Neutrons are highly sensitive to hydrogen atoms, accounting for a significant fraction of a biomolecule's atoms.
- Neutrons are sensitive to nuclear isotopes. Therefore, the scattering properties of a biomaterial can be changed (*e.g.,* by isotopic substitution of deuterium for hydrogen) while having only a minor effect on the biochemistry. This isotopic labeling allows for resolving specific parts of a complex biomolecular structure. Neutron scattering is the only low-resolution technique that can provide structural information localized to individual components, allowing a targeted understanding of this structure and dynamics. Atomistic resolution of these assemblies is recovered through modeling and complementary data, e.g., from x-ray scattering, crystallography, or cryo-electron microscopy.
- Because neutrons do not disrupt atomic bonds, beam damage from neutron scattering experiments is minimal. The non-destructive nature of neutrons allows for a continuous study of samples under changing environments, such as using temperature ramps, freezing, shear, and adding co-factors. Thereby, complex and time-dependent industrial and biological processes can be studied under native conditions.
- Neutrons interact relatively weakly with the sample material, often reducing the number of scattering events experienced by a single neutron in a sample to just one. This phenomenon results in small systematic measurement errors and allows for a wide range of neutron-compatible materials for sample environments. In structural biology, this property allows for *in situ* characterization of biological processes using biomimetic environments.
- In biological molecules and assemblies, energy differences among states are often less than thermal energy; thus, samples comprise many independent states of varying occupancy. The weak interaction of neutrons with these materials produces an unbiased superposition of all such states. Neutrons are, therefore, optimal for studying flexible and weakly interacting systems.
- The range and versatility of neutron techniques allow for the non-destructive study of biopharmaceuticals either to study key intermediates from the manufacturing processes, relevant formulation conditions, or within the primary containers in which they are manufactured (vials, pre-filled syringes, and autoinjectors).

3.5. Science drivers in the biosciences

The panel and others [1-3] identified three major science drivers for current biological research with neutrons.

The need to understand the structure and dynamics of biological molecules and systems, such as proteins, nucleic acids, membranes, cells, and tissues.
Neutrons are powerful and versatile probes that can reveal the atomic and molecular details of biological materials, such as their shape, size, orientation, interactions, and motions. Neutrons can also distinguish between different isotopes of the same element, such as hydrogen and deuterium, which is useful for studying hydrogen bonding and exchange processes in biological systems.

Structural biology research with neutrons includes:

- Protein structure, particularly the chemical mechanism of enzyme active sites, and conformational and colloidal stability in solution under relevant stress conditions.
- The organization and dynamics of the bilayer lipid membranes that separate cells from their environment and enclose subcellular structures.
- Membrane proteins and protein complexes with bilayer lipid membranes.
- The organization of large molecular assemblies in solution.
- Elucidating the mechanisms of disease and thereby informing drug development.

The need to develop new biotechnologies and biomaterials and advance the biopharmaceutical industry.
Neutrons help characterize the properties and performance of traditional and novel therapeutic modalities (antibodies, multispecific therapies), vaccines (adjuvants, mRNA, lipid nanoparticles (LNPs)), and biomaterials (biopolymers, biocomposites, and biofilms) in fundamental, applied, and industrial research [4]. Current research fields and applications include:

- Engineered proteins with novel modalities require structure and dynamics measurements to establish structure-function relationships.
- Complex mixtures or assemblies of mRNA, LNPs, therapeutics for cell therapies, antigen-antibody complexes, and co-formulations require neutron scattering techniques as part of a broader characterization effort. This effort broadly advances the design, manufacturing, and delivery of therapeutics.
- The characterization of therapeutic proteins for use in medical diagnostics.
- The study of biologics in relevant formulation conditions, such as in buffered solutions with stabilizing excipients to optimize biopharmaceutical formulations and processes.
- Facilitating the development of novel nanoscale vehicles for drug delivery and gene therapy.
- Supporting screening for small molecules that alter or disrupt macromolecular assemblies.

- Investigate the properties of new proteins/enzymes from extremophiles that can be utilized in biomanufacturing and bioconversion applications.
- Study biopolymers and food components for developing robust food storage, handling, and supply mechanisms.
- Assessment of recycled biopolymers in support of a sustainable circular bioeconomy.

The need to address the challenges and opportunities of the 21st century.
National and global challenges such as COVID-19 and the climate crisis severely impact our daily lives and national economy. Current scientific and technological solutions are insufficient to solve current and future national problems of such magnitude. Neutrons contribute directly and indirectly to addressing those challenges:

- Further innovation in biotechnology by providing complementary structural and dynamics information for multi-modal analyses that enable structural tracking of individual components in a complex sample or product.
- Help advance health equity and biomedical innovation by supporting the development of diagnostics, vaccines, therapeutics, and biosensors.
- Help mitigate climate change impacts by supporting the development of clean energy solutions and bioremediation strategies.
- Promote American leadership in science and technology by supporting the innovation and entrepreneurship of the biotechnology sector, STEM education, diversity and inclusivity, and workforce development.

3.6. Techniques and instrumentation

Reference [2] identifies five major neutron scattering techniques supporting biological neutron scattering. Small angle neutron scattering (SANS) is used to characterize biomolecules and biological assemblies in solution at a resolution of ~10 Å. Neutron reflectometry determines the structure of thin biological interfaces and obtains one-dimensional structural profiles along the surface normal. Neutron macromolecular crystallography yields the structure of biomolecular (protein) crystals at atomic resolution. It distinguishes itself from x-ray crystallography by its ability to resolve hydrogen atoms that are critically involved in enzymatic reactions or energy transfer in proteins. Inelastic neutron scattering techniques, and prominently neutron spin echo spectroscopy, reveal the structural dynamics of biomolecules ranging from atomic motions to collective dynamics of biomolecules and their solvent.

Technique	Sample Form	Length (Time) Scale	Information
Small angle neutron scattering (SANS)	Soluble, powder	1 nm - 10,000 nm	Low-resolution structure, Validation of atomic models
Neutron reflectometry (NR)	Thin film	1 nm - 1,000 nm	Low-resolution structure
Neutron macromolecular crystallography (NMX)	Crystallized	0.1 nm resolution	Atomic structure
Neutron spin echo spectroscopy (NSE)	Soluble	0.1 nm - 100 nm (0.01 ns - 1000 ns)	Collective dynamics
Inelastic neutron scattering	Powder	0.5 nm - 5 nm (0.01 ns - 5 ns)	Diffusive dynamics

3.7. Challenges

The advantages and scientific potential of neutrons in the biosciences are tempered by a series of challenges identified previously [1-3] and by this panel:

3.7.1. Technical challenges

- Low flux of current neutron sources. A combination of large sample size, high sample concentration, or long data collection times are typical experimental requirements, limiting the applicability and accessibility of the technique to the broader bioscience community.

- Lack of automation in sample handling and data analysis. Low measurement speeds have led to an underinvestment in this area so far.

- Complex data analysis. Multicomponent systems such as biopharmaceutical formulations, protein complexes, or complexes with RNA and DNA pose difficulties in data analysis as the information the scattering experiment provides is often insufficient for a complete description of the biological system. Advanced modeling techniques of the scattering data and integration of complementary techniques are required and add to the complexity of the problem.

3.7.2. Infrastructure challenges

- Limited lab and staff support for biological experiments conducted by a traditionally non-scattering-affine community, limiting the number of projects a scattering facility can support.

- Lack of comprehensive biological and chemical deuteration facilities.

- Methods in biological neutron scattering are inaccessible, difficult to learn, and not taught as part of standard curricula. The expertise required for experimental design and data analysis is often not part of the biology or pharmaceutical curriculum.

Biological, biopolymer, and biocomposite materials differ in their requirements from other soft materials and pose particular challenges for neutron measurements:

1. Sample quantity requirements for measurements should be as small as feasible, as their availability is often limited.
2. Sample timing and handling of fragile systems are critical for successful measurements, such as loading into sample cells, sample stability (degradation), shipping, storage, controlling and assessing polydispersity.
3. The sample complexity, flexibility, conformational and assembly dynamics are often significantly higher than in soft matter samples.
4. Biological matter can be (biologically) active, requiring tight control over experimental variables (time, concentrations of small molecules such as ATP, RNAses, co-factors)
5. Sample quality and deterioration are exacerbated, requiring in-line sample validation and a biologically compatible sample environment.

The Strategic Investments recommended by this panel address many of the listed challenges, in addition to solutions suggested previously [1-3]. The Strategic Investments are also designed to address emerging challenges arising from long-term trends and external pressures, as detailed in the following section.

3.7.3. Biomolecular simulations

The distinct advantages of neutron scattering for the structural characterization of biological materials also make neutron scattering data particularly valuable for validating and calibrating simulations. The biomolecular simulation field is a rapidly growing, multi-billion-dollar industry with applications in drug discovery and screening [5]. However, discrepancies between simulated and experimentally determined structures have hampered the more widespread utilization of biomolecular simulations. In addition, accurate biomolecular simulations, especially when coupled with continued anticipated improvements in computing capabilities, would, in turn, provide new opportunities for advanced data analysis techniques for neutron methods.

3.8. Long-term Trends and External Pressures

The panel identified several trends and external pressures that will most likely persist into the foreseeable future. A new reactor source should be planned with these in mind; however, addressing these trends and pressures should start immediately:

1. The global research environment is **increasingly reacting to emergencies** and expects impactful applied research outcomes on short timescales. This development comes at a cost to sustaining long-term basic research, as evidenced in an increase in short-term, high-volume funding initiatives by national funding agencies and the U.S. government (e.g., brain and cancer initiatives, calls to address the COVID-19 global pandemic, CHIPS act). The panel feels that the current research infrastructure at the NCNR lacks the agility to address this trend, which is expected to be a key requirement for the design of future facilities over the next several decades. Furthermore, U.S. research priorities include

responding to public health crises and preparing for future threats from natural or engineered pathogens (see Societal Impact and National Benefits).

2. Biological neutron scattering studies involve **increasingly complex samples**. While this is not a new trend, its impact has reached a critical level. Due to the ensemble-averaging nature of neutron scattering experiments, the ability to separate neutron scattering contributions from individual components is reaching a technical limit and a concerted effort involving deuteration, complementary instrumentation, multi-modal measurements, and new measurement methods are required to overcome it. A solution to this problem is essential for supporting advancements in the biotechnology and biomedical sectors central to public health and economic growth, the food sciences, and addressing climate change (see Societal Impact and National Benefits).

3. The last years have seen the advent of transformative changes to U.S. research triggered by an explosion in performance of **machine learning methods and artificial intelligence**. This leap in performance was powered by increased computing power, the high availability of broadband internet, and progress in computer science and proprietary and open-source software development. While the exact impact of this revolution is hard to predict, the panel feels that it has the potential to dramatically change the type of experiments conducted in the future. The panel expects many single-shot experiments to be replaced by measurement campaigns that collect large datasets amenable to machine learning techniques. The panel also feels that the NCNR infrastructure is insufficiently prepared for this change and recommends a strategic investment in this transformation as explicitly outlined in the U.S. research priorities (see Societal Impact and National Benefits).

4. The panel believes that experimental efforts will become increasingly distributed, with **remote experimentation** becoming common and even expected from large-scale user facilities. Several developments fuel this trend:

   - Scientific journals in the biosciences have a strong requirement to report multi-technique experimental data. Thus, reduced expertise of biological users to individual techniques, such as neutron scattering, is expected.
   - Employers put strong incentives in place to reduce their organization’s carbon footprint, leading to decreased travel.
   - Other large-scale facilities have demonstrated that remote experimentation is feasible and provides efficiencies and cost-savings.

   Further, remote data collection increases accessibility, which is most impactful for industry, four-year colleges, MSUs, and HBCUs, addressing the U.S. Research priority towards increasing equity and access (see Societal Impact and National Benefits).

3.9. Strategic Investments

In response to the long-term trends, external pressures and current challenges in biological neutron scattering that the panel identified, it recommends six strategic investments supporting the biosciences at a new reactor-based neutron scattering facility.

3.9.1. Investment 1: Kinetics measurements

Kinetics measurement capabilities allow for the study of out-of-equilibrium, actively driven, or cyclic processes that change the sample structure or affect the sample dynamics in a time-dependent manner. Such measurements are typically implemented via time-stamping of individual scattering events. The time resolution and observation times of a kinetics measurement vary depending on the neutron flux on the sample, the scattering technique, the detection hardware, and the observed process. In addition, kinetics-ready beamlines allow continuous data collection during motor movements between various instrument configurations.

A recent scientific case for kinetics measurements at the NCNR has been provided as part of the NSF CHRNS Initiative for Non-Equilibrium Structure of Materials [6]. Biological applications include the study of the time-dependent permeabilization of biological membranes by antimicrobial agents or the short-term stability of pharmaceutical formulations responding to external stimuli. The panel fully supports the CHRNS Non-Equilibrium Initiative and, in addition, emphasizes the importance of kinetics measurements as a tool to disentangle the complexity of modern biological samples and industrial biologics characterized with neutrons, even if the time-dependence is not the main target of the neutron measurement. The panel recommends providing kinetics capabilities for all neutron scattering instruments.

3.9.2. Investment 2: Interactions and Dynamics

Structural biology has long centered on single-representative or equilibrium ensemble structures of biological molecules. Various techniques have been utilized, including NMR, cryo-electron microscopy, x-ray, and elastic neutron scattering. However, understanding molecular dynamics and how they modulate structure and interactions between macromolecules has progressed more slowly despite being fundamentally important. Inelastic neutron scattering is an ideal technique to study macromolecular dynamics, but several factors have limited its widespread adoption:

- Limited access to inelastic neutron scattering instrumentation.
- Lack of applicable theories and tools for data interpretation that connect dynamics to function, especially for multi-component complexes.
- Requirement of large quantities of (often scarce) sample material.
- High costs and limited capacity for selective deuterium labeling, which deconvolutes data and reveals molecular interactions.

Recently, the importance of biomolecular dynamics has come into focus as its essential role in defining protein function emerged in key applications:

- The dynamics of biomacromolecules and cell membranes are crucial for understanding protein transport and disease mechanisms. Determining these dynamics is vital for therapeutic design, but accurately capturing biomolecular dynamics remains challenging.
- Biomacromolecules often exist in crowded environments, where interactions with adjacent molecules and their dynamics are crucial to their functionality. For instance,

therapeutic proteins, such as antibodies, are typically administered to patients in highly concentrated solutions and complex formulations. Hence, deciphering the interactions among these molecules presents a continuing challenge for the pharmaceutical sector.

In both examples, dynamics measurements are essential for dissecting the scientific problem. Still, we cannot fully translate measured dynamics information into a longer-term evolution of the structures and interactions in the studied system. Therefore, the panel recommends the following developments to close this gap:

- Instrumentation that covers a broader energy range.
- Source optimizations that provide higher flux and thereby require less sample material.
- Instrumentation that probes longer correlation times at lower momentum transfer for large-size biomolecules.
- Expansion of deuteration facilities.
- Theories and computational simulation tools needed for data analysis and interpretation.

3.9.3. Investment 3: Measurements yielding large datasets

Recent dramatic advances in artificial intelligence (AI) and machine learning (ML) have transformed biological research. We have seen the emergence of protein structure prediction models that are accurate enough to be widely applied, sometimes in place of an experimental structure determination. There are notable limitations of these models concerning catalytic residues, disordered regions, small molecule ligands, nucleic acids, and engineered proteins outside the scope of the training data. Protein-protein and protein-membrane complexes are also often inadequately covered for the same reason. However, they often constitute high-value health, national security, and fundamental science targets. Further, machine learning and automation are revolutionizing how biological research is performed. They are shifting the type of experiments conducted from single-shot, single-result experiments to large-scale campaigns that explore complex parameter spaces and yield large data sets.

The panel recognizes the magnitude of the changes affecting the research landscape and urges the following actions in response:

- AI/ML integration in data processing and analysis. As high throughput capabilities (Investment 5) are implemented, we envision that these advances will expand access and productive application of neutron scattering for non-expert biological scientists, removing current barriers from data collection to publication and dissemination. Transformative advances include:
    - Real-time feedback on the experiment, sample quality, and results.
    - Automatic production of reports that provide raw data and routine, standardized metrics from data analysis for developing industry or data standards.
    - Automatic deposition (with opt-out) of experimental data into databases with standardized metadata that accelerate publications or anonymized use by analysis methods.

- AI/ML may yield currently inaccessible information concerning, e.g., induced conformational dynamics, quantitative conformational flexibility, protein-specific hydration, and assembly dynamics. In addition, AI prediction algorithms provide increasingly accurate atomic structures for comparison to scattering data and should be an integral part of neutron scattering data analysis.
- Developing more accurate force fields or circumventing their use with AI/ML-based approaches requires a comprehensive basis of experimental structural data on membrane-associated proteins, ideally under pharmaceutically relevant conditions. Designing a new neutron facility to enable increased measurement throughput would uniquely position that facility to provide the requisite data.
- Neutron scattering should provide training data for improving ML applications. Multimodal data (Investment 4) will complement this effort.
- Leverage recent developments in active learning to drive autonomous measurement campaigns. Active learning introduces real-time, automated decision-making based on previously collected data. Such an algorithm is being developed within the ROADMAP project at NCNR.

3.9.4. Investment 4: Lab-on-beam

For complex biological samples, a single probe, such as a neutron scattering experiment, usually does not provide a comprehensive understanding. Samples with short shelf lives that change quickly with time or are otherwise in non-equilibrium conditions are thus excluded from neutron characterization if complementary data from other modalities are not collected simultaneously. At the same time, as experimental paradigms shift to *in vivo* or *in situ* kinetic measurements, exact sample conditions are not easily reproduced. Therefore, there is an urgent need to provide a multimodal measurement approach during the neutron experiment.

Addressing this need, the panel envisions a lab-on-beam concept. The sample at the beam is surrounded by a laboratory-like space, allowing for the integration of multiple characterization tools (e.g., x-ray scattering, light scattering, including multi-angle (MALS) or quasi-elastic (QELS), UV/Vis, Raman, and infrared spectroscopy, refractometry, circular dichroism, fluorescence) that measure the sample before, during, and after the neutron experiment. Such additional data provides complementary time and length scales. Adding multiple instruments requires significant planning, so integrating a laboratory environment at the beamline must be a fundamental design principle of the facility.

Design requirements:

1. Physical space, particularly transverse to and on both sides of the beam path. An enclosure would provide hazard containment but must be large enough to house multiple benchtop instruments and their supporting infrastructure, including power, communications, and chemical waste streams.
2. Flexibility in beam characteristics. Focusing, collimation, and wavelength range, as far as is practical, should be selectable to accommodate varying sample requirements.
3. Modularity of complementary characterization tools. The beamline requires a high degree of standardization, including software, data, user interface, and hardware

interfaces with proprietary software. Automated handling of industry-standard containment vessels, such as vials or 96-well microtiter plates, would streamline the lab-on-beam beamlines. Staffing with expertise in instrumentation, engineering and software development is required to support this effort.

4. Data management integrating data and metadata from multiple measurement modalities.

3.9.5. Investment 5: Measurement Pipelines

The panel notes that industrial users of the NCNR require reproducible and standardized measurements with instruments having good long-term stability of experimental response and beamline configuration. The target biomaterial characteristics for these measurements are often relatively simple analyses, such as the radius of gyration, P(r), Porod, and Kratky plots, among others. The panel feels that there is a potential for a high demand for such routine measurements, which is currently not met.

The panel proposes the establishment of measurement pipelines on dedicated instrument beamlines. A measurement pipeline is a standardized workflow that covers the entire process, from the arrival of samples at the facility to the dissemination of experimental results. A measurement pipeline would have the following characteristics:

1. Standard measurements. Beamlines are regularly tested with standard samples and workflows, including beamline re-configurations.
2. Pre-experiment planning. Sample characteristics (e.g., amino acid sequence) can be automatically tested for suitability and optimal conditions. This assessment may include fast, realistic, and validated instrument simulations and rapid sample simulations.
3. A comprehensive sample handling and tracking procedure.
4. Automated, routine analysis of experimental data, with transparent data reduction and analysis.
5. A deliverable product, including results of standard/validation measurements, complete pre-experiment analysis, and experiment results.

Support for measurement pipelines requires significant changes to current operation procedures, including dedicated staff for analyzing and creating processes and workflows. Access to these beamlines requires changes to the current proposal system for routine measurements and quick approval. Data handling requires the proper legal framework to handle proprietary samples and protect the intellectual property of industrial stakeholders.

The adoption of measurement pipelines is expected to yield many additional benefits. Trust in neutron measurements will be built by adopting best practices, standards, and verified procedures. Lowering barriers to industrial users will increase the economic impact of the new facility. By improving the accessibility of standard neutron measurements, measurement pipelines will constitute a vehicle for scientific outreach and visibility, thereby increasing the user base and facilitating the recruitment of talent. Eliminating barriers to the application of neutrons by labs without the resources to invest in obtaining neutron expertise will improve equity in using the nation’s neutron resources.

The panel also notes that implementing measurement pipelines is the ideal vehicle to realize Investments 3 and 4 within a limited-scope environment, greatly enhancing their chance of success. Significant expertise from the nSoft consortium should be leveraged.

3.9.6. Investment 6: Fundamental Science and Method Development

The panel recognizes the continued importance of fundamental science and method development as they significantly contribute to the NCNR's societal impact, including STEM education and workforce development (see Societal Impact and National Benefits). The panel recommends the continued support and development of established techniques and sample formats. After in-depth discussion, it recommends additional investments in the following areas of the biosciences:

- Dynamics
- Interactions in crowded environments
- Extreme environments, such as ultra-cold temperatures and high-pressure
- Food science

The panel also recommends the exploration of applying neutron scattering in potential expansion areas:

- Anaerobic biochemistry
- Synthetic biology
- Tissues, tissue engineering, and bioengineering
- Organisms and cells
- Hybrid biological/solid-state interfaces for new materials and biosensors
- Rhizosphere, plant/other organisms, soil-water interaction in climate change

3.10. Societal Impact and National Benefits

The U.S. administration's memoranda for multi-agency R&D priorities for the FY 2023-25 budget submissions [7-9] define the U.S. research priorities that support a set of beneficial societal impacts. The memoranda express the need to harness the power of science and technology to address the challenges and opportunities of the 21st century while strengthening American competitiveness, innovation, sustainability, and security. The administration emphasizes pandemic readiness and prevention, tackling climate change, catalyzing innovation in critical and emerging technologies, innovation for health and equity, national security, and economic resilience. They provide guidance on strengthening and diversifying the R&D ecosystem, promoting public participation and engagement in science, and ensuring that Federally funded R&D is open, trustworthy, and beneficial to the public. They encourage STEM education and engagement, highlighting the importance of promoting diversity, inclusion, equity, and accessibility in STEM learning and workforce development. The memoranda urge agencies to coordinate and collaborate on multi-agency R&D activities while balancing their agency-specific, mission-driven R&D, including fundamental research.

Specifically, we identified the following U.S. research priorities and societal impacts of neutron scattering in the biosciences:

1. Advancing biotechnology and biomedical research for public health and economic growth.
2. Supporting emerging technologies such as artificial intelligence, quantum information science, and biomanufacturing.
3. Preparedness for future public health emergencies.
4. Promoting American leadership in science and technology.
5. Advancing health equity and biomedical innovation.
6. Supporting fundamental research and scientific discovery.

The Strategic Investments identified by this panel directly address current and future challenges and pressures to meeting these national research priorities:

Strategic Investment	Challenge or External Pressure	Societal Impact or U.S. Research Priority
Kinetics measurements	Sample complexity	Fundamental research and scientific discovery
Interactions and dynamics	Sample complexity	Fundamental research and scientific discovery, Advancing biotechnology
Measurements yielding large datasets	Sample complexity, AI revolution	Artificial Intelligence, Advancing biotechnology, Biomedical innovation
Lab-on-beam	Sample complexity Research agility	Advancing biotechnology, Supporting biomanufacturing, Biomedical innovation
Measurement pipelines	Public health challenges, Research agility, Remote work	Advancing biotechnology, American competitiveness, Equity and accessibility, Workforce development, Artificial Intelligence
Fundamental Science and Method Development	Public health and climate challenges	Fundamental research and scientific discovery, Emergency Preparedness, American competitiveness, Workforce development, STEM Education

3.11. Recommendation for new instrumentation and assessment of the new reactor’s ability to facilitate science

3.11.1. Reactor Characteristics

The panel supports the stated plan to increase the capacity and capability of a new reactor-based neutron source. For the biosciences, the panel emphasizes optimizing the source and guides for cold neutron flux, particularly for the kinetics and dynamics capabilities outlined in Strategic Investments 1 and 2. Beam-focusing optics that provide higher flux at the sample position are a viable option for many biological experiments that can tolerate a higher beam divergence. Any increase in cold neutron flux at the sample enables measurements using flux-limited sample environments such as size-exclusion chromatography SANS or high-pressure SANS, allows for higher throughput for automated systems (Investments 3 and 5), and supports more researchers at the facility (access and equity, see Societal Impact and National Benefits). The panel endorses an increased capacity (number of beamlines) at a new facility, particularly to allow for specialized measurement pipelines (Investment 5) in addition to flexible fundamental science beamlines (Investment 6). The panel advocates for ample space at the beamlines supporting the proposed Lab-on-Beam initiative (Investment 4).

3.11.2. Instrumentation

The panel recommends utilizing the higher capacity at a new facility to optimize existing scattering techniques for research in the biosciences. The table below summarizes the recommended instrumentation. The panel recommends separate beamlines for measurement pipelines (Strategic Investment 5) and fundamental research (Investment 6). The panel identified an access gap for NSE at the current facility and recommends building a second instrument specifically supporting dynamics method development (Investment 2).

Technique	Purpose	Features
Reflectometry (CANDOR-type)	Measurement pipelines	Optimized for biology (lower Q resolution, larger samples)
Reflectometry (CANDOR-type)	Fundamental research (shared with non-biosciences)	Optimized for biology
SANS (general)	Measurement pipelines	Optimized for throughput, modular pipelines
SANS (general, shared), vSANS-type	Fundamental research	Optimized for flexibility and complex sample environments
SANS (focused beam)	Biomacromolecular complexes	Focused beam for small samples
SANS (industry/pharma)	Measurement pipelines	Optimized for throughput, compatibility with industry samples, streamlined accessibility
USANS	Hierarchical structures	Small samples, live cells, viruses
NSE	Fundamental research	Highest possible flux
NSE	Fundamental research and method development (Investment 2)	Explore design changes for high vs low Q
Inelastic	Confined water dynamics associated with biomacromolecules	Broad energy range, separate coherent and incoherent
Imaging/microscope	In situ studies of living systems, therapeutic devices	<1 µm resolution
Quasi-Laue Diffractometer	Protein crystallography	Room temperature, small crystals

The panel identified further instrumental developments to pursue:

- Optimizing and exploring a broader deployment of wide-band energy-dispersive solid-state detectors (such as the one developed for CANDOR) to counter the low neutron flux [2] and provide a lower scattering background.

- Routine separation of coherent and incoherent scattering at SANS experiments, requiring investments in detector technologies, beam polarization, and data reduction.
- Assess complementary capabilities at x-ray facilities and align neutron instrumentation accordingly. Explore hybrid neutron and x-ray beamlines or stand-alone complementary x-ray instrumentation.

3.11.3. Sample Environment

The panel states its strong support for the role of sample environments at a new scattering facility. It urges the provision of sufficient resources for their design and commissioning as part of a new reactor project. The panel recommends the following new sample environments supporting the biosciences:

- Liquid handling for automation (Investments 3 and 5).
- Design and adapt sample environments for pharmaceutical containers (vials and syringes) to support biomanufacturing and Investment 5.
- *In-situ* lyophilization with simultaneous neutron and FTIR measurements supporting industrial and fundamental research.
- Extreme environments (Investment 6).
- Design of size-exclusion chromatography SANS coupled with light scattering (MALS-QELS) and in-line spectroscopic methods and refractometry. Providing flow capillaries or microfluidics scattering cells.
- Software for beamline integration and automation of laboratory instruments (Investments 3-5). Adaptation of open hardware interfaces and software APIs in-house and commercial sample environments and laboratory instrumentation.

The panel notes that the current staffing is insufficient to support these new environments comprehensively and recommends dedicated staff for each of the projects listed above (see also next section).

3.11.4. Accompanying Facilities

3.11.4.1. Biodeuteration

Deuterium labeling is critical for successful neutron scattering experiments. Currently, deuteration laboratories are associated with all major neutron scattering facilities worldwide. [10] It will be necessary to upgrade and expand the NIST BL2 deuteration user facility to meet the future needs of the biology community, using a multi-tiered approach based on user expertise, ranging from training students in bio-deuteration techniques to a fee-based service model for industrial users. D-labeling needs can be broadly broken down into two major areas: biomacromolecule deuteration and small molecule chemical synthesis.

Biomacromolecule deuteration relates to proteins, nucleic acids, biopolymers, and their complexes. Some of the challenges that need to be addressed are the development of deuterium oxide-tolerant higher eukaryotic systems for expressing membrane proteins and post-translationally modified proteins. Similarly, there are opportunities for developing high-efficiency cell-free protein expression systems for routine production of toxic proteins in milligram quantities needed for neutron scattering experiments. A subset of a related development is for domain-selective deuteration of multidomain proteins. New biochemical approaches are required for efficient in-vitro ligation of protiated and deuterated domains of multidomain proteins that do not currently exist. This success would enable novel SANS and NSE experiments. The ability to selectively deuterate cellular components using gene editing tools can revolutionize our understanding of biomolecular structures in their native environment, as exemplified in a recent study that showed the feasibility of this approach for in vivo structural characterization of biomembranes [11].

Small molecule deuteration capabilities will benefit several different areas. For instance, controlled incorporation of deuterium into different classes of lipids will enable new neutron scattering experiments aimed at understanding the fundamental properties of biomembranes, their interactions with other synthetic and bio-based molecules, as well as deconvoluting the complex architecture of LNPs. Similarly, the availability of deuterated amino acids, sugars, and nucleotides (or other excipients) is important for producing synthetic peptides for biopharmaceutical or biomaterial research and deuterated DNA and RNA molecules for LNP studies, as well as studying protein/nucleic acid complexes. Currently, the building blocks for these materials are either not commercially available or are cost prohibitive.

During its discussions, the panel recognized the difficulties of implementing such a comprehensive approach to bio-deuteration by a single-user facility. It also recognized significant overlap with efforts in other communities, such as NMR, or institutions, such as the NIH. Therefore, the panel recommends strong cross-facility coordination (see below) to provide bio-deuteration to its users. Ideally, the NCNR would pursue the creation of a National Isotope Labeling Center for Chemistry and Biology.

3.11.4.2. Support Staff

Most of the investments and developments recommended by the panel are not directly concerned with the scattering experiment but rather in support of it, addressing needs in sample environment, computation, and administration. The panel believes that current staffing in those areas is insufficient to support the transformative changes outlined in this report. It, therefore, recommends including dedicated staff for the following activities in the proposal for a new reactor-based scattering facility:

- Beam-on-lab support teams (Investment 4)
- Computation and theory group (Investment 2)
- Autonomous experimentation and artificial intelligence group (Investment 3)
- High-performance computing (NCNR computing infrastructure)
- Data management group (Investments 3-5)
- Workflow and process development group (product management) for measurement pipelines; administrative support for alternative beam access; logistics and sample handling (Investment 5)
- Industry liaison with support for intellectual property protection (Investment 5 and 6)

- Academic liaisons and outreach to NIH-funded investigators (Investment 5 and 6)

3.11.4.3. Cross-Facility Coordination

Many of the recommended activities in this report require profound structural changes at the NCNR and there are likely similar efforts underway at other institutions. We therefore recommend extending the NCNR's cross-facility coordination efforts, particularly in the following areas:

- Deuteration facilities
- Data structures, shareable data, databases
- Standardization of measurement pipelines
- Standards for measurement pipelines for seamless data quality and transfer
- Sample environment and adaptation of industry standards, e.g., 96-well plate handling

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4. Energy and Environment

4.1. Panel

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4.2. Glossary of Terms

Density Functional Theory (DFT): a quantum-mechanical computational method used to predict the electronic structure of materials.

Machine Learning: a field of study in artificial intelligence concerned with developing algorithms that can learn from data.

MOFs: metal organic frameworks; a class of porous materials of interest for hydrogen and carbon storage

Molecular Dynamics (MD) modeling: a computer method used to simulate the motions of atoms.

POFs: another class of porous materials that, in contrast to MOFs, are constructed solely from organic building blocks.

Wolter optics: this involves grazing incidence reflections from two concentric, mirrored, conic sections such as a paraboloid.

4.3. Summary

Energy is fundamental to all human endeavors and has profound impacts on the US economy, human health, and our quality of life. Neutron science is key to designing, developing, and deploying the materials and technologies of the future that address issues of energy, sustainability, and environmental stewardship. This includes the catalysts used in chemical industries totaling nearly a third of US gross domestic product (GDP), emerging electrochemical devices that will transform our transportation sector and energy grid, and new classes of structural materials for continued innovation in the domestic built infrastructure. For example, 10-15% of total US energy usage is devoted to separation processes; neutron scattering can help understand structure and dynamics in the adsorbent materials to enable efficient separation processes, from cleaning water to distilling hydrocarbons. For continued innovation, scientists and engineers will require a new and optimized research reactor and an accompanying suite of state-of-the-art instruments to study how material systems function under real-world conditions. The next generation neutron research facility will be key to the development of new energy storage systems, materials for energy conversion, sustainable processes for decarbonizing our industry, and materials for the production and transportation of alternative fuels such as hydrogen.

To fully address these challenges, the neutron instrumentation and source will need to provide structural and dynamic information over a multiple length scales and time scales and be built to anticipate future needs in energy and environment research. The unique characteristics of neutrons make them an indispensable resource. Their special sensitivity for hydrogen and other light elements enables studies of materials such as biomass, petrochemicals, polymers, and absorbates. Neutron scattering is also a nondestructive technique, necessary for the study of precious or delicate samples and real, operating devices. The next generation facility will enable new frontiers in science as it will be a brighter source with higher neutron flux focused on smaller sample sizes. Spanning several energy scales, from cold to thermal neutron beams, the new facility will bridge multiple length and time scales to study condensed matter relevant to energy and the environment with unprecedented accuracy, sensitivity, and speed. This report highlights key science drivers, societal impacts, national benefits, new instruments, and reactor characteristics that will enable leading edge energy and environmental science research far into the future.

4.4. Science Drivers for Neutron-Based Research

Industrial development—intensified in the past century with the industrial revolution, advent of large-scale chemical processing, rapid changes in transportation, and increasing energy demand fueled by new technology—has applied stress to both natural and built environments and jeopardized human health. Moving to a sustainable, circular economy on all levels of production and consumption is necessary to address these challenges and support the economic, health, and social well-being of U.S. citizens into the 22nd century. These efforts rely in large part on the development of novel high-performance materials and chemical processes to achieve three key objectives: (i) develop renewable, environmentally benign energy sources, (ii) increase the efficiency with which we utilize these resources, and (iii) remediate the impacts of energy use on society and the environment. In all of these objectives, neutron scattering science has the potential to make enormous contributions by virtue of the unique characteristics of neutrons (Table 1).

Table 1. Unique characteristics of neutron probes and their benefits to energy- and environment-related research

Neutron characteristic	Benefits to energy research
Sensitivity to light elements (H, Li, C, etc.) and high contrast between neighboring elements	Find where the elements are and how they evolve as a function of time
Broad range of energies/wavelengths	Probe a range of time and length scales
Isotope contrast	Identify specific elements, kinetic effects, contrast match for enhanced sensitivity
Highly penetrating	Probe materials in complex *in situ* / *operando* environments
Non-destructive	Probe materials without changing their intrinsic nature or chemical state
Large incoherent cross-section for elemental hydrogen	Analyze dynamics in a range of hydrogen-rich materials (e.g., polymers)
Prompt gamma interaction	Analytical chemistry and elemental analysis

4.4.1. Advancing Energy Sources

Developing next generation technologies for clean energy conversion and storage are critical for realizing a carbon neutral society while meeting rising energy demands by mid-century. Decarbonizing the nation's energy infrastructure will require a multi-pronged approach, which will simultaneously lead to a more resilient energy infrastructure. This includes the effective conversion and storage of energy from chemical (hydrogen/ammonia/methane conversion), electrochemical (fuel cells and batteries), nuclear (molten salts and fusion materials), renewable (photovoltaic and winds), and thermal (phase change, thermoelectric materials etc.) resources.

4.4.4.1. Electrochemical Energy Storage and Conversion

Among various electrochemical energy storage technologies, Li-ion batteries have yielded significant societal benefits over the past three decades. To meet the increasing power demands of applications including electric vehicles, portable electronics, and grid energy storage, it is crucial to further reduce costs and resource demands, while enhancing energy density and maintaining safety. A mastery of structure-property relationships in key materials is vital for improving current Li-ion technology and developing transformative next-generation storage techniques. These include Na-ion and multivalent cation batteries, all-solid-state Li metal batteries, aqueous batteries, and redox flow batteries. Tools are required to quantify chemical concentrations with precise spatial and time resolution which are difficult to determine because of complex microstructures, prevalence of key processes at buried interfaces, and the importance of light elements.

4.4.4.2. Renewable Energy Generation

Renewable energy will continue to play a pivotal role in the energy transition, strengthening US energy independence. Renewable sources, including (but not limited to) solar, wind, hydropower, and geothermal, rely heavily on understanding materials and processes across a broad range of length- and timescales in constituent materials and across functioning devices. For example, wind energy research requires tools to understand and control the manufacture of efficient, high-yield, lightweight and durable composites for turbine blades. In solar research, process-structure-property relationships and interface stability for new layered materials must be developed. In all cases, researchers need to understand how materials and interfaces evolve over the course of decades in a range of environmental conditions.

4.4.4.3. Biomass

Lignin is a major component of plant cell walls that aggregates and causes problems during the production of cellulosic ethanol, a renewable substitute for gasoline. When enzymes are used to release plant sugars necessary for ethanol production, the lignin aggregates bind to the enzymes and reduce the efficiency of the conversion. Understanding how these aggregates form from the molecular to macroscopic scale and the mechanism of biomass breakdown are needed to optimize biomass conversion.

4.4.4.4. Hydrogen Production, Storage and Utilization

Hydrogen storage is a key enabling technology for fuel cell applications including stationary power, portable power, transportation, and industrial materials processing. Hydrogen's low mass density results in a low energy per unit volume and hence requires advanced storage and transportation methods. For instance, mixing small amounts of hydrogen into the nation's existing natural gas infrastructure could avoid generating an entirely new infrastructure robust to hydrogen embrittlement, but would require new separation processes. Electro/catalytic conversion of H_2 to ammonia or other liquid carriers could also enable high density transportation and storage of hydrogen. These processes are expected to be at giga-joule scales; optimization will yield enormous cost savings but will require new advances in chemical and electrochemical catalysis and chemical separation.

4.4.4.5. Thermal Energy Storage and Conversion

Roughly 67% of the energy generated in the U.S. is wasted in the form of heat. Efficient storage, transport, and re-use of heat or conversion of waste heat into useful electricity is therefore essential for society. Heat sources include (i) primary sources, such as thermophotovoltaics and concentrating solar-thermal power; (ii) low-quality (waste) heat from other primary sources, such as engines, power plants, and low-temperature geothermal sources, and (iii) cooling loads, such as for microprocessors, data centers, and radiation detectors. This power can be used at many scales, for example, powering sensors in Internet-of-Things applications, providing residential heating from smart building materials, and facilitating load balancing of grid-scale renewable energy. Enabling efficient and cost-effective thermal energy processes such as these will require new advances in thermoelectric materials that operate across a range of temperatures, thermophotovoltaics, and phase-change materials with the ability to absorb and release heat on-demand. Research tools must be able to examine material properties across a large range of length scales and monitor interfaces across a range of extreme temperature and pressure variations.

4.4.2. Increasing Energy Efficiency

The energy demands of modern society are enormous and continue to grow as more countries industrialize and new resource intensive technologies are connected to energy grids - such as edge computing for artificial intelligence. Catalysis and molecular separation processes, which are inextricably linked with many of the previously discussed technologies, are resource intensive in and of themselves. Thus, new and improved energy sources will require advances in chemical and electrochemical catalysis and chemical separation.

4.4.2.1. Chemical Catalysis

Catalysts have played a key enabling role in industrial chemical processes by promoting difficult reactions and lowering energy costs. The current petroleum, chemical, and biopharma industries would not function without catalysts. Catalyst development to reduce power, temperature, and pressure requirements for industrial processes are key scientific drivers in this area but require improved understanding of conversion processes and mechanisms. Transition metal or rare earth-based catalysts are used in large scale industrial processes, but new, cheaper, more efficient catalysts are needed. Optical spectroscopies are a core research tool in catalysis but are limited by photoreaction/ photo-desorption issues, difficult optical access to samples, poor sensitivity to hydrogen and other light elements, and energy deposition in the sample. Therefore, new and better measurement techniques are required to decipher the mechanisms of chemical reactions, identify transition states and intermediates, improve selectivity and performance, and understand catalyst end-of-life processes.

4.4.2.2. Separations

Separation processes are key to the manufacture of many commodity chemicals. Currently 50% of the energy used by the US chemical industry, and 10-15% of total US energy usage, is devoted to separation processes [1]. The development of new adsorbent and membrane materials could dramatically decrease this energy consumption, and reduce US economic vulnerability to global energy prices, by facilitating a move away from thermal separation processes. Effective materials for separations can also better facilitate the extraction and recovery of critical metals to reduce geopolitical conflict, and environmental remediation by enabling cost effective greenhouse gas capture and water decontamination [1].

4.4.3. Addressing Adverse Impacts of Energy Use

Energy industries have historically produced a tremendous amount of waste. Future energy sectors must be managed in ways that safeguard human health, minimize impacts on the environment, and ensure sustainable supply chains for critical materials through reclamation and recycling processes. Simultaneously, maintaining a livable habitat will require remediation of adverse impacts from previous energy use paradigms. Efforts span the conversion of non-recyclable waste materials into usable heat, electricity, or fuel through combustion, gasification, pyrolization, anaerobic digestion, landfill gas recovery, and other processes; and encompass efforts towards industrial decarbonization and the circular carbon economy, including green construction materials, the recycling of plastics, and chemical-, electro- and photo-conversion of CO_2.

4.4.3.1. Industrial Decarbonization

Industrial decarbonization is an enormous challenge that the world must solve to limit temperature rise. This includes decarbonizing a range of heavy industries, including chemicals, petroleum refining, cement, iron and steel, and food and beverage. Combined, these are responsible for 25% of all anthropogenic CO_2 emissions. Required technologies span from new catalysts for CO_2 up-cycling to renewable chemicals and fuels, separation materials and processes for atmospheric CO_2 removal, to green cements and new furnace technologies for iron and steel production. As one example, concrete is a complex multiscale, heterogeneous, and porous material that continues to evolve days, months, and years after creation. Alternative cement technologies, including carbonate cements based on mineralization processes and alkali-activated cements, lack the 150 years of experience with Portland cement concrete. The insight that materials research provides on the fundamental processes that control macroscopic performance is indispensable for development of these ‘green’ materials and predicting their long-term performance.

4.4.3.2. Carbon Capture and Sequestration

Research on CO_2 sequestration is currently focused on (i) reversible capture in cheap liquid or solid materials with high capacity and easy regeneration or (ii) chemical capture (e.g., as carbonates) for subsequent disposal in oceans or in geological repositories. The development of capture materials and evaluation of the environmental impact from geological storage are directly related to fundamental questions in chemical synthesis, molecular/atomic structure at ambient and high-pressure conditions, aging, and microstructure. It is estimated that the capacity for underground storage of fluid CO_2 is substantially more than near-future demand and that the costs are reasonable [2]. Research challenges include incompatible pipeline metallurgy (e.g., susceptibility to carbonic acid attack and other degradation reactions), predictive models for complex fluid flow in porous rocks (for example, for supercritical CO_2 and water, where one fluid is partly soluble in the other), and CO_2 reaction with subsurface minerals. *Operando* imaging with sensitivity to light atom species is needed to examine the reactions in real time within subsurface structures. For solid storage materials, structural probes are required to investigate metal site activation and bespoke porous frameworks with fitted pore sizes and functionalized surfaces, and to study activated membranes and interfaces, along with their uptake efficiency under specific conditions as well as the kinetic pathways and limitations for optimization. To address these problems, researchers require sophisticated sample environments mirroring real world conditions, with controlled and variable temperature, pressure and environmental process variables paired with sensitivity to N, C, O, H, in presence of heavy metals and rare-earth metals.

4.4.3.3. Circular Carbon Economy

An attractive alternative to sequestration is chemical (including electro- and photochemical) conversion to value-added products (e.g., fuels such as methanol, or chemical feedstocks such as CO, formic acid, or other simple organic molecules). The chemical conversion of CO_2 is limited by its poor reactivity. The development of novel catalysts for its activation is still in its infancy. Current catalysts are based on expensive Pt-group metals and processes using them are still energy, resource, and waste intensive. Increasing selectivity and efficiency is required to avoid elaborate purification streps and minimize environmental impact. Hybridized MOFs and POFs are promising candidates for creating innovative bifunctional catalysts for CO_2 separation and adsorption [3]. CO_2 recovered from industrial activities or direct air capture is typically mixed with reactive gases such as SO_2, NO_x, and water vapor. Extracting and concentrating CO_2 at a sufficiently high rate from these mixtures requires energy intensive treatment. New classes of materials and systems under study for this purpose include porous frameworks for gas separation, catalysts, membranes for separation and concentration, and pressure swing absorption. Material and process development from conceptual studies to commercial applications will remain an active area of research for materials scientists, chemists, and chemical engineers for years to come.

4.4.3.4. Critical Minerals for Energy Independence

The United States' energy portfolio is increasingly reliant on "critical minerals", driven by the global efforts to reduce carbon emissions and meet future energy demands. Critical minerals encompass any non-fuel minerals, elements, or substances that (i) have a high risk of supply chain disruption; and (ii) serve an essential function in one or more energy technologies. Key energy technologies that rely heavily on critical minerals include (but are not limited to): catalysts and electrolyzers (Pt-group metals, Ir, Rh); batteries for electric vehicles and stationary storage (Co, Li, Mn, Ni); magnets for wind turbines and electric vehicle motors (rare-earths, lanthanides); and light-emitting diodes (Ga, As). Significant research is needed to accelerate the circularity of materials (e.g., recycling, reconstitution, and reuse) to offset the need for raw minerals. The development of new functional materials that reduce or eliminate the use of critical minerals in key technologies is essential to advance energy technologies, improve environmental and sustainability outlooks, and mitigate the US's dependence on critical materials. A rich, foundational understanding of both materials and devices across a range of length- and timescales will advance technological design principles that improve both atom- and energy-efficiency.

4.4.3.5. Environmental Science

Mitigating the deleterious effects of climate change is predicated on a foundational understanding of anthropogenic impacts in the broader global ecosystem, ranging from environmental geology, hydrology and plant biology to aerosol and atmospheric chemistry. The sensitivity of neutrons to lighter elements—especially hydrogen—is particularly well-suited to environmental science, as it permits study of organic species and hydrogen-rich environments. Neutron science has enabled crucial advances towards understanding and mitigating anthropogenic impacts to the environment. Neutrons have provided key insights into pollutant speciation, including heavy metals and organic pollutants, in water and aqueous environments [4]. Additionally, structural and dynamics studies by neutrons have provided key insights into the role of particulates in cloud condensation and ice formation [5], both of which are critical for climate moderation.

4.4.4. Science of Synthesis

The science of materials synthesis crosscuts all energy and environment categories introduced above, foundational to enabling further advances in energy conversion, energy storage, and environmental stewardship. Increasingly, the stability or properties of desired new compounds are being assessed computationally; yet there remains an enormous gap in establishing methods to prepare a new material in single-phase form *a priori*. Optimizing material synthesis to yield a desired outcome remains a tedious and lengthy endeavor as it involves complex multiparameter spaces. Even conventional synthesis approaches often lack well-established mechanisms, missing kinetics data at reaction conditions that would inform them. In situ synchrotron diffraction and local structure studies have been demonstrated in the last decade to provide data that informs synthesis by design and accelerating materials discovery [6-8]. Neutrons offer larger sample sizes, unique atom and isotope sensitivities, and a wide variety of sample environments (high/low temperatures, magnetic fields, reactive/inert gases, etc.). High-throughput *in-situ* neutron diffraction [9-11] will provide rich opportunities to reveal reaction mechanisms and kinetics for industrially relevant samples, paving the way to synthesis by design and data-driven automated synthesis. Furthermore, neutron total scattering can be utilized in concert to follow local ordering, amorphous phases, nucleation intermediates, and solute complexes and clusters in these processes.

4.5. Societal Impact and National Benefit of Neutron-Based Research

Advancing the scientific drivers detailed above will have an immediate and broad impact on the US economy and society in general. In the space of energy storage systems, neutron scattering emerges as a pivotal tool for addressing some of the most critical, not yet well-understood, challenges due to their highly penetrating nature. In the area of catalysis, new neutron techniques will decipher the mechanisms of chemical reactions, improve selectivity and performance, and understand catalyst end-of-life processes. Neutrons will also play a crucial role in the development of new technologies that will substantially lower industrial-based CO_2 emissions through the development of renewable fuels, green cements and alternative furnace technologies for iron and steel manufacturing. New separation technologies will be developed from hybridized metal-organic frameworks in combination with other framework materials. Finally, *in situ* neutron capabilities will aid in the discovery of the materials to meet all the above challenges by advancing the science of synthesis. Each scientific goal is driven by the benefits and positive outcomes conferred to the U.S. economy, industry, and research infrastructure.

Energy independence is one of the most critical problems facing the USA, powering our economy while curbing pollutants and maintaining the country's high standard of living. Research needs to be closely aligned with industrial priorities and partners to have near-term or immediate impact. NIST has a rich history of working closely with industrial partners to use neutron scattering and imaging instruments to accelerate product development. One example includes General Motors' use of neutron imaging at NCNR yielding over 40 patents in hydrogen fuel cell research. The *n*Soft consortium has facilitated industry's use of neutron scattering tools for soft matter research, including projects by Toyota, Aramco Services, Chevron-Phillips, Exxon-Mobil, 3M, Solvay, Dow, and Dupont. Meanwhile, as the USA's national metrology institute, NIST plays a key role in hosting reference databases and producing standard reference materials. Emerging efforts in defining lithium phase diagrams and carbon uptake in cements will generate similar efforts beyond 2050. Thus, NIST's strong performance in engaging with industrial partners will need to be a focus of the NNS to be fully successful.

4.6. New instruments and reactor to enable cutting edge energy/environmental science.

To address outstanding challenges in the aforementioned areas, we need new measurement capabilities that provide insights into fundamental material processes. These processes, organized into the appropriate length and time scales, fit into the following four categories:

1. ***Atomic to Nanoscale Material Structures**:* Scientists and engineers must learn how to manufacture materials with finely tuned properties and predictable long-term evolution. This, in turn, requires development of process-structure-property relationships to guide energy-efficient, environmentally benign manufacturing processes.
2. ***Interfaces***: The prevalence of interfacial processes in a multitude of energy and environmental applications demands that scientists and engineers understand how to design material interfaces that: (a) are chemically selective, (b) promote relevant charge and mass transfer processes, and (c) are chemically and thermally stable. These interfaces must span various phases including solid, liquid, and vapor interfaces.

3. ***Ion, Charge, and Mass Transport:*** Scientists and engineers need to be able to correlate material structure (crystal and polycrystalline structures in solids, solvation structures in liquids) with atomistic transport mechanisms. They must also understand the movement of molecules and ions within dimensionally confined micro and nanostructures such as pores and vacancies in relevant energy materials.

4. ***Multi-Modal Capabilities:*** With *operando* and *in situ* techniques, materials can be studied under realistic operating conditions, allowing for a deeper understanding of their synthesis, stability, and functionality. Having multiple probes such as high-energy X-rays in combination with neutron techniques simultaneously would result in powerful advances in the study of materials relevant for energy and environmental applications.

Summarizing many of the science drivers mentioned in **Table 1**, the new instruments and new reactor should supply a broad array of measurements capabilities including:

a. Chemical sensitivity, especially for low atomic number elements

b. Measurements on a broad range of length scales, from sub-nanometers to meters for material structure and chemical composition.

c. Measurements on a broad range of time scales, from picoseconds to days and even weeks.

d. Measurements must be repeatable and provide fast feedback.

e. Multi-modal capabilities are required to probe different aspects of the same system (*e.g.,* chemical, structural, or range of time or length scales in a single shot).

f. Measurements of materials in relevant thermal, chemical, magnetic, and electrical environments (*in situ*) and of devices and materials away from equilibrium (*operando*) to understand the relationship between material properties and their role in key energy processes.

These capabilities are well matched to the relative strengths of neutron scattering (see **Figure 1**), but additional bandwidth and advanced capabilities are required to meet the full scope of challenges in energy and environment research. Conversely, failing to properly invest in neutron scattering capabilities in the US will profoundly harm US competitiveness and quality of life in a range of key areas related to energy and environment, ranging from human health to economic competitiveness, to workforce training in science and engineering. Detailed below are the four areas identified above that the new instrumentation and new reactor at NIST must address to have maximal impact on energy applications and environmental science.

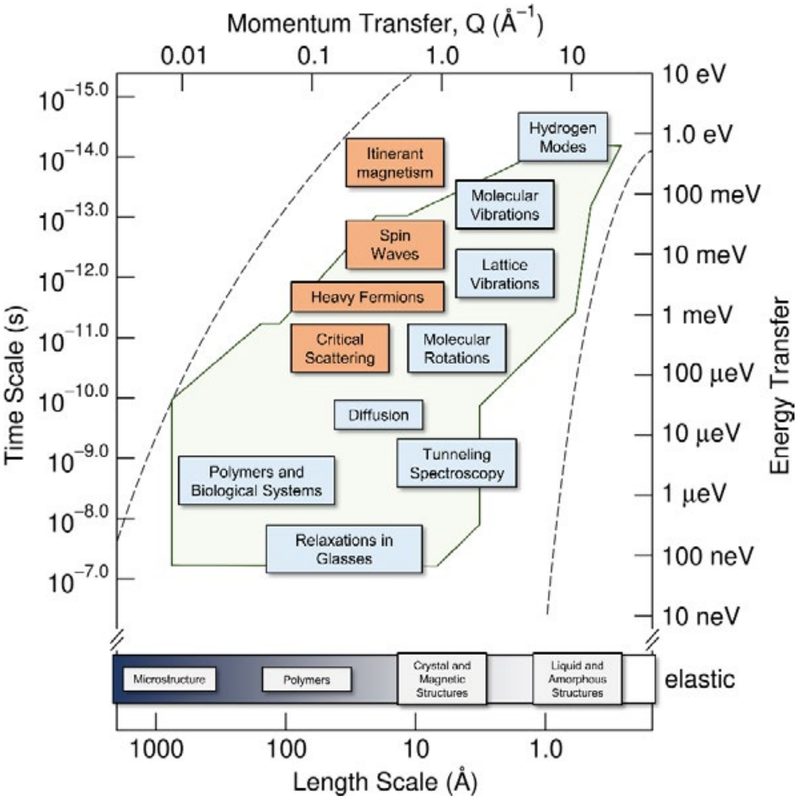

Figure 1. The length scales and time scales probed by neutron science measurements. Many of the scientific and engineering questions fall into the momentum transfer (Q) and energy transfer characteristics of neutron instrumentation covered in this report.

4.6.1. Atomic to Nanoscale Materials Structures

Understanding the atomistic to nanoscale structures is necessary to advance the next generation of functional materials for applications in energy and the environment. Diffraction, imaging, and small angle neutron scattering (SANS) investigate atomic-level structure statistics and changes, spatial distribution information, and microstructure with nucleation and formation processes, respectively.

4.6.1.1. Diffraction Suite

Neutron diffraction, with its high sensitivity to light elements like lithium, hydrogen and carbon, and excellent contrast to neighboring transition metal cations (*e.g.,* Mn, Fe, Ni, and Co in cathodes), plays a crucial role in determining the structure of battery electrode/electrolyte materials. This information serves as the foundation for a deeper understanding of the ionic transport and electrochemical performance of electrodes. Neutron total scattering (pair distribution function), encompassing both short-range and long-range structure information, is significant in comprehending how local order impacts the performance of electrodes and electrolytes. Interfaces play a critical role in governing battery performance requiring selectivity and stability, but debates surrounding the composition, structure and even thickness of these interphases impede targeted design or tailoring for specific functionality to enhance various battery performances. Neutron reflectometry and small-angle neutron scattering are powerful tools for unraveling the detailed composition/structure of battery interfaces. Quasi-elastic neutron scattering is an essential tool for studying Li/Na-ion transport dynamics in battery electrode and electrolyte materials. Neutrons, being highly penetrating, non-destructive, and non-disturbing to electrochemical reactions, also present an ideal probe for *operando*/*in situ* monitoring of structural changes in battery materials during operating conditions.

The panel identified the following critical instruments for the future diffraction suite:

a. High-Intensity, High-Resolution Materials Diffractometer: The purpose of this instrument is to provide accurate structural information on relatively small sample quantities. Small sample sizes are a must, as many novel materials are produced in very small quantities; often, materials relevant for separations are produced as thin films or membranes. To achieve these capabilities, this instrument requires a thermal neutron source with high flux on the sample, wide detector coverage, and a suite of doubly focused monochromators so users may select optimal wavelengths. This is a critical "workhorse" instrument for the diffraction suite.

b. Fast Materials Diffractometer: This instrument will provide rapid data collection to follow chemical processes. *In situ* and *operando* experiments enable understanding of how materials systems evolve under real conditions, including applications in catalysis, kinetics, energy transformation, energy storage, and rapid materials discovery. A cold source ($\lambda > 3.0$ Å) and focused neutron beam with energy-discriminating detectors will provide limited Q-range and resolution but will enable rapid collection suitable for kinetics, *in situ*, and *operando* studies.

c. Local Structure Diffractometer: This instrument will provide the capability to study local structure to complement the global structure studies enabled by the High-Resolution and Fast Materials Diffractometers discussed above. The dynamic and static local structural order of materials often deviates from the global structure, and frequently drives unique materials functionalities. This capability will be critical for materials that exhibit limited crystallinity, *e.g.,* heavily disordered materials, liquids. An understanding of local structure will advance the development of novel materials for a variety of energy and environmental applications. This instrument will require hot-source neutrons ($\lambda < 1.0$ Å) to achieve high resolution at high-Q ranges with a focused beam that can accommodate small sample sizes.

d. Small Angle Neutron Scattering Instrument: The purpose of this instrument is to uncover nano, meso, and microstructural features that inherently control macroscopic performance of materials that are critical to energy and the environment. High brightness and wide Q-range small angle neutron scattering is crucial for discovering these multiscale features and how they temporally evolve. Multimodal measurements with small angle X-ray scattering will enhance our understanding of these complex evolving systems, while the ability to use a diverse set of sample environments will enable access to nascent material properties.

4.6.1.2. Imaging Capabilities

Neutron imaging is rapidly developing the ability to generate multiscale images, measuring average microstructural properties at the voxel level. Bragg edge imaging allows one to measure the local lattice spacing to determine local crystal phase volume fraction and possibly enabling the measure of strain. Dark-field imaging using a neutron grating interferometer yields the correlation function in each voxel, so that one can analyze heterogenous, thick samples. Environmental and energy systems are inherently hierarchical structures, and such a measurement capability would be a boon for *operando* or *in situ* studies in these fields. To move these multiscale methods to *operando* studies, the apparatus will require the highest source brightness that can be produced, in addition to focusing optics for image formation. Further development in these "Wolter optics" will improve the spatial and temporal resolution of neutron imaging to be on par with second generation synchrotron imaging instruments, *i.e.*, few micrometers in a few seconds. To pair an X-ray source with such a high-performance neutron imaging station demands more than laboratory X-ray tubes. To this end, a compact light source based on inverse Compton scattering would be a powerful tool to include in neutron imaging capabilities, and such a configuration would only be feasible at a neutron source.

4.6.2. Interfaces

Interfaces play critical roles in governing the performance of batteries, fuel cells, and catalysts. Debates surrounding the composition, structure, and even the thickness of these interfaces hinder targeted design and tailoring for specific functionality to enhance overall performance. With more accurate neutron instrumentation that can probe shorter length scales and faster time scales, scientists and engineers will be able to study interfaces with low atomic number elements prevalent in such systems, *e.g.*, water, carbonate electrolytes, Li ions, and hydrogen. Such studies will enhance energy and environment applications ranging from electrochemical energy storage to catalysis to geochemistry. The panel has identified several neutron instruments that would play an important role in studying such interfaces.

a. Wide Angle Candor Reflectometer**:** The current Candor reflectometer opens new capabilities for the studies of the time evolution of the depth profile of near surface layered structures. By measuring the reflectivity at a single detector bank angle, a range of Q-values can be measured simultaneously with integration times short enough to support kinetics measurements. An instrument must capture Q-ranges needed to characterize features of thin layers at high-Q and the features of thicker layers with greater roughness at low-Q. This broad Q-range can be extended in two ways, first by increasing the wavelength bandwidth, which requires analyzer crystals other than graphite. Second, it is also important to increase the angular range of the incident beam as much as possible. An optimized reflectometer would measure large samples at simultaneous Q-ranges by coupling large wavelength bands with a broad incident beam divergence.

b. Grazing Incidence Small Angle Scattering (GISANS): With recent advances in software to model and fit GISANS data, the case for GISANS is becoming more widespread and accessible. This technique has unique applications in the study of batteries, fuel cells, catalysis, and corrosion. Including slit geometry and sample alignment stages needed for GISANS into one of the SANS instruments would lead to having this extra capability to probe interfaces.

c. Neutron depth profiling (NDP): Highly complementary to neutron reflectometry, NDP provides depth profiling of materials on larger length scales, with smaller sample areas and for samples with greater interface roughness. Having both instruments at the same facility allows for a synergistic program with shared ancillary equipment where proposed experiments can be optimized. The NDP should receive a high flux end station and a sample chamber with multiple detectors to increase measurement throughput.

4.6.3. Ion, Charge, and Mass Transport

The transport of ions and molecules through a material limits the performance across a broad range of devices including batteries, fuels cells, catalysts, adsorbents, and membrane materials. To optimize by design, for example, ion transport in a solid-state battery electrolyte, or molecular transport in a molecular sieve used for separations, it is necessary to understand the transport mechanisms. Neutron scattering data probing local and average structure, along with dynamics, can provide the insights needed for this improvement by design when coupled with computation. The following techniques should be included in the suite of instruments needed to understand such transport phenomena.

4.6.3.1. Quasielastic neutron scattering (QENS):

This technique measures atomic and molecular displacements in space (Å to nm) and time (ps to ns). The method probes dynamics from vibrational modes down to slow diffusive motions and is unique to the field of neutron scattering. There is no X-ray equivalent to QENS. As such, QENS plays a prominent role in ion diffusion studies in energy-related materials, from electrodes to electrolytes, solids to liquids. The charge transport in these materials is tied to single-particle and correlated motions of the charge carriers, which give rise to the incoherent and coherent neutron scattering signal, respectively. In hydrogen-bearing materials, incoherent scattering dominates, whereas for many other elements, including deuterium and many metal cations, incoherent and coherent signals are comparable in strength. Traditional neutron scattering experiments cannot distinguish between coherent and incoherent QENS signals. Polarization analysis can separate coherent and incoherent signals, and it has become common at some neutron spectrometers, but not with the very high energy-resolution spectrometers dedicated to QENS measurements. This lack of polarization analysis capability significantly hinders application of QENS to studies of collective charge transport phenomena in energy-related materials. The future instrument suite should include at least two QENS instruments:

a. High intensity QENS: A direct geometry instrument affording adjustable elastic resolution, intensity, and dynamic range and directly useful for QENS. In conjunction with modeling, QENS provides information on diffusive transport mechanisms in materials, which are not accessible in other ways. Most studies have focused on the diffusive motion of protons, but battery research requires Li (^{7}Li for neutron scattering) and soon will focus on Na and Mg, all of which are weaker scatterers than H. It complements and extends the time scale attainable with other techniques, *e.g.*, NMR or Spin Echo.

b. High-resolution QENS: A backscattering instrument with higher energy resolution is essential for energy research, including batteries, fuel cells, catalysts, and porous materials. High-resolution QENS is intensity-limited and would benefit from implementation at a high flux source.

4.6.4. Multi-Modal Capabilities

In addition to the specific instruments and capabilities outlined above, the facility design must also support new use cases, both anticipated and unanticipated. One area requiring support is multi-modal measurements that enable combinations of complementary measurements on the same sample to understand complex and evolving material systems. Ideally these measurements should occur simultaneously on the same instrument platform. Here, a new facility provides an opportunity for innovation that we must seize, to support cutting-edge research in the 21st century and beyond. For example, recent advances allow compact light sources with a footprint on the order of 30 m^2. Combined neutron and high-energy X-ray scattering would be game-changing for multiple instrument types, alloying the temporal, spatial, and chemical sensitivities of both probe types. This capability would allow measurements of multiple phenomena in a single shot and aid in data reduction and analysis to help deconvolute complex phenomena.

Similarly, SANS and wide-angle neutron scattering (WANS) in a single instrument using both thermal and cold neutrons would lead to unprecedented information on single samples undergoing complex changes. Development of such an instrument could utilize an over-illuminated beam port (i.e one that accepts neutrons from both the cold source and surrounding thermal moderator) to allow for both thermal and cold neutrons to impinge on a single sample. WANS + SANS would provide structural information across an unprecedented range of length scales, facilitating new insight into how materials evolve and respond to driving forces from the atomic scale to the micron scale.

Given the significant capital investment, long lead time, and infrequency of new neutron sources in the US, it is critical that we explore and embrace ambitious concepts such as these during the design phase. This also requires that ample space is included in the facility design for signature large-scale instrument concepts, including those we can name today and those sure to develop over the facility lifetime. Multi-modal capabilities must also be supported via more traditional means. Staging and measurement areas must be constructed with sufficient space, instrumentation, and technical support to enable users to incorporate complementary measurement instrumentation, for example FTIR on a Neutron Reflectometer, either that they brought with them or as provided by the facility. To the extent possible, transferable sample environments should be designed and built that can be deployed *across multiple instruments*, without exposing the sample to ambient conditions.

4.7. Enabling Infrastructure

To efficiently and effectively use neutron scattering to address the scientific challenges outlined above, a robust suite of supporting capabilities is essential. These include sample environment, beam line automation, software, and computing hardware to support on the fly decision making during a neutron measurement, laboratory space for experiment preparation, storage space for user equipment, and routine sample characterization facilities, such as XRD, that can be used to examine samples before and after they are exposed to neutron beam. The facility needs to be designed to be future proof, with space to accommodate new needs and developments over time.

It is imperative to emphasize the vital importance that staffing and support (*e.g.,* for sample environment and data analysis) has played in the success of the NIST neutron scattering program, to date. The staff at the NCNR, including instrument scientists, sample environment, reactor operations, health physics and many others, has been indispensable to the NCNR's success, and they are a shining example that other user facilities should attempt to replicate. While marquee instruments and superb facilities are no doubt essential to advances in neutron scattering, building instruments without sufficient staffing and support will result in a facility with limited scientific impact. ***For the future facility, it is crucial that planning includes ample staff support to preserve the strengths of the current NCNR program.***

Sample environments covering a wide range of temperatures, pressures, chemical environments (*e.g.*, reactive gases), and electrochemical environments are essential, given the need for in-situ and in-operando measurements, including those that mimic process operations conditions. This equipment needs to be designed with the efficient use of beam time in mind. Novel designs to facilitate rapid temperature changes, and precision mounts to reduce positioning issues and enable the interleaving of experiments by quickly switching between environments should be considered. Infrastructure, such as power, cooling water, gas lines and chemical exhaust needs to be in place and easy to access. To the greatest extent possible, changes in samples, sample conditions, and the operation of beam lines, should be automated so that the scientist can focus on science goals and not operations, and remote users can work effectively without requiring extensive staff support on site. Software developments to support Machine Learning/Artificial Intelligence (ML/AI) logic for direct feedback and autonomous experiment navigation during cycling and external stimuli will provide insight into transient phenomena and behavior under extreme conditions. The added understanding serves Density Functional Theory (DFT) and Molecular Dynamics (MD) modeling to develop adequate, predictive system representations.

Access to complementary specialized sample characterization tools, such as prompt gamma analysis will also be of value. This is an extremely accurate method for elemental analysis. While this subject is covered by another breakout group, we would like to emphasize its importance to energy-related research.

Finally, to properly support industrial research, efficient processes for dealing with proprietary measurements, and intellectual property, must be in place.

4.8. Conclusions

The importance of energy and environmental research for its broad benefits to society, human health, and to the future US economy cannot be overstated. Neutron scattering is a rare and precious national resource offering unique and critical capabilities for discovering, advancing, and accelerating future energy technologies, in addition to reducing, remediating, or eliminating adverse ecological impacts. It is essential to equip the nation and the broader scientific community with a modern and forward-looking neutron suite offering.

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5. Hard Condensed Matter Structure

5.1. Panel

Chairs:
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5.2. Glossary of Terms

AI: Artificial intelligence

Antiferromagnets: materials in which neighboring magnetic moments align antiparallel.

Atomic number: the number of protons in one atom of a specific element.

Hard condensed matter: solid and rigid materials like metals, minerals, and glasses that generally lack carbon-hydrogen bonds.

Ferromagnets: materials in which all magnetic moments align in the same direction.

In situ: refers to measurements made after a sample is modified incrementally.

Isotopes: nuclei with identical numbers of protons but different numbers of neutrons.

Magnetic moment: a quantum-mechanical property analogous to that of a bar magnet.

ML: Machine learning

Quantum materials: materials that exhibit topological properties and/or entanglement.

Scattering cross section: the probability that a neutron will scatter from an atom.

Operando: refers to measurements made while a sample is being changed in some way.

Polarized neutron: neutrons which have their spin aligned along a specific direction.

Quasiparticles: collective behavior of fundamental units which results in particle-like properties.

Spin: a quantum mechanical property that gives rise to magnetic phenomena in materials.

Spintronics: an analogue of conventional electronics that uses spin and magnetism, instead of, or in addition to, the charge of electrons in the storage and processing of data.

Structure: how atoms or collections of atoms, and/or magnetic moments, in a material are spatially organized.

Topology: A phenomenon in which the behavior of electrons in certain materials are protected against changes or in some way mutually coupled.

5.3. Summary

The study of materials has propelled humankind forward from the stone-age to today's electronic age. Around the world, scientists and engineers are pushing matter to new frontiers. Hard condensed matter structural science is central to materials discovery and technology transfer and will remain so into the foreseeable future. Using neutron scattering techniques, the structure and behavior of materials can be probed statically, or while being manipulated *in situ* or *operando,* thereby expanding our understanding into new regimes. These efforts are interdisciplinary and serve as a bridge between fundamental research and industry that spans biology, medicine, chemistry, epidemiology, engineering, archeology and much more. The next burgeoning revolution is in quantum materials. As noted by the DOE Basic Research Needs Workshop on Quantum Materials for Energy Relevant Technology (https://doi.org/10.2172/1616509): "*Just as the discovery of semiconductors revolutionized computation and information storage, and ushered in today's hundred-billion dollar electronics industry, quantum materials have the potential to revolutionize energy and energy-related technologies.*" Being a leader in quantum materials research is a national mission, driving widespread investment from federal funding agencies in the many billions of dollars to grow and support the diverse research areas needed to develop the next generation of technologies that will meet the urgent demands for a sustainable and safe society. Beyond quantum materials, research into nano-structured materials, interfaces, spintronics, clean energy, cancer, space missions, and countless other areas will sustain and propel our society into the future. To achieve these scientific, technological, and societal benefits, the U.S. research community needs the ability to measure the average and local atomic and magnetic structures of matter with high precision. This is achieved with neutron scattering. Unlike X-rays, neutrons are uniquely sensitive to magnetism and light elements (i.e., those having a low atomic number such as oxygen and hydrogen) and can penetrate the walls of large magnets, furnaces, cryostats, and pressure vessels needed to establish extreme sample-environment conditions while still resolving the magnetic and structural properties inside a material.

The Hard Condensed Matter Structure panel recommends: substantially increasing the number of spin-polarized neutron scattering instruments, optimizing the neutron beam brightness at the sample position to enable spatially resolved measurements, building diffraction instruments for high demand and high throughput, provide *in situ* and *operando* lab capabilities on beamline instruments, building instruments capable of multimodal measurements spanning multiple time and length scales, providing extreme sample environments with the ability to induce novel and metastable states, building a dedicated steady-state high magnetic field beamline, and providing pulsed and pump-probe capabilities. A key enabler integral to all future instruments will be the implementation and development of AI/ML. AI will close the feedback loop on experiments, providing ultra-high throughput and information-rich measurements. Taking advantage of the full polarized neutron cross section with fine resolution will also provide reliable training data sets for AI models with predictive power for material structure and function.

5.4. Science Drivers for Neutron-Based Research

5.4.1. Future Neutron Research for Hard Condensed Matter: Two Basic Requirements

There are two basic requirements needed to advance hard condensed matter structural science with neutron scattering: (1) state-of-the-art neutron instruments that provide world-leading material research capabilities, including the ability to resolve smaller structures, measure smaller signals, and conduct *operando* measurements; (2) high-throughput techniques to accelerate materials discovery. These requirements, when simultaneously satisfied, will enable the scientific, technological, and societal advancements necessary to address current and emerging national priorities.

The need for (1) state-of-the-art neutron instruments is discussed in the following two sections: *Quantum Materials* and *Functional Materials*. Numerous science cases are provided to highlight the benefits that new, specialized, and more advanced neutron scattering instruments will have on science and technology research of national importance. The need for (2) high-throughput techniques to accelerate materials discovery is discussed in the subsequent section: *Materials Discovery*. Current U.S. capacity for neutron measurements has been curtailed as facilities have been shuttered, leaving only three domestic neutron scattering facilities, contrasted against nine European sources and five sources in Asia. This bottlenecks the U.S. research community, crippling its ability to remain a world leader in materials structure research. In a recent survey of U.S. neutron users [1], 77% of the respondents reported problems caused by the scarcity of neutron measurement time, resulting in an inability to complete their research, losing or under-utilizing grant funding, and reductions in information obtained. Nearly 20% of these researchers took their research overseas. The lack of U.S. neutron measurement capacity has also stretched the time between project inception to beamtime to more than six months, which is far too long to conduct ‘cutting edge’ research and wholly incompatible with industrial research and development. An important scientific case can be made for high-throughput techniques by leveraging the materials genome paradigm. This approach, sometimes called materials by design, uses AI to design materials with specific and predictable properties. It has relevance to virtually every facet of materials science: designing better structural materials, better magnets, better semiconductors, better battery materials, new quantum materials, new thermoelectrics, and new superconductors, among others. Implementing such a research paradigm requires extensive, accurate and detailed datasets to inform and train the AI models. Many of these insights rely on the unique capabilities of neutron scattering, such as its sensitivity to magnetism and light elements. Arguments can also be made that large segments of the science and technology community advance by pushing the boundaries of system design or innovation, which does not necessarily coincide with the cutting-edge of neutron scattering techniques. In other words, increasing the throughput of neutron measurements, rather than its capabilities, drives science forward. This motivates investment in numerous high-throughput (high flux, fast measurements, flexible environments) neutron instruments.

Neutron scattering provides researchers with a wealth of information, much of which cannot be obtained using any other method including X-ray, light, and electron scattering, which are techniques that yield complementary, not substitutional, insights. A new reactor will offer enormous opportunities to push the boundary of materials science and physics forward by increasing the neutron flux delivered to modern instruments thereby making it possible to probe much smaller structures with higher accuracy and to improve the throughput of scientific investigations. For structure and magnetism this means collecting data across a large dimensional space that includes three spatial translation directions, three momentum directions, three spin directions, and time, as well as the externally applied conditions such as temperature, pressure, magnetic and/or electric field, and out-of-equilibrium perturbations.

5.4.2. Science Drivers: Quantum Materials

The National Quantum Initiative (https://www.quantum.gov/) was established to provide continued leadership of the United States in quantum information science (QIS) and its technological applications. The unique information provided by neutrons, specifically those from a new reactor, would support, strengthen, and advance this leadership. Quantum materials exhibit fundamentally new physical states and behavior, for example topological quasi-particles, that will create new technological paradigms beyond conventional silicon-based computing. Quantum materials can be used for information transfer, taking advantage of entanglement and topological protection, energy efficient information technologies based on antiferromagnetism (high information density, fast (THz) spintronics), and high-temperature superconductivity to enable efficient power transmission. A new reactor equipped with state-of-the-art neutron instrumentation would facilitate the development of new methodologies for quantum materials exploration and discovery and deepen our understanding of quantum effects. It would also serve both fundamental research and industry in their common goal of advancing quantum materials and exploiting quantum effects for real-world applications, potentially motivating synergistic or collaborative activities.

Advanced neutron instruments with improved beam characteristics provided by a new reactor source could begin to probe “driven” quantum states, such as those pushed through non-thermal pathways at quantum phase transitions, which are currently a challenge to access. Stroboscopic investigations of how magnetism and structure evolve in quantum materials upon application of an optical, microwave, or electrical-pump perturbation are in their infancy, but these could become routine. Key to such future neutron-scattering studies are methods that exploit neutron-spin-polarization analysis, which is the gold standard neutron measurement. Advances in quantum-materials research require exquisite knowledge of the atomic, spin, and orbital structure of materials. Neutron scattering methods, particularly those that use spin-polarized neutron beams, are ideally suited to disentangle these distinct properties. The following discussion details some of the science cases and technological advancements in quantum materials that a new reactor would enable.

5.4.2.1. Science Case: Unique insights into quantum materials with neutron polarization

Modern complex quantum materials harbor unique spin and orbital-dependent properties that can give rise to efficient, potentially controllable, spin-to-charge interconversion for new devices. For example, antiferromagnetic materials show significant promise in fast, low-dissipation (e.g., energy efficient) devices because they are insensitive to stray magnetic fields and operate on THz frequencies. Similarly, geometrically frustrated magnets can stabilize complex spiral or non-coplanar magnetic order parameters that respond to external magnetic or electric fields even in the absence of a net magnetization, thus affording writability. Specific challenges exist in determining the spin structure of a material with standard unpolarized diffraction, such as confirming chirality, characterizing domain structures, probing local magnetization density, and understanding spatial inhomogeneities from complex multi-Q structures. The solution is to use spin-polarized neutron beams to gain access to the full spin polarization matrix. Unfortunately, the United States lags far behind the rest of the world in polarized neutron capabilities. A new reactor would provide a great opportunity for the U.S. to regain leadership in this area and apply it to quantum materials research. Moreover, a new reactor would allow for novel neutron instrument concepts to be designed, tested, and deployed. Using highly focused beams to provide small beam spots would resolve the complex magnetism that exists in the ever-miniaturizing sample sizes needed for realistic technological applications. Small beams and detectors with fine spatial resolution could enable Bragg raster scanning or far-field tomography to probe the domain structure within a material. As a specific example, topological materials, including topological magnets and topological insulators, possess quantum states that exist only at the surface (top 1-2 unit cells) of the material and are responsible for the exotic behavior. The high-resolution measurements proposed in this report could spatially distinguish different the bulk and surface, or ‘edge,’ states significantly improving our understanding of these materials. Systems with exotic magnetism often require multiple simultaneous parametric investigations. The applications of electric and magnetic fields, strain and temperature, pressure and temperature or pressure and magnetic fields, expand the phase space for a more accurate description of the system through *operando* measurements.

5.4.2.2. Science Case: Magnetic interfaces for spintronics

Heterostructures and interfaces between different materials have played a critical role in the discovery of new physical behavior and form the basis for a wide range of microelectronic, spintronic, and optoelectronic devices. Polarized neutron reflectivity is the gold standard technique for probing magnetism at interfaces, providing quantitative information on the magnitude of the magnetization density and how it changes spatially with distance from the interface. Developing a more complete understanding of quantum material interfaces will require improved measurement capabilities to detect smaller magnetization values, probe samples with smaller areas, and collect time-resolved reflectivity under applied fields and external stimuli. These advances will yield new insights into magnetism at interfaces between topological or correlated materials, the ability to manipulate magnetic order with electrostatic or electrochemical gating, the generation of spin currents or torques from topological or antiferromagnetic materials, and emergent magnetism in Moiré lattices of twisted two-dimensional heterostructures.

5.4.2.3. Science case: Spintronics for low power electronics

Spintronic technologies use the electron spin, rather than its charge, to perform data logic processing and data storage operations. These technologies are already present in many devices, such as hard drives and magnetic random-access memory (MRAM) and offer a promising route to achieve energy-efficient computational technologies. Expanding the use of spintronic devices beyond data storage and into information processing would be transformative to U.S. energy consumption. Notably, current electronic computing technologies consume ≈ 5% of all the power generated in the United States, and this is expected to exceed 20% by 2030 as data centers, cloud computing, and data storage grow. The recent and rapid expansion of artificial intelligence will significantly increase demand for networked computational power and exacerbate energy needs. Spintronics, due to their use of spin, are predicted to consume merely ≈1% of the time-integrated power of analogous electronic devices. Thus, research capabilities that advance the materials and heterostructures upon which spintronic technologies are based serves society by reducing power demand, enabling new approaches for computational platforms, and reducing consumer costs. Commensurate with the demand for increased energy efficiency in consumer devices is a demand for miniaturization. For spintronic devices this requires identifying strategies to switch the direction of the magnetization locally at faster timescales and with minimal energy dissipation. A leading approach uses spin-orbit torques in which a charge current is passed through a material adjacent to a ferromagnet; the charge current generates a perpendicular spin current that imparts angular momentum to the ferromagnet, causing the magnetization to switch. Polarized neutron reflectometry plays an essential role in our efforts to understand and engineer the magnetic materials used in these applications by providing a detailed picture of the depth-resolved nuclear and magnetic structure within these device structures, leading to new insights into spin-orbit torques. Additionally, antiferromagnetic materials that lack a net magnetization have emerged as leading candidates for these applications. Advanced neutron diffraction instruments are needed to probe the spin structure within ultrathin layers of antiferromagnets that will be used in emerging spintronic technologies.

5.4.2.4. Science Case: Advanced Neutron diffraction to study accurate changes in lattice parameters and competing spin, orbital, and charge orders

Spin, orbital, and structural degrees of freedom are often highly entangled in quantum materials. This coupling can play different roles depending on the material. For instance, in Kitaev magnets, spin-orbit coupling entangles the spin and orbital degrees of freedom and stabilizes a quantum-spin-liquid state; at the other end of the spectrum, the orbital degree of freedom can couple to the lattice and effectively quench quantum effects. The ground states of quantum materials can be extremely sensitive to perturbations and impurities. Understanding subtle structural distortions is crucial. For example, the quantum-spin-liquid state often lies close in energy to that of valence-bond crystal states and/or magnetic order. The valence-bond crystals may exhibit large distortions of the unit cell. Here, neutron diffraction measurements on single crystals at a high-brightness source could allow for the discovery of complex singlet/dimer states or incommensurate magnetically ordered states.

Neutron diffraction is commonly used to determine the lattice parameters and structure of solids. However, current instruments lack the ability to resolve extremely small structural changes. Neutron Larmor diffraction, which uses polarized neutrons to measure such structural changes, can achieve ultra-high resolutions with a $\Delta d/d$ value of order of 10^{-6} and is extremely bulk sensitive [2]. Using this technique, one can accurately determine the tiny lattice distortions induced by uniaxial pressure needed to de-twin unconventional superconducting iron pnictides [3]. Interesting quantum states may involve subtle rotational symmetry breaking, such as nematic order or ferro-quadrupolar order that Larmor diffraction can detect in the structural response [4]. Recently, neutron Larmor diffraction was used to detect minute lattice distortions in a Kagome-lattice magnet [5], as shown in Fig. 1. Neutron Larmor diffraction is very difficult to implement at a spallation neutron source, but it is ideally suited to the characteristics of a reactor.

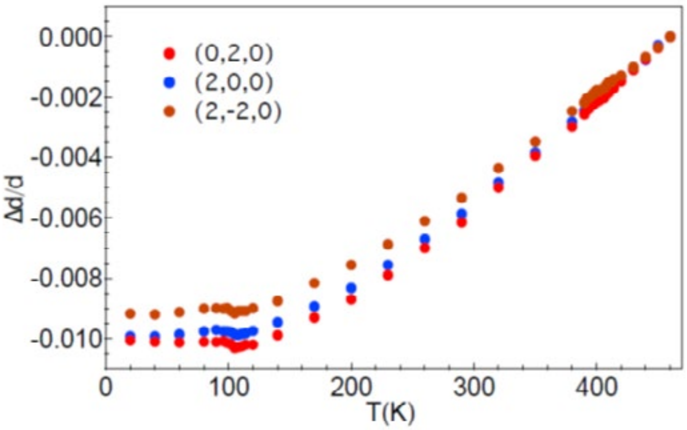

Figure 1. Neutron Larmor diffraction can be used to determine the temperature dependence of the lattice distortions with high accuracy. This example shows data measured on the Kagome-lattice magnet FeGe [5].

5.4.2.5. Science Case: Using entangled neutron beams

The extreme quantum limit of quantum materials is defined by the presence of a macroscopically entangled wavefunction. Such a state has not been proven to exist in any material because there is currently no way to probe entanglement of the many-body electronic wavefunction directly inside a material. Such research could create new quantum information technologies where quantum states are protected from decoherence by this many-body entanglement. It is possible to prepare beams of neutrons in entangled spin states [6, 7]. The Einstein–Podolsky–Rosen pairs comprising the neutron entangled state are delocalized laterally across a neutron beam, separated by the coherence length, such that each member of an entangled neutron pair can interact with a different region of the material. The transmission of the neutron beam through a sample will exhibit a “quantum erasure” of a double slit diffraction pattern that is sensitive to entanglement within the material across the coherence length of the entangled neutron, offering a completely unprecedented view of nature. Future neutron instrumentation should be constructed to take advantage of this possibility.

5.4.2.6. Science Case: Single-molecular magnets for qubits in quantum information sciences

Single-molecular magnets (SMMs) are candidate materials for qubits in quantum computers. The magnetic anisotropy is the most important ingredient dictating the behavior of a SMM. Below a certain temperature, which depends on the magnetic anisotropy and the total ground-state spin, SMMs exhibit magnetization hysteresis loops with resonant steps due to quantum tunneling. Recently, molecules that exhibit long-range magnetic coherence times have come to the forefront as potential molecular qubits for quantum information science (QIS). Understanding the correlations between the molecular structure and magnetic anisotropy is crucial to the development of better SMMs and molecular qubits. Electron paramagnetic resonance (EPR) spectroscopy is a typical method of choice to establish the direction of the anisotropy axis in a molecule, but EPR lacks the ability to interrogate each individual metal ion in such molecules with multiple metal centers. In contrast, polarized neutron diffraction offers the ability to measure the susceptibility tensors on each magnetic site and thus establish the full magnetic anisotropy for both individual ions and the entire molecule [8]. As an example, see Fig.

3 of Ref. [8] (https://doi.org/10.1002/chem.201803300). Such methods would inform research aimed at finding optimized Qubit materials.

5.4.2.7. Science Case: Probing and harnessing disorder for new material properties

Conventional materials design often focuses on systems that are structurally and chemically well ordered. However, recent work has shown that disorder can be used as a handle for materials design. Disorder is also intrinsic to many (potentially all) synthesized materials. Local magnetic order has been shown to drive fundamentally new behavior in frustrated quantum magnets where the long-range ordering of spins is suppressed due to the lattice geometry. This leads to a macroscopically large number of degenerate ground states and, consequently, local spin fluctuations, as the material is not restricted to a single energetically favorable long-range ordered state [9]. The unambiguous extraction of the magnetic pair-distribution function (mPDF) (powder) and 3D-delta-mPDF (single crystals) signal offers opportunities for deep and transformative insights into complex materials with short-range spin ordering. Studies where mPDF is expected to have a strong impact include those trying to understand why geometrically frustrated quantum magnets select a mesoscale ground state to break degeneracy, how subtle structural and magnetic interactions couple to the ferroic phenomena in multiferroics, how doping introduces local spin alterations in magnetic semiconductors, how structural disorder suppresses long-range order in spin glasses, how spin-stripe correlations arise in cuprate superconductors, and how short-range correlations drive long-range order in magnetic materials.

5.4.2.8. Science Case: Unconventional Superconductors to transform the energy landscape

Despite decades of intense research, there is still no comprehensive theory that can explain or predict high-temperature (“high-T_c”) superconductivity. A major problem complicating these efforts is the fact that these materials are inherently “dirty”, i.e., rich in defects such as vacancies, substitutions, and dislocations, and subject to significant structural, electronic, and magnetic inhomogeneity. In many exotic superconductors, competing ordered states involving the charge and spin degrees of freedom may co-exist with the superconducting phase at low temperatures. The balance between these competing orders may evolve in intriguing ways as a function of doping. Multiple phases may coexist due to disorder or microscopic phase separation. For example, charge-density-wave (CDW) and spin-density-wave (SDW) phases are known to be closely related to the superconducting state in high-T_c materials. However, information about the interplay between these phases that brings about (or inhibits) superconductivity is lost using current neutron scattering techniques due to spatial-averaging effects. Instrumentation employing highly focused spin-polarized neutron beams at the future NIST neutron source could provide new insights into this mesoscale inhomogeneity and mechanisms that enhance high-T_c superconductivity.

5.4.3. Science Drivers: Functional materials

Materials are often categorized into two groups by their societal utility: structural and functional. Since structural materials are expected to be a focus of the Engineering Panel report, this report will only consider functional materials. Technologies based on functional materials leverage their electronic, optical, thermal, and magnetic properties. These technologies play critical roles across society, spanning energy, information, biomedical, and defense applications. Understanding the structure and response of a material is essential to efforts to optimize their functional properties and eventual performance in devices. Neutron scattering measurements, particularly those performed in operating conditions representative of real-world applications, are required for the detailed insights they provide. A new reactor source at NIST would enable these measurements to be performed faster and more effectively, thereby accelerating the development of new technologies. The following science cases provide context for this motivation.

5.4.3.1. Science Case: Designing novel materials with improved functionality and lifecycles

Solid-state fast-ion conductors underpin a broad range of energy storage and conversion technologies; applications include solid-state batteries, electrode catalysts, electrochemical capacitors, oxygen pumps, and gas/ion sensors. Designing novel materials with improved functionality and lifecycles is impossible without a detailed understanding of how the microscopic structures in the bulk as well as at the surface of battery materials changes under operating conditions. Neutron diffraction, neutron reflectometry, and small-angle neutron scattering continue to provide crucial and unique insights, as they are particularly sensitive to hydrogen and lithium, key constituents of battery materials. The ability of neutrons to penetrate and probe deep within materials and devices is fundamental to *in operando* studies of defect formation and clustering and how they lead to failure modes. Thermoelectric and optoelectronic materials are ubiquitous in energy conversion technologies and sensor applications. Neutrons provide important, and often unique, insights about the microscopic structure of such materials, which often contain both light and heavy elements, a situation for which X-rays often cannot assess the effects of the lighter elements on the materials properties. Many functional materials properties are derived from local disorder and short-range correlations. The large configurational degeneracy that results from such complex disorder can enhance various responses to external stimuli, yielding materials that are extremely sensitive to external perturbations and that have fast, energy efficient, or other highly sensitive functionalities. To achieve these desirable functional responses requires a detailed understanding of the physical principles that govern the properties of materials in the presence of complex disorders, and this can only be done if we have the ability to measure the resulting materials structures under various operational conditions. Increased neutron flux and advanced instrumentation are essential to such structural investigations from the nanoscale to the microscale in bulk materials, thin films, and heterostructures and will require the use of neutron diffraction, advanced real-space analysis (such as 3D-deltaPDF), small angle neutron scattering, and neutron reflectivity techniques.

5.4.3.2. Science Case: Electronics and Beyond CMOS

Silicon-based electronic technologies are a marvel of modern manufacturing. Leading these technologies is the MOSFET transistor. This device is the building block for all processors, solid-state memory, and many sensors. The architecture underlying these devices is an atomically thin, defect-free, insulating, oxide layer that separates the silicon layer from the metallic gate that controls the device. The metal-oxide layer and its interface govern device operation, but as these are buried structures they can be challenging to study. Flash memory has a similar structure, but rather than a simple insulating oxide layer, the layer between the gate and the silicon is a tri-layer oxide/metal/oxide structure. Devices based on the giant magnetoresistance effect rely on an atomically thin metallic spacer layer, and optoelectronic sensors rely on a high-quality interface to allow electrons to move between the electronic and optically sensitive layers. In virtually all electronic, magnetic, and optical devices, the interface is central to device function. Therefore, interface design is of paramount importance to the success of these technologies.

Neutron reflectometry can probe buried interfaces with atomic resolution and unique sensitivity to light elements such as hydrogen, oxygen, and carbon. However, to obtain sufficiently large signals that can be analyzed, current neutron measurements require large samples (>25 mm^2), which are not representative of actual devices. The capabilities afforded by a new reactor and an advanced, polychromatic reflectometer, would allow much smaller structures to be measured. Critically, this new capability would permit electronic devices to be probed *in operando*. That is, using the higher neutron beam brilliance, single devices could be probed, and the interface structure measured, while the device is actively under test. This would allow the functionality to be directly correlated to the interface structure. A key example of this is the tri-layer structure of a FLASH memory cell, which fails over time as the interface degrades. This degradation is a consequence of oxygen ion migration, which is challenging to study with other techniques like X-rays. Neutron reflectometry performed on a single device can measure this migration and provide insight into the lifetime and failure mechanisms of these devices. Understanding the structure-performance relationship in these systems would yield better devices that could operate faster, at higher efficiency, and for longer periods, and/or be made smaller (miniaturization). In turn, this would allow deployable consumer electronics and facilitate the so-called ‘internet of things.’

5.4.3.3. Science Case: Neuromorphic computing for the needs of an advanced society

Modern computing architectures use the MOSFET transistor as an on/off switch, forming the hardware foundation of binary data storage and processing, including computer logic. These architectures have separate data depositories and computational nodes, a design that works very well for addressing some computational problems. However, this is not how biological computers, e.g. brains, operate. In these systems, the computational and data storage nodes are co-located. This architecture offers significantly higher efficiencies with problems such as pattern recognition, a field that is increasingly important as society adopts increased automation. Naturally, attempts have been made to design a computational analog of the brain, which comprise the field of neuromorphic computing. Leading efforts in this field use defective oxides and an electric field to move the oxygen defects within the material. Oxygen is, however, a light element and therefore challenging to measure with X-ray techniques. Neutrons have a strong sensitivity to oxygen and can be used to measure ion migration, providing new insights that can be leveraged to design neuromorphic materials and corresponding devices. Hardware-based neuromorphic computing would transform civilization. Many menial tasks currently performed by humans, such as reading and evaluating documents, transportation, quality control (for example in food quality, waste management, and manufacturing oversight) could be performed by neuromorphic computers. Doing so would free the people currently doing these tasks to pursue other goals. It would also reduce the cost to consumers because these tasks could be performed around the clock and with reduced staffing and overhead.

5.4.3.4. Science Case: Nanoparticles and Quantum Dots For Advanced Electronics, Medicine, and Energy

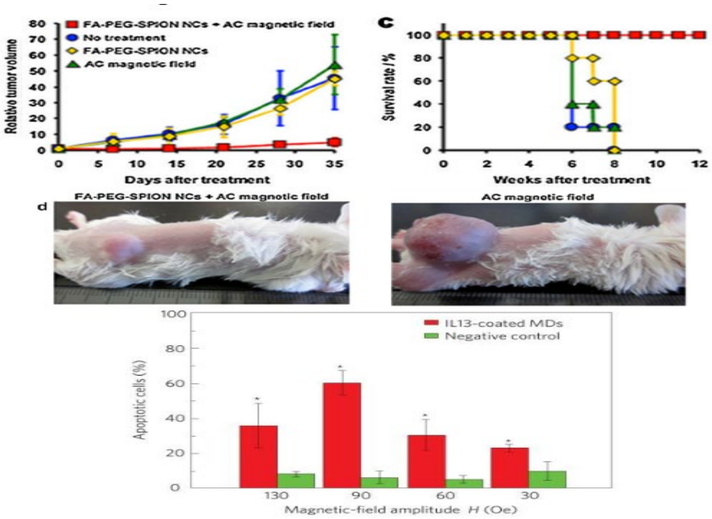

Figure 2. Application of magnetic nanoparticles to treat cancer. From https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3677408/

The functional behavior of materials is determined by a balance of different fundamental energies, and as a material is made smaller this balance changes. These changes can be leveraged to achieve new functionalities, allowing new technologies to emerge that serve the greater society. Nowhere is this as apparent as in the field of nanoparticles and nanomaterials. The quantum dot is a prototypical example of this effect and exists in today's cutting-edge technologies. Quantum dots are often made of semiconductors and are only ≈30 atoms across. This very small structure confines the electrons so much that their behavior is dominated by quantum effects. One consequence is that the 'color' of a quantum dot is explicitly tied to the size. This feature is used in electronics such as in high-end displays. Biomedical applications exist where quantum dots encased in an antibody shell attach to bacteria or even cancer cells; by looking for specific colors, doctors can diagnose these diseases with incredible fidelity, even at very low concentrations. Quantum dots can also be used to increase the efficiency of solar-cell technologies. Since solar cells absorb light in a very narrow color band and quantum dots are constrained to have only one color, they can absorb higher energy light and emit at a wavelength that matches the solar cell, increasing the efficiency. This benefits society by improving clean-energy production and can drive new innovations, such as providing energy to realize new frontiers in space exploration.

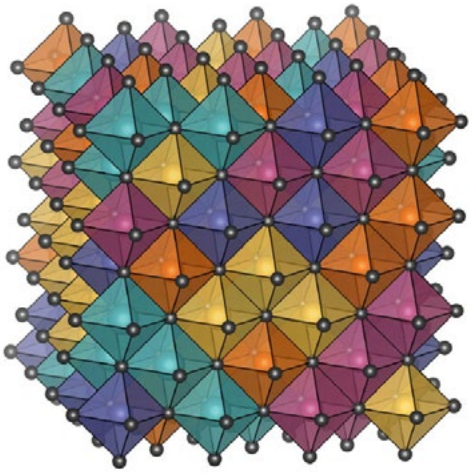

Figure 3. The crystal structure of a high entropy oxide, in which five different chemical elements shown in five different colors share a single crystal lattice (Ref: https://doi.org/10.1021/jacs.2c11608).

Another biomedical example involves using magnetic nanoparticles to treat cancer. Whereas large magnetic particles cannot transmit through the body because they tend to stick together (agglomeration), nanometer-scale magnetic particles lose a some of their magnetic stability, which discourages their agglomeration and allows them to pass through the body. By attaching antibodies to the surface of a magnetic nanoparticle, the particle can attach to, and target, cancerous cells. When an oscillating magnetic field is applied, the nanoparticle generates a small amount of heat. This raises the temperature of the cell to ≈ 43 °C, enough to kill it while leaving the rest of the tissue unharmed. Thus, cancer is treated without the unpleasant side-effects of radiation treatment or chemotherapy. This application has already been well demonstrated on mice. These same nanoparticles also improve the contrast in MRI and PET scans and can even enable multimodal imaging. As with quantum dots, this allows early and accurate diagnosis of medical issues.

In all these examples, the structure of the nanoparticle is explicitly tied to the application. For the quantum dots, increasing the diameter of the dot by even a few angstroms, essentially the size of one atom, significantly affects the color. Understanding the homogeneity of these dots, the smoothness of their surface, and the quality of the material inside the dot are all critical to making a monochromatic quantum dot with high light yield. For the magnetic nanoparticles, similar arguments exist, but with the added caveat that the magnetic structure inside the dot matters. How the magnetism swirls inside the nanoparticle determines how the nanoparticle interacts with the magnetic field and thus its efficacy in hyperthermia, MRI, or magnetic switch applications. Polarized-beam neutron scattering is uniquely suited to determining the structure of the dot and the magnetism within. New neutron instruments and sources would allow for the improved design of these systems, benefiting medicine and advanced electronics for years to come.

5.4.3.5. Science Case: High Entropy Oxides for Catalysts and Batteries

One emerging class of functional materials for which knowledge of the structure is especially important is high-entropy oxides (HEOs). In an HEO, multiple chemical elements are randomly distributed across the sites of a single crystal lattice. They are characterized by their large configurational entropy, as the elements can be arranged in an enormous number of different configurations. HEOs exhibit a remarkable coexistence of ordered and disordered phenomena. On the one hand, the average structure of an HEO is well-defined, as in a conventional ordered crystalline material. But on the atomic scale, local distortions are expected to be abundant. While it is still early in the life cycle of their development and optimization, HEOs have already shown remarkable potential for use in a wide range of applications including catalysis and energy storage. The advantage conferred by a high-entropy material over more conventional crystalline materials lies in its resistance to degradation. Achieving a structure-function understanding of high-entropy oxides requires a deep understanding of their ordered and disordered phenomena on all length scales, with a particular emphasis on knowing the positions of the oxygen atoms. This insight has been achieved using a variety of neutron scattering techniques including neutron diffraction, PDF, and SANS.

5.4.3.6. Science Case: Local Structure in Relaxor Ferroelectrics

The local-structure analysis first pioneered by B. E. Warren close to 50 years ago made use of X-ray diffraction. The technique became popular for studying disordered systems. With the advent of spallation neutron sources, the use of local-structure analysis spread beyond disordered systems to highly ordered systems, with improved intensity and spatial resolution. One class of materials to which local-structure analysis has made important contributions is relaxor ferroelectrics, which lie at the border between order and disorder. Relaxor ferroelectrics exemplify a class of functional materials where the interplay between disorder and phase instability results in inhomogeneous nanometer-sized regions of electric polarization known as polar nanoregions (PNRs). Although known for about 30 years, there is no definitive explanation for PNRs. The direct observation of the formation of polar nanoregions in $Pb(Mg_{1/3}Nb_{2/3})O_3$ using neutron pair-distribution-function analysis while cooling from 1000 K to 15 K demonstrated the existence of local polarization and the formation of PNRs having a local rhombohedral symmetry. The PNRs volume fraction increased from 0% to ≈30% on cooling from 650 K to 15 K. Below 200 K, the PNRs freeze into a spin-glass-like state [10].

5.4.4. Science Drivers: Materials discovery

Neutrons are widely recognized as the best probe for determining the crystal and magnetic structures of many classes of materials under well-defined equilibrium conditions. However, the utility of neutrons to inform materials discovery, investigate out-of-equilibrium metastable states, optimize growth processes, and measure simultaneously with other probes has not yet been widely established. In all sectors of hard condensed matter, there is an ongoing need to improve the methods used to discover new materials.

Currently, materials synthesis in hard matter research faces a series of significant challenges, including the ability to grow high-quality materials in a systematic, efficient way; mapping the phase space of materials properties and compositions quickly and with high detail; coupling probes and experiments without compromising results; providing robust, standardized measurements with high fidelity and availability; leveraging AI or ML to conduct efficient experiments or to notice important trends in data quickly; and coupling data collection, reduction, analysis, and interpretation.

The development of a next-generation reactor at NIST with state-of-the-art instrumentation would rapidly accelerate materials discovery and optimization. The following points are identified as enabling and accelerating materials discovery with neutron scattering.

1. The next generation of condensed matter experiments will be highly reliant on the efficient growth of high-quality materials. Neutron scattering has much to offer to modernize and accelerate this process. A next-generation suite of neutron instruments would offer facilities for *in situ* growth and characterization that spans wide length (centimeters to microns) and time (seconds to hours) scales. Such capabilities would provide significant advantages in detecting and stabilizing metastable states. These advances would also allow topotactic reactions, such as anion substitution, to be studied *in situ*, taking full advantage of the neutron's ability to resolve anions like nitrogen and oxygen, which is impossible with X-rays.

2. An increased neutron beam flux would make feasible focusing and time- and location-resolved rastering, or wide-beam tomography, thereby enabling mapping modes for measurements that are currently performed using a single beam and that have no spatial resolution. Many next-generation materials rely on hierarchical structures or mesoscale features that can be understood only with this type of spatial, high-throughput measurement. Its use on heterogeneous samples would greatly expedite the surveying of large composition spaces.

3. Next-generation neutron sources with an order-of-magnitude improvement in flux would allow for more flexible instrument designs to facilitate a broad array of *in situ* and *in operando* property measurements coupled with neutron measurements. This is particularly interesting in the case where the operational conditions of a material can alter its structure, such as electric-current-induced effects on crystal structure or photo-induced decay of films. On a continuous source with event-mode data collection, stroboscopic measurements become possible. *In situ* measurements of gas loading, pulsed measurements, driven materials with standardization for NIST would be feasible. Driving and studying metastable states is currently challenging but should become routine at a new reactor source.

4. Improved stability, performance, flux, and brightness of a next-generation neutron source would lead to more robust, standardized measurements of novel materials and metrology of high-value samples and devices. Massive improvements in throughput would lead to capacity gains that fundamentally change the barrier of entry to neutron measurements, expanding the user base, which is especially important for industrial and new users.

5. Incorporating AI, ML, and automation from the ground up would make for transformative advances in hard condensed matter structure research. Current neutron scattering users often experience long delays between data collection, reduction, and analysis. Fundamentally new advances could be made to interpret results and identify unexpected features and trends via real-time data reduction and analysis tools. Use of robotics and automation would enable high throughput measurement. Ongoing progress in AI and ML will lead to massive advances in our ability to analyze datasets that are ever larger and more complex. Developing standardized, transferable data structures will significantly decrease the time between data collection and scientific and technological insights.

5.5. Societal Impact and National Benefit of Neutron-Based Research

The National Science and Technology Council has put forth a list of critical and emerging technologies that are central to the national security and economic leadership of the U.S. [11]. These technologies include advanced engineering materials, quantum information technologies, renewable energy generation and storage, and materials for microelectronics, all of which depend on the research and development of new materials. Across the wide range of material functions required for these technologies, an immutable principle is that the properties of materials (electronic, optical, thermal, magnetic, and more exotic quantum behavior) derive from their local and macroscopic structure. As such, the ability to quantify and predict the structure of hard condensed matter materials is central to maintaining leadership in many of the listed critical technologies. Neutron scattering offers unique insights that no other technique can provide and is an indispensable tool in performing these evaluations.

The societal and economic impacts of these technologies are immense. For example, quantum information technology had an investment of $35.5 billion in 2022 [12], which is expected to grow exponentially. Much of this investment has focused on quantum hardware and the specific materials that are expected to enable high-performance quantum applications. Neutron scattering has and will continue to play a role in defining this future. These materials are highly sensitive to defects, interfacial structure, and crystalline quality, all of which can be probed in unique ways by neutrons. The propagating effects of quantum computing will lead to further advances in our ability to model complex materials and chemical reactions (especially those of catalytic reactions with high economic value), and model financial and geopolitical behavior.

The global microelectronics industry is predicted to grow by 6 to 8 percent a year and reach $1 trillion in revenue by 2030 [13]. Historically, advances in silicon electronics have come through understanding the physics of semiconductors. The next generation of high-performance microelectronics beyond silicon will revolutionize manufacturing and fabrication in the United States. New fabrication facilities (“fabs”) typically have a construction investment of about $1 billion such as the Wolfspeed silicon carbide plant [14] in upstate New York. These new materials will have much more complex electronic, magnetic, and chemical behaviors. Neuromorphic computing is projected to grow at an annual rate of over 20% by 2030 to $15 billion [15] and relies on subtle transformations of materials structure to store and process information in a faster and more energy-efficient way than traditional transistor logic devices. Probing these emerging materials requires unique insights enabled by neutron scattering. Strengthening domestic electronics development is a critical goal for economic growth and national security. Chips and sensors are critical components in many technologies (automotive, aerospace, healthcare, etc.) beyond the semiconductor industry itself.

Neutron scattering techniques enable the acceleration of materials discovery, with new materials having been central to societal progress for millennia. New electronics for the development of quantum computation, storage, communication, and transduction will take us beyond CMOS technologies. Spintronics for fundamentally new devices and energy efficiency will contribute to improving and enriching lives. All these efforts will grow the workforce, by providing training in cutting-edge technologies that will enable and maintain United States' global leadership.

In addition to the societal and technological benefits discussed above, there will be major impacts on the condensed matter and wider scientific workforce. Neutron users are hired to fill important R&D positions; neutron users gain valuable experience by designing and building unique experiments and working on cutting-edge science; neutron-enabled technologies create jobs; and hard condensed matter scientists have played historical roles in technology and policy leadership.

5.6. New instruments and new reactor's ability to facilitate science

A next-generation neutron reactor is ideally positioned to satisfy the full cross-section of state-of-the-art instruments needed to provide a comprehensive view of the structures of all solids. We note there is enormous overlap between the use cases described here and other panels, including energy materials, engineering materials, as well as soft matter.

Key characteristic needed for beamlines to address U.S. scientific and societal priorities

Polarization: Making optimal use of neutrons to characterize magnetic structures requires full neutron polarization capabilities. Such capabilities are relatively rare globally. Taking full advantage of the neutron's spin degree of freedom to develop these new beamline capabilities using spin-entangled states of neutrons would provide unique opportunities for future materials research.

AI and Machine Learning: Better and faster measurements are needed for hard condensed matter structural and magnetic studies. This requires automated sample changers and AI/ML driven automation. AI can help design and improve experiments by concentrating measurements on key regions of phase space and distinguishing weak signals from background. At the same time, high-efficiency instruments can be used to build training datasets of material structure-property relations. All instruments should have a digital twin to plan and support measurements and aid in the analysis of experimental data.

High Brightness and low backgrounds: Maximizing signal/noise/scattering volume is essential to make full use of neutron measurements. The ability to focus the neutron beam to very fine spot sizes will allow for the study of small single crystal samples (<1 mm) and single devices (< 10 micron), thereby pushing new instruments beyond the current state of the art.

Event-mode data: the ability to tag neutrons and the state of the sample synchronously in time*:* Utilizing event-mode data collection and stroboscopic measurement modalities will enable the study of transient, metastable, and/or out-of-equilibrium states. In many cases, such time-structured measurements can be carried out more efficiently at a high-integrated intensity continuous neutron source where there are no timing constraints.

Sample environment requirements: The ability of neutrons to travel through the walls of large sample environment equipment such as furnaces, cryostats, and magnets is a key advantage over comparable X-ray measurements. Measurements of hard condensed matter structures are typically performed under one or more non-ambient perturbations, including temperature, magnetic field, electric field, pressure, or a variety of dynamic stimuli such as microwaves, pulsed lasers, or pressure waves. The requirements are ever more extreme environments with optimization of signal to noise driven by low background and focused beams. Below is a table of target sample environments. Combinations of these are required. Supporting lab space is crucial and flexibility to do new science with new equipment is a prerequisite.

Instruments for Hard Structure (*List is not in any order of priority*)	**Characteristics**
High-throughput Powder Diffraction (hot and cold source)	Multiple high-throughput instruments for accelerated discoveries
High-throughput Single crystal	Multiple high throughput instruments for accelerated discoveries
Versatile beamline	Small beam, multi-modal, optical access, open beam area for pushing boundaries with neutron scattering.
Polarized Powder/crystal diffractometer (XYZ analysis)	Fully polarized instruments needed for magnetic studies.
Polarized single crystal (Cryopad compatible)	Fully polarized instruments needed for magnetic studies.
High Magnetic field Beamline >35 T	Provide unique capability at any neutron source
Polarized Mag-SANS	Fully polarized instruments needed for magnetic studies.
General Purpose SANS	Multiple high throughput instruments for accelerated discoveries
SANS interference	Enabled for realistic device investigations. Probe domains.
Grazing incident SANS	Nanomaterials and surfaces in thin films
Hot source diffractometer (high Q multipolar, mPDF)	Disorder structure and magnetism studies.
Polarized reflectometer	Thin films and magnetism in devices
Spin coherent beamline	Ultra-high resolution and advanced polarized scattering (e.g. Larmor procession, Interferometry for QM)
Development beamline	Essential for continued neutron leadership
Extreme environment beamline	High pressure, pulsed field. Multi-modal capabilities
WAXS (Wide angle SANS to high-Q)	Access cross-over regions in momentum space simultaneously

New Sample Environments
World leading steady state high magnetic field of 35 T
Pulsed magnets (>100 T). Can be well suited to CW – collect data during whole cycle using event mode
Automated sample changers for most environments: low temperature, high temperature, high magnetic fields
Optical access, Pump probes, Electric field. Multi-modal: X-ray (XAS, XMCD), ESR/EPR, Conductivity, etc
High pressure (> 100 GPa) at low temperature. Cells optimized for neutron measurements.
Gas atmospheres

5.7. References

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6. Hard Condensed Matter Dynamics

6.1. Panel

Chairs:
Martin Mourigal – *Georgia Institute of Technology*
Chen Li – *University of California, Riverside*

Panel Members:
Collin L. Broholm – *Johns Hopkins University*
Andrew Christianson – *Oak Ridge National Laboratory*
Olivier Delaire – *Duke University*
Jason S. Gardner – *Oak Ridge National Laboratory*
Sara Haravifard – *Duke University*
Raphael Hermann – *Oak Ridge National Laboratory*
Allyson Fry-Petit – *California State University, Fullerton*
Dmitry Reznik – *University of Colorado, Boulder*
Allen Scheie – *Los Alamos National Laboratory*
Hillary Smith – *Swarthmore College*

Scribe:
Rebecca Dally – *National Institute of Standards and Technology*

6.2. Glossary of Terms

AI: Artificial Intelligence

Antiferromagnets: materials in which magnetic moments are antiparallel.

Dynamics: the time-dependent motions of electrons and atoms in a solid.

Emergent property: one that “emerges” from many particles, none of which has that property.

Hard condensed matter: solid materials such as minerals, metals, glasses, etc.

Ferromagnets: materials in which magnetic moments are parallel.

Isotopes: nuclei with identical numbers of protons but different numbers of neutrons.

IT: information technology

Magnetic moment: a quantum-mechanical property analogous to that of a bar magnet.

Multimodal: providing two or more measurement capabilities at the same time.

Multicalorics: materials that exhibit thermal changes if subjected to magnetic or electric fields.

Operando: under operating conditions.

Phonon: a quasiparticle used to describe, for example, sound waves in materials.

Quasiparticles: fictitious particles used to simplify the descriptions of dynamics in materials.

Scattering cross-section: the probability that a neutron will scatter from a nucleus.

Spin: a quantum-mechanical property that gives rise to magnetic phenomena in materials.

Topological: related to geometry and symmetry of continuous deformations.

6.3. Summary

Modern technology is deeply anchored in our mastery of select materials like semiconducting silicon. As the quest for energy and quantum materials continues, integrating novel materials into revolutionary devices remains a developing area. The New Neutron Source (NNS) at NIST would facilitate significant leaps in technological advancements, transitioning materials from conceptual frameworks to tangible industrial applications. The NNS would empower the U.S. research community to identify and interpret novel states of matter through AI-enhanced, high-throughput experiments and tools designed to manipulate matter under extreme conditions. Moreover, the NNS would enable studies of dynamics spanning longer time scales than possible before with improved energy resolution, facilitating a deeper comprehension of nanostructured and driven materials in practical scenarios, thereby unraveling the intricacies of these systems to maximize their utility. Building on NIST's legacy of innovation and collaboration, the NNS would not only significantly augment research capacity in critical areas by maximizing the number of beamlines, but also establish new models for neutron scattering research. It would exploit the distinctive attributes of neutrons while pioneering instruments for multi-modal experiments and AI-driven discoveries and fostering an ecosystem of operando experimental setups. Neutrons are poised to decode the enigmas of condensed matter physics, from innovative electronic storage solutions to the subtleties of superconducting materials vital for quantum computing. Such research promotes and supports crucial U.S. economic domains, as it promotes energy autonomy, revolutionizes electronics, defines materials suitable for space exploration, and guarantees unparalleled data security. Fundamentally, the New Neutron Source at NIST is poised to reshape our understanding of materials, fortifying U.S. leadership in seminal scientific and technological domains.

6.4. Science Drivers for Neutron-Based Research

Overview: The study of the motions (dynamics) of atoms and electrons in materials holds the promise of discovering exciting new physics and transformative applications. While dynamical measurements are one of the most sophisticated and powerful tools of neutron-scattering research, their full potential to benefit industrial applications remains largely untapped due to a multitude of challenges. The next generation of instrumentation at the NNS aspires to elevate and broaden the U.S. research community, pushing the boundaries of hard-condensed-matter physics by exploring the dynamics of unique states of matter over unprecedented time scales and operating conditions. Moreover, it offers significant potential to investigate materials that deviate from the ideal, exhibiting atomic-scale defects, nonperiodic structures, and meso-scale complexity, shedding light on physics that transcends the conventional notion of infinitely lived, resolution-limited quasiparticles, which are commonly used to understand the properties of hard condensed matter. Furthermore, a significant challenge lies in aligning AI-based automation with the principles of solid-state chemistry, device physics, and the complexities of quantum many-body physics. *AI* integration is essential for accelerating innovation and supporting research that is both motivated by practical applications and driven by pure curiosity, but it requires the ability to verify and validate the "ground truth" in materials research. Neutrons offer an unparalleled capacity to investigate and validate these truths. Consequently, the NNS at NIST would play a crucial role in providing this certification, ensuring that the empirical realities align with the computational advances in the field.

Core 1 (new phases): The IT revolution that has shaped modern society is largely based on understanding and manipulating the electronic properties of semiconducting silicon. But there is a sense that we have only scratched the surface. We now understand that nature offers a vast variety of electronic states of matter with distinct properties that could fuel a new generation of advanced technologies. Neutrons will be the key to unlocking this potential. Capable of covering six orders of magnitude of time scales, inelastic neutron scattering provides a unique view of ultra-fast collective electronic properties that are the basis for understanding and applying such novel materials. Long-term electronic memory systems are currently based on forming, switching, and reading domain structures in ferromagnetic materials. By virtue of their net zero magnetization, antiferromagnetic materials offer great opportunities to increase energy efficiency, information density, and speed by orders of magnitude. Neutron scattering is key to understanding the electronic structure and dynamics of antiferromagnets, enabling a revolution in electronic information storage systems. Technologically relevant superconducting materials would transform transportation and energy distribution systems, and, again, neutron scattering is a key method with which to probe and understand the collective-electronic phenomena that promote electron pairing and superconductivity. The quantum spin liquid is a radically different electronic state of matter wherein the electronic spins, the basis for magnetism in solids, form a coherent quantum fluctuating state. The spin liquid supports emergent quasiparticles that are unique carriers of energy and information; their topological nature makes them of interest as a basis for quantum computing. Finding quantum spin liquids and characterizing their emergent quasiparticles requires extreme conditions of high pressure, low temperature, and high magnetic fields for which neutron-scattering methods are uniquely compatible. These extreme conditions are needed to tune quantum interactions and coherence in relevant materials so that researchers can map their ground-state and excited-state energy landscape. For example, magnetic fields can control topological and quantum properties by modifying the quantum wave-functions of particular states. In this case, the application of pressure can modify the size and hierarchy of quantum interactions to provide access to proximate quantum critical points that are not realized in materials under ambient conditions.

Core 2 (longer timescales): The Heisenberg principle of quantum mechanics endows the atomic world with intrinsic dynamics, deeply affecting how energy, information, and particles flow in materials at very short time scales. However, in most current applications of materials, for instance in devices and complex systems, it is the long-time-scale properties of equilibrium and driven steady-states that are relevant. Exploiting the quantum properties of real materials and driven systems requires connecting short-time quantum dynamics with long-time, often quantum-incoherent, behavior. Neutron scattering is a quantitative probe of quantum dynamics, but the coarse energy resolution of current cold and thermal neutron instrumentation is only matched to a narrow window of short time scales. The absence of measurements that can bridge this enormous timescale gap has significantly hampered the wide adoption of quantum materials in mainstream technologies and industrial applications. More fundamentally, theoretical models based on idealized quasiparticles, i.e. infinitely long-lived, coherent oscillations, are unable to explain or predict the properties of quantum materials in realistic systems and devices. High-resolution next-generation instrumentation will allow researchers to study directly the effects of decoherence, defects, imperfections, and interfaces in equilibrium and driven materials and thus accelerate the use of quantum materials in industrial applications. As an example, neutrons are ideally poised to reveal how energy flows through materials on multiple timescales. Neutrons traditionally measure the extreme short-time response (~10^{-12} s) of materials, but with high-resolution instruments it will be possible to probe these responses on much longer timescales, as the energy propagates farther through the material. Given recent proposals to use magnetic excitations as high-efficiency carriers of information ("spintronics"), it is crucial to understand not only the velocity and direction that energy flows, but also how far the excitations that carry the energy can propagate before decaying into a less useful form of energy. This is directly measured with neutron scattering methods and would show whether a material that *in principle* is useful for electronics can be so *in practice*. Thus, neutron scattering can provide the essential information needed to choose and design new materials for next-generation electronics.

Core 3 (embracing disorder): Solid-state electronic and energy technologies are built on a theoretical foundation based on the famous Bloch theorem, which simplifies the physical description of the collective motion (i.e. dynamics) of atoms and electrons in terms of quasiparticles. While this simplification has spawned elegant theoretical treatments that can capture the properties of bulk, ideal crystals such as silicon, departures from the perfect crystal often give rise to new and useful properties. For instance, the silicon transistors used in microelectronic chips rely on the extra electrons or holes that are introduced into the material via extrinsic dopant atoms. Relaxing the limitations of ideal crystalline periodicity forces us to develop new paradigms and to explore a vast space of material properties tuned by intentional imperfections. These imperfections, such as lattice defects (dislocations, surfaces, interfaces) or chemical variations introduced by doping and alloying, present a challenge to the current theoretical descriptions of crystalline solids. New behaviors and functionalities can also emerge from the complexity of nanoengineered materials or superstructure assemblies. Precisely stacked layers of twisted sheets of graphene, for example, can create a superconducting device. Tuned multilayers can also lead to phonon localization and coherent transport, enabling one to control heat flow. Neutrons are uniquely suited to help scientists probe the microscopic structure and dynamics of such novel complex materials, especially under externally driven conditions and in operating devices. Microscopic disorder can arise from synthesis conditions, but it always arises from dynamic motions of atoms at finite temperatures or even from the intrinsic uncertainty of quantum mechanics. Correlated deviations from a perfect crystal give rise to diffuse scattering, which informs us about the systematic, local rules that atoms or spins tend to adopt, and these correlations, in turn, affect their dynamical properties. Whether or not quasiparticles can form, or what types of collective behavior emerge, depend strongly on the nature of the disorder. Disorder can thus provide a means of controlling the behavior of materials and generating previously unattainable magnetic, electronic, or phononic properties. Using next-generation advanced neutron spectrometers, we will be able to understand how the properties of non-ideal and engineered materials emerge from the underlying complex, inhomogeneous structure and how we can tailor the interactions between the fundamental degrees-of-freedom of electrons, spins, and atomic vibrations.

Concluding Paragraph: Research on hard condensed matter dynamics is uncovering a vast expanse of challenges and questions, many of which are uniquely suited to investigation by neutrons. The examples discussed above are merely a few of many, as the capabilities of neutrons stretch far beyond this list. In the future, neutrons will serve as an indispensable tool to help us understand quantum processes, notably as materials transition from quantum coherence to classical behavior. The neutron scattering cross-section, which can be measured and quantified on an absolute scale, provides a valuable and rigorous benchmark with which to validate the accuracy of computational methodologies that aim to predict material behaviors. Furthermore, the synergy of neutron scattering with concurrent measurements, such as optical spectroscopy, paves the way for multidimensional views into material systems. The concept of "lab-on-a-beamline" will herald a transformative approach in which real-time, dynamical observations made under operational conditions are conducted at the facility, thereby bridging the gap between fundamental research and real-world applications. The potential for high-throughput studies with neutrons is deeply intertwined with automation and advanced AI methodologies. This combination promises accelerated discoveries and a deeper understanding of materials. Finally, the importance of extreme conditions—ranging from high-magnetic fields, ultra-low temperatures, and high pressures—remains paramount. These conditions push materials to reveal novel phases and uncharted behaviors.

6.5. Societal Impact and National Benefit of Neutron-Based Research

Overview: From semiconductors to superconductors, artificial intelligence to quantum computers, high-efficiency batteries to renewable energy sources, all hold the promise to reshape our future and profoundly affect our daily lives. Just as telescopes grant us stunning glimpses of distant galaxies, neutron-scattering techniques are invaluable tools capable of delving deeper into the complex behavior of emerging materials. Neutrons are a gateway to the quantum realm, unveiling the atomic-scale details of materials in a non-destructive and quantitative manner. With neutron scattering, researchers can achieve a much deeper understanding of the exotic and groundbreaking properties exhibited by novel materials. This knowledge, in turn, empowers the U.S. technological ecosystem and the public to realize the full potential of these materials in applications. The connection between scientific exploration with neutrons and real-world applications has the potential to reshape our technological landscape.

> *Core 1 (Manufacturing)*: Manufacturing currently makes up 12% of the total U.S. GDP, [1] and the U.S. is firmly situated as first-in-the-world in the production of chemicals and pharmaceuticals, computers, electronics, optical products, and coke and refined petroleum products. As we move into the future, these manufacturing areas will continue to evolve as our dependence on each shift. Advances in these fields help to secure our financial freedom as a nation and create U.S. employment. However, these advances depend critically on understanding the complex atomic-scale dynamics that drives the properties of electronics, optics, and catalysis. Research performed at neutron facilities has taught us that the dynamics of materials plays a fundamental role in all these U.S.-leading manufacturing areas, but funding and building advanced neutron instruments equipped with the ability to achieve sample environments under extreme equilibrium and nonequilibrium conditions will allow us to understand the dynamics of materials in regimes relevant to the manufacturing process.

Core 2 (Energy Independence): The U.S. is interested in gaining energy independence to ensure the economic future of the nation while also driving technologies to sustain that future. To reach full energy independence, a multi-technology approach must be adopted that includes electrification, solar power, hydrogen storage, fuel cells, and multicalorics. Understanding the atomic-scale dynamics of hard condensed matter materials used in energy technologies will allow optimization of such materials. But this understanding cannot be realized until we can probe the dynamics on a wide range of length and time scales under operating conditions, which are often extreme relative to traditional laboratory conditions. Moreover, moving to smaller samples and devices based on these materials is imperative, as both the size and fabrication method of devices can change their properties. Neutrons are the ideal probe with which to measure and understand the dynamics of these impactful materials, as outlined below. A modern high-flux reactor source coupled with state-of-the-art neutron scattering instrumentation will provide data with a higher signal-to-noise ratio (and thus the ability to work with smaller samples) and at a faster rate, thereby advancing the novel science needed to ensure U.S. energy independence and improved sustainable energy technologies.

Core 3 (Future Information Technologies): Society, including individuals and large corporations, will increasingly depend on electronic devices. Improving these devices requires enhancing their speed, information storage capacity, data privacy, safety, and encryption, as well as reducing their power consumption. New information management schemes will require novel materials. One currently promising avenue is the emerging field of spintronics. Future devices will require novel spin storage or spin-charge-transduction technology and spin-transport channels, such as those provided by spin waves in antiferromagnets or by edge modes in topological insulators, as well as novel electric insulators (so-called high-*k* dielectrics) and materials with tailored thermal transport to dissipate heat. Neutron scattering plays a critical and central role in understanding and improving spin and heat-conduction phenomena, as well as the resilience of stored information with respect to external perturbations.

Core 4 (National and Data Security): Neutron scattering emerges as a vital component of our national security strategy when we consider its relevance to the fields of quantum information science and cryptography. Quantum-information science is poised to revolutionize the way we secure data and communications. Unlike classical computers, quantum computers have the potential to solve complex mathematical problems much faster, which could threaten current encryption methods and potentially compromise sensitive information in strategic sectors, including finance, healthcare, and national defense. Neutron scattering's role here is multifaceted. Firstly, it aids in the development of new materials crucial for quantum technologies. By examining the atomic structures and dynamics of these materials with neutron scattering techniques, we can learn how to fine-tune their properties to optimize quantum operations, thus ensuring the secure transmission of information. Secondly, neutron scattering contributes to the creation of materials for quantum key distribution, a cryptographic method that harnesses the principles of quantum mechanics to achieve unbreakable encryption. By understanding and enhancing the properties of materials used in quantum key distribution systems, we can fortify the security of our data and communications. Additionally, quantum entanglement security, a cutting-edge field in quantum cryptography, relies on the entanglement of particles for secure communication. Neutron scattering offers a promising avenue with which to enhance the security of these quantum systems. Neutrons can interact with matter without disturbing the quantum entanglement between particles. This unique property makes neutron scattering an ideal tool for studying the effects of environmental factors, such as eavesdropping attempts, without compromising the quantum information being transmitted. By leveraging neutron scattering, we can better understand the vulnerabilities and safeguards of quantum entanglement-based security protocols, ultimately strengthening the security of future quantum communication technologies. The future NIST facility will equip U.S. researchers with capabilities necessary to study such quantum phenomena with respect to national security.

Core 5 (Novel Computing Paradigms): Novel computing paradigms are required to maintain national security and competitiveness. On the one hand, advanced cryptography will be essential with the advent of quantum computing to guarantee data security and integrity of sensitive technological and personal data and financial transactions. On the other hand, the increase in the rate of data generation, which passed the mark of 100 zettabytes (10^{23} bytes) per year globally in 2023, and the need to manage, analyze, and make decisions based on these data calls for new computing paradigms for machine learning and artificial intelligence that require novel materials. Developing quantum computing poses formidable challenges, notably in developing materials with increased qubit stability and qubit-transport channels. Novel schemes for artificial intelligence might be based on neuromorphic computing, featuring artificial neurons and complex interconnects. This approach appears to be necessary simply from the perspective of managing the global energy used in information technology, which is becoming unsustainable. By mimicking information handling as performed in the human brain, a decrease by a factor of about 1 million in energy consumption might become possible. Neutron scattering provides essential insights in developing novel 2-dimensional materials that feature the basic physical phenomena, such as charge density waves and metal-insulator transitions, that are needed for the material realization of neuromorphic computers.

Core 6 (Truthfully documenting the materials landscape): The hard-condensed-matter-physics subfield presently lacks a validated experimental-data repository for inelastic neutron scattering experiments. This type of repository, which exists for elastic scattering data from inorganic compounds, would greatly benefit U.S. researchers who are developing new computational models, training machine-learning algorithms, and designing new materials. With the new NIST facility, we envision the sophistication of measurement and data quality evolving to the point that we can produce and archive standard data for the phonon density of states and vibrational entropy for a wide range of materials. This type of work aligns closely with NIST’s mission “to promote U.S. innovation and industrial competitiveness by advancing measurement science, standards, and technology in ways that enhance economic security and improve our quality of life,” and with its long-standing commitment to open-data practices and the newer FAIR data initiative. We foresee the new facility providing this valuable service to the materials-science community by establishing clear protocols for measurement, analysis of data, and dissemination to the community for a large subset of inelastic-neutron-scattering data collected at the new facility.

Core 7 (Space exploration): Technological developments that allow humans to push the boundaries of space exploration place unique demands on the underlying materials. Materials interact with the environment in specific ways, many of which can modify the atomic and magnetic structures, electrical and thermal conductivities, vibrational modes, and free energy. A detailed understanding of the dynamics of materials will allow us to design and develop new materials that can withstand extreme environments in space and on neighboring planets. The successful development of such materials requires measurement conditions that include extreme temperature and thermal gradients, high pressure, corrosive atmospheres, and long-term exposure to high-energy galactic cosmic rays.

Concluding Paragraph: Advances in U.S. manufacturing, energy independence, electronic devices, national security, and space exploration hinge on broadening and deepening our understanding of materials dynamics, a challenge for which neutron studies are critical. Achieving this objective is impossible without cutting-edge instrumentation that enables innovations like high-throughput and multimodal measurements. High-throughput methods validate results across diverse sample conditions while multimodal techniques provide concurrent measurements. The NNS facility aims to pioneer studies on hard condensed matter dynamics under extreme conditions with specialized instrumentation. This includes probing materials under high fields, over a wide range of temperatures and pressures, and those subjected to reactor irradiation or thermal shocks. Such advanced measurements demand state-of-the-art data collection methods and rapid-analysis pipelines in line with theoretical models.

6.6. New instruments and the new reactor’s ability to facilitate science

Overview: By maximizing the number of beam ports available to the U.S. community for innovative experiments, the NNS will redefine the neutron-scattering landscape. All instruments should provide access to event-mode, multimodal, and *operando* functionality. They should also exploit the neutron scattering cross-section to the fullest by, for instance, relying on polarization-analysis techniques and high-resolution measurements in absolute units. Users of the NNS will want access to data obtained with better energy resolution across a broader range of momentum and energy transfer than is presently available. Therefore, advanced neutron-scattering techniques, such as Resonant Spin Echo and Larmor precession, will be essential, as will traditional spectrometers with tunable energy resolution. Some instruments should specialize in rapid sample throughput and serve as flexible laboratories-on-a-beamline; others should combine high resolution with high signal-to-noise ratios, facilitating the study of samples previously deemed too small to measure. Within a concerted national strategy, the availability of extreme sample environment conditions such as high pressures and high magnetic fields, as well as the novel use of neutrons to probe quantum entanglement, would expand the application of neutrons to the material sciences.

Core 1 (Using the neutron scattering cross-section to the fullest): The intrinsic spin, or magnetic moment, of the neutron plays a crucial role in scattering experiments. It allows neutrons to interact with electronic and nuclear magnetic moments, thereby making neutrons invaluable probes of the orientation and strength of these magnetic moments as well as their associated dynamics in magnetic materials. In experiments based on the spin-echo technique, spin-polarized neutrons are used wherein the spin orientation of the neutron beam is controlled. This enables scientists to measure different aspects of the magnetic and vibrational dynamics of the sample with exceptionally fine energy resolution. The zero electric charge of the neutron provides yet another notable advantage as, unlike X rays, neutrons can easily penetrate the walls of a variety of equipment used to create controlled sample environments, such as cryostats, furnaces, magnets, and pressure cells.

The well-known isotopic dependence of the neutron scattering cross-section allows one to study light elements within a matrix of heavy elements and materials composed of elements with similar atomic numbers with high accuracy, which can be problematic for X rays. Neutrons provide a non-invasive means of investigating materials, leaving the sample unaltered and facilitating the analysis of material dynamics without causing damage. An additional advantage of neutron scattering is that it provides a statistically averaged measurement so that the overall effects of defects on the bulk response of a material can be determined. Given these unique properties of neutrons, a guiding principle of the instrumentation development at the NNS should be to exploit the many advantageous aspects of the neutron-scattering cross-section to the fullest extent.

Core 2 (Multimodal measurement capabilities): Experiments in which multiple measurement techniques are employed simultaneously with neutron scattering can greatly enhance the range of time, length, and energy scales over which the dynamics of materials can be studied and help to optimize the use of precious neutron beam time. Next-generation neutron spectrometers should therefore revolutionize the ways neutrons are used. Their design should consider the integration of intricate sample environments and/or support a wide range of equipment that provides high and low temperatures and magnetic fields, the ability to apply temperature and chemical gradients, hydrostatic and uniaxial pressure, electric fields, and pass electric currents through the samples. Operando experiments are instrumental in both physics and material science and engineering. They provide crucial insights into the real-world performance and behavior of materials such as metals, ceramics, composites, and quantum materials. These experiments help researchers optimize the structural integrity, durability, and wear resistance of materials.

Core 3 (Maximizing event mode approaches for operando studies): Next-generation spectrometers that operate in event mode, where the wall-clock time of arrival of the neutron is recorded, will significantly enhance the flexibility in data analysis, enabling novel instrument design and harnessing time-dependent information for *operando* experiments. This includes optical pump-probe experiments, as well as measurements of solidification processes and kinetics. These new instruments would have the ability to investigate steady-state driven systems, metastable materials, the dynamics involved in chemical reactions, and other time-resolved measurements. An example would be phonon measurements made while a high electrical current is passed through the sample or a temperature gradient is applied. Neutron instruments featuring innovative multiple operation modes that are, for instance, capable of acquiring wide- or small-angle information while performing inelastic measurements, would also provide multidimensional insights into the physics of materials.

Core 4 (Resolution control): Controlling the energy resolution of a neutron-scattering measurement is key to understanding technologically important material transport properties originating from spin and lattice dynamics. Similarly, controlling the Q-resolution (i.e., the angular resolution) is crucial to quantifying the length scale(s) of the corresponding dynamics. This requires instruments with a dynamic range that is sufficiently large to access the pertinent combination of energy and Q. In many cases, this may necessitate the development of instruments with a large footprint to achieve large scattering angles, especially when dealing with bulky sample environments. To attain superior energy resolution across all Q values, different types of spectrometers are needed, such as classical spin-echo instruments and triple-axis spectrometers equipped with Larmor devices for ultra-high energy resolution at high Q.

Core 5 (High-signal-to-noise ratio): The NNS, equipped with state-of-the-art neutron-scattering instruments, could significantly improve the signal-to-noise ratio in experiments. This would facilitate investigations of smaller samples, a critical capability in the early stages after novel materials are discovered when large crystals are difficult or impossible to grow. It would also accelerate studies of as-synthesized materials and thin-film materials as they would be used in an electronic device. Thin-film geometries are known to change the transport properties of materials, but the ability to probe the band structure of such materials via neutrons would open entirely new opportunities to study, understand, and predict this striking behavior.

Core 6 (High-throughput capabilities): Instrument development should emphasize enhancing high-throughput capability. The flux of contemporary neutron sources makes it feasible to complete measurements on, for example, a powder sample in less than an hour. To capitalize fully on this potential, appropriate sample-handling equipment and sample-environment equipment will need to be designed. This step is crucial, as it would expand the user base, streamline workflows for greater cost-effectiveness, improve overall efficiency, and enable wider explorations of entire phase diagrams.

Core 7 (Novel uses of neutron beams): Efforts should also be made to advance neutron-scattering applications, such as using the neutron as an entanglement probe and applying neutron interferometry for material science. A similar focus should extend to pioneering techniques in instrument design, such as methods to enhance the out-of-plane Q-resolution and the creation of rotary monochromators to optimize neutron utilization.

Concluding Paragraph: The NNS, equipped with a comprehensive array of instruments optimized to study the dynamics of hard condensed matter and rapidly address pressing science challenges, would transform our understanding of materials. Neutron-scattering techniques offer unparalleled insights into the fundamental properties of materials. The power of these methods stems from the unique properties of the neutron that enable it to probe both magnetic and lattice-dynamics on length scales ranging from atomic to microscopic dimensions and energy scales from a millionth of an electron Volt to one electron Volt, all while penetrating deeply into materials subjected to a multitude of different and extreme sample environments.

6.7. References

[1] https://www.nist.gov/el/applied-economics-office/manufacturing/total-us-manufacturing/manufacturing-economy/total-us

7. Neutron and Neutrino Physics

7.1. Panel

Chair:
Brad Plaster – *University of Kentucky*

Panel Members:
Stefan Baeßler – *University of Virginia*
Tanmoy Bhattacharya – *Los Alamos National Laboratory*
Nathaniel Bowden – *Lawrence Livermore National Laboratory*
Vincenzo Cirigliano – *University of Washington*
Maynard S. Dewey – *National Institute of Standards and Technology*
Joseph A. Formaggio – *Massachusetts Institute of Technology*
Vladimir Gudkov – *University of South Carolina*
Michael G. Huber – *National Institute of Standards and Technology*
Takeyasu M. Ito – *Los Alamos National Laboratory*
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Wolfgang Korsch – *University of Kentucky*
Emanuele Mereghetti – *Los Alamos National Laboratory*
Hans Pieter Mumm – *National Institute of Standards and Technology*
Jason J. Newby – *Oak Ridge National Laboratory*
Jeffrey S. Nico – *National Institute of Standards and Technology*
Alexander Saunders – *Oak Ridge National Laboratory*
Danielle Schaper – *Los Alamos National Laboratory*
William M. Snow – *Indiana University*
Fred E. Wietfeldt – *Tulane University*
Albert R. Young – *North Carolina State University*

Scribe:
Shannon F. Hoogerheide – *National Institute of Standards and Technology*

7.2. Glossary of Terms

aCORN: An experiment to measure the angular correlation between the electron and antineutrino produced in neutron beta decay, known as the “little a” coefficient. A measurement of “little a” can be combined with other measurements in neutron beta decay to test the validity and self-consistency of the Standard Model.

Alpha-Gamma device: A device for very high precision measurements of neutron beam fluence.

Antineutron: the antiparticle of the neutron, which consists of three anti-quarks.

Ballistic neutron guide: A neutron guide with a cross-section that varies along its length to minimize neutron transport losses within the guide.

Baryon number (B): a number describing the relative number of quarks and antiquarks contained within a subatomic particle.

Baryons: subatomic particles that consist of three quarks bound together by the strong force, examples of which are protons and neutrons.

Beam Lifetime: An experiment to measure the lifetime of the free neutron that uses a beam of cold neutrons and counts the number of protons that result from neutron decay within a specific volume.

Berry phase: A purely quantum phenomenon where a phase shift is introduced that depends on the particulars of how a quantum state came to be.

Beta (β) decay: radioactive decays mediated by the weak force in which an electron or positron is emitted from the atomic nucleus with the accompanying transition of a neutron into a proton or vice versa.

BSM: beyond the Standard Model : Any physical theory that includes particles or forces not already included in the Standard Model of particle physics. The fact that the Standard Model is incomplete implies that BSM physics must exist.

CEvNS: Coherent Electron neutrino Nuclear Scattering. It is possible that a neutrino can scatter coherently from a nucleus. This process has only been recently observed.

Cheshire cats: These arise when one can separate a particle's properties (e.g., its spin and momentum) in unconnected physical paths inside an interferometer. Just like in the classic fairy tale Alice in Wonderland where the Cheshire cat's 'grin' unexpectedly separates from its body.

CKM matrix: a matrix of numbers that provides information on the relative strengths of weak force interactions between the quark flavors.

CP violation: the combination of the operations of charge conjugation C (transformation of a particle into an anti-particle, or vice versa) and parity P (see above). A change in the laws of physics under these combined operations is termed "CP violation," which has connections to the question of, for example, why the universe consists of more matter than antimatter.

Dark matter models: theories of physics involving dark matter, a form of matter hypothesized to explain why not all mass in the universe is observable directly.

DUNE: The Deep Underground Neutrino Experiment is an experiment to make precision measurements of neutrino oscillation parameters with a primary goal of better understanding the origin of neutrino mass.

emit: An experiment to search for Time-Reversal symmetry violation in neutron beta decay by measuring electron-proton coincidence events from the decay of polarized neutrons.

Endstation: An instrument placed at the end of a neutron guide.

Energy Frontier: fundamental physics research at the highest-available energies, such as at particle colliders.

Fission daughters: Any of the isotopes produced by fission. Fission daughters are generally unstable and subsequently beta decay yielding additional isotopes and neutrinos.

GHZ states: Greenberger-Horne-Zeilinger States: entangled quantum states with 3 qubits used in quantum communication.

Hadronic parity violation: weak force interactions between protons, neutrons, and nuclei that differ upon the operation of parity.

Large Hadron Collider: a particle accelerator located underground, deep beneath the France-Switzerland border, designed to carry out tests of particle physics at the energy frontier through very high energy collisions between Standard Model hadrons.

Magnetic moment: The intrinsic magnetic dipole moment (combination of magnetic strength and orientation) of a particular particle. Elementary particles have an intrinsic magnetic moment due to their spin and electric charge.

Majorana mass term: a mathematical method for describing the masses of Majorana particles (particles which are their own antiparticles). Neutrinos are hypothesized to be Majorana particles, which would make them unique among Standard-Model particles.

Matter-antimatter symmetry: The universe developed with a slight excess of matter over antimatter. This fact cannot be explained with the Standard Model and has generated many searches for BSM physics.

Moderator: A material that reduces the speed of fast neutrons (such as those created directly during fission within the reactor), ideally without capturing any, leaving them as thermal or cold neutrons. In UCN production, cold neutrons are first generated by a cold (pre)moderator and then further slowed (cooled) by another material (UCN converter) until they reach UCN energies.

Monochromatic beam: a neutron beam of a single discrete wavelength.

Monochromator: a crystal placed in a neutron beam that selects a specific neutron wavelength using Bragg's law of diffraction.

Neutrino and neutrino oscillations: Neutrinos are one of the elementary particles that make up the universe. They are electrically neutral, nearly massless and interact with other matter only very weakly. They exist in three types or flavors (electron neutrino, muon neutrino, tau neutrino) and can change their type (oscillate) as they travel. The fact that neutrinos change flavor is the first direct evidence that the Standard Model is incomplete.

Neutrino flux: The number of neutrinos traveling through a fixed area. The neutrino flux from a reactor carries information about the operation and nuclear physics of reactors.

Neutron Beta Decay: A type of radioactive beta decay, mediated by the weak force, whereby a neutron decays into a proton, an electron, and an electron anti-neutrino.

Neutron guide: Neutron waveguides for transporting neutrons from a reactor to instruments typically residing in a guide hall.

Neutron Interferometry: An instrument for investigating the wave-particle duality of the neutron.

Neutron Orbital Angular Momentum: A quantum state with a phase associated with its azimuthal coordinate and perpendicular to is trajectory. Maybe useful in quantum state selection and in studying quantum materials.

Neutron selection rules: The governing rules for driving one quantum state into another. Specifically for neutrons, where different OAM values could change the likelihood of a neutron being absorbed by an atom.

Parity: an operation in which the three dimensions of space are simultaneously inverted.

Permanent electric dipole moment (EDM): a property of a subatomic particle related to the distribution of positive and negative electrical charge within the particle. A non-zero EDM would violate certain symmetries.

Polarized helium-3 spin filters: a device for producing polychromatic neutron beams with a unique spin state.

PROSPECT antineutrino experiment: The Precision Reactor Oscillation and SPECTrum experiment was designed to test the possibility of sterile neutrinos altering the number of observable neutrinos emitted by reactors, to measure the neutrino energy spectrum, and to demonstrate the technology to observe reactor neutrinos in a small detector at the earth's surface.

Quantum Chromodynamics (QCD): the theory describing the strong force interactions between quarks.

Quark: an elementary particle with six flavors (up, down, charm, strange, top, bottom) which combine to form observable matter, such as protons, neutrons, and atomic nuclei.

RDK: An experiment to measure the Radiative Decay of the Neutron, that is, a neutron beta decay event that produces a photon in addition to the usual proton, electron, and electron anti-neutrino.

Reactor-based neutrino physics: the investigation of neutrino properties and applications based on the utilization of nuclear reactors as a high-intensity neutrino source.

Rest mass energy: The amount of energy equivalent to the mass of a particle. E= mc2

Spin ½ particle: particles possessing a spin, an intrinsic property of quantum mechanics related to magnetism, equal to ½. Examples are electrons, protons, and neutrons.

Spinor: A quantum state, such as the neutron's spin, requiring a rotation of 720 deg (not 360 deg) to return to its original state.

Standard Model of particle physics: the theory unifying three of the four known fundamental forces (electromagnetic force, strong force, weak force) and describing the interactions between the elementary particles.

Sterile neutrino: A hypothesized type of neutrino that does not interact with other matter except though oscillation with the Standard-Model neutrinos. Sterile neutrinos are theoretically well-motivated BSM particles.

Time Reversal Invariance: The concept that, at a microscopic level, interactions between particles appear the same under the reversal of time. The matter-antimatter asymmetry implies that this symmetry is violated.

Ultracold neutrons (UCN): neutrons with kinetic energies below 340 neV (nano-electron volts)

Weak interaction: one of the four fundamental forces (the three others being gravity, electromagnetism, and the strong force). It is responsible, for example, for radioactive decay and it differs upon the operation of parity.

Weinberg mixing angle: Also known as the weak mixing angle, a fundamental parameter in the Standard Model that describes the strength of the weak force.

7.3. Summary

The NIST Neutron Source (NNS) offers a prime opportunity for U.S. leadership to address some of the most pressing questions in fundamental physics as well as to develop the new technologies necessary to realize next-generation metrological and measurement capabilities. Investment in targeted facilities and continued engagement with the neutron physics and neutrino physics communities is required to take full advantage of this unique opportunity. The opportunities afforded by the NNS will continue and expand upon the decades-long leadership by the NIST Center for Neutron Research (NCNR) in fundamental neutron physics, as experiments conducted at the NCNR have driven the subfields of neutron β decay, the hadronic weak interaction, and neutron interferometry. The recent (October 2023) release of the nuclear physics community's Long-Range Plan [1] highlighted the impact of the NCNR on the field with the document noting "...major DOE- and NSF-funded nuclear physics experiments in neutron decay (e.g., beam lifetime, emiT, RDK, aCORN), hadronic parity violation, and neutron interferometry have operated and obtained important results at the NCNR ..." With the nuclear physics community's scientific vision for the next decade captured in the Long Range Plan, implementation of the needed infrastructure, facilities, and workforce identified in this document will position the NNS to maintain and extend NIST's world-leading role in the field of fundamental neutron physics, together with an opportunity to establish a new world-leading facility for reactor-based neutrino physics, utilizing the antineutrinos emerging from the fission and β decay processes in the reactor. The science program outlined here will have multiple direct societal impacts, including workforce development for U.S. national interests, support of the U.S. nuclear data effort, development of advanced technologies with applications to a broad range of disciplines, and advancement of the core NIST mission of metrology.

To achieve our vision for the future of neutron physics and neutrino physics at the NNS, we make the following recommendations (at equal priority):

> **Recommendation 1:** Construct new instruments to continue and expand NIST's decades-long leadership role in neutron physics, including a cold-neutron endstation, an environmentally isolated neutron interferometry facility, and monochromatic beams. These instruments must be designed so that they can serve a diverse program of experiments with each presenting unique requirements.
>
> **Recommendation 2:** Perform detailed design studies to establish the capabilities and "physics reach" of two world-leading facilities: an Ultracold Neutron (UCN) national user facility and a neutrino physics facility able to host multi-ton scale reactor neutrino experiments. Detailed design studies are needed to maximize the UCN source output while minimizing the impact on other instruments. A compact reactor core less than a meter in size would enable world-leading neutrino experiments with sensitivity to new neutrino oscillations and BSM physics.

Recommendation 3: To maximize the return on investment in the NNS facility, make a commensurate investment in cultivating talent. With proper staffing, the physics program can provide a uniquely exceptional training environment enabled by the convergence of cutting-edge and novel technologies, end-to-end involvement in experimental design and execution, and experiment timescales.

7.4. Science Drivers for Research

7.4.1. Neutron Physics

Neutrons have played and will play a fundamental role in addressing key open questions in nuclear and particle physics. The current Standard Model (SM) of particle physics is an extremely successful theory that provides an accurate picture of nuclear and particle physics phenomena up to the TeV energy scale (i.e., down to the attometer or 10^{-18} m length scale). The SM, however, spectacularly fails to explain the origin of both baryonic and dark matter in our Universe. In addition, it does not have a mechanism for generating the tiny masses of neutrinos, and, while it can parameterize quark masses and mixings, it lacks a convincing explanation of the hierarchies between the masses of different quark families and of the structure of the Cabibbo-Kobayashi-Maskawa (CKM) quark mixing matrix. These pressing open questions have been investigated by experiments at the Energy Frontier, which try to observe new particles and their interactions in high energy collisions. A complementary strategy consists of looking for subtle deviations from SM predictions in high-precision, low-energy experiments. Neutrons are a key component of the Precision Frontier portfolio.

The properties of the neutron make it an ideal system for precision tests of physics in the SM and physics Beyond the Standard Model (BSM). Neutrons are the simplest baryons to undergo β decay, allowing for precision tests with small theoretical uncertainties. Measurements of the neutron lifetime and β-decay correlations with sub-permille uncertainties, coupled to advances in first-principle theoretical calculations, will provide tests of the weak sector of the SM that are highly competitive and complementary with direct searches at high-energy colliders, such as the Large Hadron Collider. These measurements will confirm or falsify hints of BSM physics in tests of the unitarity of the CKM matrix [2,3], currently limited by the nuclear theory error on the extraction of V_{ud} from superallowed $0^+ \rightarrow 0^+$ β decays. As spin-1/2 particles, neutrons can have a permanent electric dipole moment (EDM), which would signal the violation of the symmetries of time-reversal (T) and, equivalently, charge-conjugation and parity (CP). Being charge neutral and long-lived, neutrons constitute one of the best systems for EDM experiments [4], and their (relative) simplicity allows for a direct connection to Quantum Chromodynamics (QCD) and BSM sources of CP-violation. Neutrons could also have a small Majorana mass term [5], which would violate baryon number (B) by two units and cause the oscillation of neutrons into antineutrons. Neutron experiments could thus reveal new mechanisms for the violation of CP and B, which are necessary conditions for the dynamical generation of a baryon asymmetry in the Universe, a phenomenon the SM cannot explain.

In addition, to reach far beyond the electroweak scale, low-energy hadronic parity violating experiments can lead to a better understanding of the SM by shedding light on the nucleon-nucleon weak interaction, the least understood sector of the electroweak theory. Slow neutron interactions have been exploited in several searches for possible new weakly coupled interactions of various types, complementing similar experiments performed with atoms and molecules [6]. For example, dark matter models often propose new particles with weak coupling to the SM.

The NCNR has been a world leader over the past several decades in the quest to discover new physics scenarios such as those described above. As noted in the Long-Range Plan [1], the NCNR's world-leading role in fundamental neutron physics has yielded significant impact in precision measurements of neutron β decay observables, studies of the hadronic weak interaction, and neutron interferometry. In neutron β decay, experiments such as aCORN [7,8] and Beam Lifetime [9,10] have contributed to precision measurements of fundamental weak interaction parameters important for tests of the SM. The emiT experiment [11,12] carried out a high-sensitivity test of Time Reversal Invariance, and the RDK experiment [13,14,15] pioneered measurements of radiative neutron β decay. Magnetic trapping of ultracold neutrons [16] was also demonstrated at the NCNR. In the near future, the next generation Beam Lifetime experiment (BL3) will begin operating; it is designed to resolve anomalies in the neutron lifetime [17,18] and weak interaction physics that could unlock new BSM physics. Studies of the hadronic weak interaction via parity-violating spin-rotation measurements [19,20,21] have constrained BSM interactions.

Finally, the NCNR has been a world-leading facility for neutron interferometry (NI) studies. Neutron Interferometry exploits the wave-like properties of the neutron to study aspects of fundamental and applied physics. Measuring the neutron's quantum phase allows for precision and sensitivity not found in other neutron scattering techniques. The most widely used device is a perfect-crystal neutron interferometer that consists of several parallel silicon blades machined on a common base and is analogous to a Mach-Zehnder interferometer. Perfect-crystal NI has been used to demonstrate 4π spinor rotation [22, 23], the Berry phase [24], Cheshire cats and weak measurements [25], GHZ states [26], as well as to probe nuclear structure [27,28,29,30] and search for BSM physics in, for example, studies of 5th forces and dark matter [31,32,33].

The existence of neutron Orbital Angular Momentum (OAM) [34,35,36], which was recently demonstrated using NI, provides an exciting avenue for future research. Optical OAM, first proposed in 1992 [37], has applications in quantum information, photonics, optical tweezers, and sensing [38,39]. Neutron OAM may prove important in the study of topological materials [40] and generating "self-healing" neutron beams, and in studying neutron selection rules [41]. Advanced fabrication techniques have led to several new types of neutron interferometers. These include phase-grating interferometry for cold neutrons [42] and the use of Ni/Ti multilayer mirrors [43]. A technically challenging, perfect-crystal neutron interferometer [44] where the blades of the interferometer can be separated has also been demonstrated. Each of these holds promise for studies of large samples and weak interactions at scales not yet possible with current neutron interferometers.

7.4.2. Neutrino Physics

The nearly massless, charge-neutral neutrino is one of the most abundant particles in the Universe. Thus, even though neutrinos interact only weakly, they play a critical role in shaping our understanding of Nature through their effects on the origin of structure in the cosmos and the evolution of supernova, their place in the SM, the possible generation of the matter-antimatter asymmetry, and the generation of particle mass. The rarity of their interactions make them extremely difficult to detect, but that also means that they are unique messengers capable of carrying information through dense matter. They can tell us about extreme astronomical processes and the physics of nuclear reactor cores. Pushing the frontiers of challenging neutrino detector technology also benefits a range of activities from the exotic (e.g., dark matter detection) to the applied (e.g., nuclear safeguards technology).

Because reactors are intense well-understood sources of terrestrial anti-neutrinos, reactor neutrinos have played an especially important role in our understanding of neutrino physics and developing the contemporary view of the SM. They provided the first experimental verification of the existence of neutrinos [45], yielded world-leading precision on some of the parameters that govern how neutrino flavors mix [46,47,48,49], and offered early validation of the theory of weak interactions [50]. Reactor neutrino-electron scattering enabled measurement of the weak Weinberg mixing angle and competitive limits on whether neutrinos have magnetic moments [51,52]. Reactor experiments have also provided sensitive probes of BSM physics; for example, short-baseline experiments have set new limits on possible sterile neutrino mixing [53,54,55,56,57,58,59]. Additionally, the low energies of reactor antineutrinos allow them to scatter coherently off all nucleons in a target (CEvNS), greatly enhancing the cross-section. This gives reactor experiments the potential of unmatched sensitivity for measuring SM cross-sections at low momentum transfer and detecting data-model deviations indicative of new physics. Early reactor CEvNS experiments have already set world-leading limits on hidden sector (BSM) neutrino couplings [60,61], demonstrating the discovery potential of reactor-based neutrino physics.

Looking forward, reactor-based CEvNS offers exciting possibilities with dramatic increases in discovery potential possible. Future experiments may be sensitive to much of the same BSM physics as neutrons, which manifest as non-SM couplings. In addition, high-precision measurements of the reactor antineutrino spectrum and flux, which encode detailed information about fission product yields and the energy spectrum of β-decays of those fission daughters, could have far-reaching impacts. Such knowledge will increase the achievable precision of some reactor-based BSM measurements as well as being strongly synergistic with facets of the applied reactor physics, nuclear safeguards, and nuclear data communities [62,63,64]. The reactor electron-neutrino (ν_e) energy spectrum includes contributions from short-lived, high Q-value isotopes, some of which have received limited experimental investigation and are poorly understood. Improved measurements have the potential to test the nuclear data evaluations that underlie many areas of nuclear physics, nuclear energy, and nuclear security. Specific nuclear data needs that can be addressed with reactor ν_es have been described in recent reports [62,63]. Future neutrino experiments at short detector-core distances (baseline) can also play a unique and important role in BSM searches. Reactors provide a clean environment in which to study oscillations owing to the electron-flavor purity of the source, the low energies which prevent heavy particle states from polluting the observed signal, and the relative absence of matter effects. These features mean that short-baseline reactor experiments play a unique and orthogonal role to other searches worldwide in constraining scenarios including sterile neutrino decay [65,66], the presence of nonstandard neutrino interactions [67,68, 69], and hidden sector couplings to neutrinos [70]. An important case is a possible ambiguity in the interpretation of the U.S. high-energy physics centerpiece long-baseline experiment, DUNE, introduced by a possible sterile neutrino. Certain portions of relevant parameter space can only be accessed by a short-baseline program. Other novel aspects of reactor-based experiments, such as their on-surface location and their proximity to large reactor-produced neutron and photon fluxes, offer promise in probing the existence of a range of new particles like axions [71], hidden sector particles such as mirror neutrons [72], and new interactions. While the potential physics reach of short-baseline reactor-neutrino experiments is compelling, there are currently no dedicated sites for such measurements; each experiment must individually face unique site-specific challenges with access, backgrounds, and facility restrictions.

7.5. Societal Impacts and National Benefit

The program of fundamental neutron and neutrino physics at NIST supports the core NIST mission of metrology and fuels many NIST priorities including validating the underpinnings of the new SI, determining fundamental constants of nature, improving methods in standards and metrology, and developing novel applied technologies for commerce. The future experimental program enabled by the NNS will continue to provide significant benefits and impacts to both NIST and the broader society, ranging from technological innovations to workforce development. In particular, this research program must often push the boundaries of what it is possible to measure. In order to achieve the science and measurement goals, these types of experiments have to bring together a wide variety of expertise, and often have to develop new methods, techniques, and technologies. These new methods, techniques, and technologies often go on to play an important role far beyond the initial experiment, making advances in other areas of science and metrology possible. This dynamic environment, which brings together diverse expertise and innovative technologies at a relatively small experimental scale, also provides a unique training environment for the next generation of U.S. scientific leadership. While predicting specific future impacts of basic research is a challenge, we highlight below a few examples that illustrate what one might expect in the future.

One important example is the development of polarized helium-3 spin filters. These devices allow one to polarize polychromatic neutron beams having large spatial area and divergence while producing minimal gamma background. This technique was developed in the fundamental neutron physics community to achieve the beam polarizations required for these experiments. The technique was then expanded and applied to neutron scattering experiments, where it has become a workhorse technique across the NCNR, while continuing to play a crucial role in fundamental physics experiments.

Another example comes from the development of the Alpha-Gamma device, which can count with extreme precision the individual neutrons in a beam of neutrons striking an absorbing target. Although it was created to calibrate the neutron detector used in a neutron half-life determination, it has utility reaching far beyond that. It is being exploited in important nuclear cross section measurements (e.g., the ^{6}Li neutron capture and ^{235}U neutron-induced fission cross sections). These measurements represent the first steps in an extensive campaign to improve nuclear data for a wide range of uses. Alpha-Gamma is also a key component of an effort to recalibrate the U.S. national neutron source NBS-1, a radioactive neutron-emitting source whose precisely known neutron emission rate underpins efficiency measurements of all neutron detectors in the U.S. The Alpha-Gamma facility and its capabilities are unique in the world.

Finally, we highlight the PROSPECT antineutrino experiment. This experiment was designed to address the BSM explanations of anomalies observed in the flux and spectrum of antineutrinos from reactors. While largely motivated by the pursuit of fundamental scientific discovery, PROSPECT has now enabled remote monitoring of nuclear reactors, opening the potential to address nuclear energy and security problems. Nuclear reactors present a viable, clean energy source that can help to combat the effects of climate change, and more reactors are projected to be constructed every year. However, concern over the misuse of nuclear technologies and materials is one of several impediments to the widespread adoption of this power source. Antineutrino detection can potentially support the safe and peaceful use of nuclear energy as a non-intrusive, remote measurement method to increase confidence and transparency by verifying that reactors are being used in a manner consistent with their declared purpose. In the future, precision measurements of the reactor flux and spectrum will provide unique data in the context of global evaluations and aid in the U.S. effort to improve nuclear data.

Because of their nature, neutron experiments, such as those that run at NIST, and small-scale reactor-ν_e experiments provide an ideal training ground for producing well-rounded and highly skilled scientific generalists. The projects are relatively small-sized, allowing early career scientists to get involved in the full range of the experimental process, including design, simulation and modeling, construction, data acquisition, data analysis, and publication. The collaborative nature of the experiments, coupled with the relatively small size of the collaborations, also provides broader exposure and increased mentoring opportunities for early career researchers, while also reducing the threshold for involvement. In addition, certain aspects of the program have been especially important in meeting the needs of the emerging Quantum Information Science (QIS) workforce. The current interferometry program, for example, has an excellent track record of early career scientists moving into the private sector to pursue QIS.

7.6. New Instruments and the New Reactor’s Ability to Facilitate Science

7.6.1. Neutron Physics

7.6.1.1. Cold-Neutron Endstation

The NG-C fundamental physics beamline at the NCNR provides the highest flux of cold neutrons for fundamental physics in the U.S. and is one of only a few such high-flux facilities worldwide. NG-C (and its predecessor, NG-6) have a long history of delivering important results as discussed in the section above. It is a very important community resource in an oversubscribed field and one of the few facilities that regularly supports multi-year-long experiments. To ensure world leadership in next-generation experiments, the neutron physics program at NIST requires a flagship cold-neutron endstation for fundamental physics as part of the NNS.

Meeting the need for increasing precision in neutron β decay and other experiments requires increasing the number of useful cold neutrons, as these experiments are generally statistics-limited, as well as having a large, flexible experimental area that can host a wide variety of experimental apparatus and a host of supporting infrastructure. Specifically, we require the following:

1. The brightest source possible (an increase of a factor of 10 or more is highly desirable) combined with the highest cold-neutron flux possible.
2. A curved ballistic guide with a large cross section, similar in size to that of NG-C. This guide should ideally be located at the edge of one of the guide halls.
3. A large experimental area, to include 5 m of space on both sides of the beam, 10 m overhead space with crane access, and a 5 m deep pit centered on the beamline.

4. We also recommend that the cold-neutron endstation be placed in such a way as to allow for a potential 1 km-long flight path for neutron-antineutron oscillation experiments. It is difficult to say at this point what the need for such experiments will be in the future, but we believe such experiments may be required, and preserving the option to construct such an experiment, should the scientific need arise, seems prudent.
5. Modular radiation shielding for a wide range of experiments. Each new experiment has its own layout and geometry and a different radiation environment, which can be quite high in some cases. A set of modular shields that can be reconfigured to accommodate a variety of experimental apparatus is needed.
6. A large cross-sectional area polarized neutron beam, requiring R&D that would also benefit other avenues of research at the NCNR.
7. Various general infrastructure including significant floor-loading capability; sufficient power for dry cryogenic systems and helium recovery for wet cryogenic systems; non-magnetic structural materials in the vicinity of the experimental area; reasonable temperature and humidity stability.

7.6.1.2. Environmentally Isolated Neutron Interferometry

The NI program at the NCNR has a long history of impactful results in nuclear, quantum, and fundamental physics. There are currently two monochromatic beamlines at the NCNR dedicated to interferometry with a third (based on diffraction grating) awaiting commissioning once there is a return to normal reactor operations. Each beamline has different scientific goals: (1) - quantum measurements, materials, and polarized scattering, (2) - high precision nuclear constants and fundamental physics, and (3) - exploring field gradients and fundamental constants. To preserve long-term phase stability, the most successful beamline uses a massive, thermally, acoustically, and vibrationally isolated hutch with a foundation that is separate from the rest of the building [73]. This unique facility was designed and built by NIST physicists and has the highest phase stability and fringe visibility (contrast) in the world [74].

Neutron Interferometry will continue to provide quality results in fundamental science. A new research reactor at NIST should continue to support this technique. Specifically, we recommend:

1. A neutron interferometer facility located in a thermal guide hall enclosed in an isolated hutch with modifications to include a modern sample environment and additional safety controls.
2. A neutron interferometer facility located in the cold guide hall, preferably with a liquid hydrogen cold source, also in its own environmentally isolated hutch.
3. A monochromatic beamline composed of 8.9 Å neutrons for fundamental physics that could also be used to support a phase-grating-based neutron interferometer like those being developed by the NCNR/PML INFER project.
4. In support of these facilities, we also recognize a need for the handling of activated samples within the guide halls in a laboratory space with etching capabilities.

7.6.1.3. Monochromatic Beams

Over the past three decades, many important physics results have been obtained using a variety of monochromatic beamlines at the NCNR. The NG6-M beamline provides a well-characterized 5.0 Å neutron beam to the alpha gamma spectrometer, an instrument that can measure the absolute neutron flux to a precision < 0.06 %. This was a key ingredient for obtaining the best result in the NIST neutron lifetime experiment using the beam method [10] and has enabled high-precision neutron cross section measurements [75]. The NG6-U beam, using a potassium intercalated graphite monochromator, delivered an 8.9 Å neutron beam to the super-thermal helium ultracold neutron lifetime apparatus that first demonstrated the magnetic trapping of ultracold neutrons and detection of their β decay [16,76,77]. The NG6-A beam provided 3.8 Å neutrons to a slotted silicon crystal that measured the neutron spin-orbit interaction (Schwinger scattering) [78].

The proposed NNS with its 16+ cold neutron guides would allow for many monochromatic beams of various neutron wavelengths. Some of these should be used to support the fundamental neutron physics program. We recommend supporting at least the following three dedicated beamlines:

1. A 5 Å neutron beamline to enable a future program of precision cross section measurements that would greatly extend what has been achieved by the current Alpha-Gamma apparatus. This beamline would also support high-precision neutron source calibrations.
2. A multipurpose 4-5 Å neutron beamline for detector and metrology development and specialized physics experiments.
3. An 8.9 Å neutron beamline to be used for phase-grating interferometry that allows measurement of very large targets.

7.6.1.4. Ultracold Neutrons

Ultracold neutrons (UCNs) are defined operationally to be neutrons of sufficiently low kinetic energies (below about 340 neV) that they can be confined in a material bottle. These kinetic energies correspond to temperatures of several thousandths of a degree Kelvin (several mK). UCNs are playing increasingly important roles in the studies of fundamental physical interactions, discussed earlier in the “Science Drivers and Research” section. Even in the coldest neutron spectrum available from cold moderators at 20 K, the fraction of neutrons that are UCNs is extremely small. To overcome this difficulty, most modern sources of UCNs are based on the so-called super-thermal process [79]. In this method, a UCN converter, which operates at a temperature much higher than several mK, but lower than that of typical cold neutrons (several 10’s of Kelvin), converts cold neutrons to ultracold neutrons. Incident neutrons are down-scattered by dissipating most of their kinetic energies into the bulk medium to create phonons. The reverse process of up-scattering (i.e., neutrons gaining energy from coupling to a thermal bath of phonons) is heavily reduced as the population of phonons is suppressed by the Boltzmann factor $\exp(-\Delta/k_B T)$, where Δ is the energy difference between cold and ultracold neutrons and T is the temperature of the converter. Therefore, a typical UCN source consists of 1) a primary neutron source (reactor or spallation source), 2) thermal and cold moderators, and 3) UCN converter. Superfluid liquid helium (LHe) and solid deuterium (SD_2) have been successfully applied as UCN converters.

Currently, Los Alamos National Laboratory (LANL) operates a UCN source based on a SD_2 converter driven by spallation neutrons [80,81]. This is one of the highest performing UCN sources in the world, and it has been producing world class-science [82,83,84]. The U.S. needs to invest in future UCN sources to maintain its lead in this field.

The planning of the NNS presents a unique opportunity to design a UCN source optimized to a compact reactor core. Incorporating such a UCN source into the NNS will significantly enhance its science capability. We recommend the following two options to be considered and studied:

1. Place a UCN source, which consists of a dedicated cold moderator and a UCN converter, near the core.
2. Extract a cold-neutron beam and place a superfluid LHe-based converter in the guide hall.

Among the operating and planned UCN sources based on the super-thermal process, there are a few that use a reactor as the primary source of neutrons and place the UCN source near the reactor core. These include several sources based on solid deuterium converters: the UCN source currently operational at the TRIGA Mainz reactor [85,86], the UCN source under construction at the PULSTAR reactor at the North Carolina State University (NCSU) [87,88], and the UCN source under construction at the FRM II reactor at the Technical University of Munich (TUM) [89]. At TRIGA Mainz, which is a pulsed reactor with a maximum peak energy of 10 MJ, the UCN source assembly that consists of a pre-moderator (solid hydrogen) and the UCN converter (solid deuterium), both cooled by liquid helium, is inserted into the water pool and the graphite reflector surrounding the core. At the TUM FRM II (20 MW), a UCN source also using a solid hydrogen pre-moderator, but optimized for much larger heat loads and incident thermal neutron fluxes, is inserted into the D_2O moderator volume near the reactor face. At the NCSU PULSTAR (1 MW) reactor, neutrons from the reactor core are extracted through a graphite-lined port to the UCN source assembly, which consists of a D_2O thermal moderator, a CH_4 cold moderator, and a UCN converter based on solid deuterium. In the Mainz and FRM II source, a large cooling power is needed to keep both the pre-moderator and the UCN converter cold. However, in the case of the PULSTAR source, modest cooling is sufficient thanks to the distance between the core and the UCN source.

There is also a source designed for operation near the reactor core with a superfluid-He converter (operated near 1.4 K) and a liquid deuterium moderator. This source is under construction for the PIK (100 MW) reactor at the Petersburg Nuclear Physics Institute [90]. In this design, the use of superfluid helium for the converter permits a larger converter volume and smaller UCN loss rates (in the converter) compared to solid deuterium sources, compensating for smaller UCN production rates per cm^3 in helium.

If a UCN source is incorporated in the design of the NNS (rather than retrofitting a UCN source after the reactor is built and operational), it is conceivable that the performance of the UCN source at the NNS will exceed any of the UCN sources currently planned in the world. As in the case of these other sources, the UCN source at the NNS will consist of a pre-moderator (i.e., a cold source) and a UCN converter. A dedicated thermal moderator may be necessary. A detailed design study is needed to maximize the UCN source output while minimizing the heating and the effect to other instruments.

Another possibility (not mutually exclusive to the option discussed above) is to extract a cold neutron beam and generate UCNs by placing a liquid-helium-based UCN converter in the guide hall, as is done by the super-SUN source at the ILL [91]. In this case, while the expected performance will not likely exceed that of the highest planned source, it is conceivable that it will exceed the performance of the super-SUN source because of the expected improvements in the cold neutron transport efficiency.

7.6.1.5. Neutrino Physics

Nuclear reactors are a uniquely powerful, abundant, and electron-flavor-pure source of MeV-scale antineutrinos. Electron-flavored antineutrinos ν_e are produced in reactors as the unstable, neutron-rich products of nuclear fission that undergo β-decay reactions. While only a few percent of the excess rest mass energy from one nuclear fission is ultimately expressed as ν_e kinetic energy, this equates to a total release of 2×10^{17} ν_e per MW_{th} power generated. The energy spectrum of ν_e emitted by an operating reactor core reflects the decay schemes of the decaying isotopes, as well as the relative abundance of these isotopes in the nuclear fuel, which is driven primarily by the likelihood of their production (or yield) in the core's fission reactions [92,93,94,95]. Knowledge of the total number of neutrinos emitted depends on precise knowledge of the reactor power and fuel burnup. Research reactors can be relatively compact (~m scale) and well-understood neutrino sources. They also offer the especially important characteristic of being operated with a limited duty cycle, affording valuable opportunities to study experimental backgrounds.

Despite their attractive features, short-baseline experiments at reactors face significant experimental challenges. The extremely low neutrino interaction rates of 100s per tons of active volume per day for a typical arrangement mean that backgrounds are an enormous challenge. As there are no plans for a buried reactor facility, experiments must operate near the earth's surface and close (~ several meters) to an operating core. Raw background rates can be five orders of magnitude higher than the signal. Nonetheless, technological advancements have successfully allowed for precision experiments in these environments for some limited detection mechanisms [58,57,96]. Despite these recent successes, a purpose-built facility promises to facilitate dramatic increases in both sensitivity and data quality. An ideal facility at the NNS would have the following features:

1. Neutrino flux: neutrino experiments are always starved for statistics. The neutrino flux is proportional to reactor power and inversely proportional to the baseline squared. The current NBSR running at 20 MW_{th} and hosting an experiment at a 3-4 m baseline is competitive with other research facilities world-wide. Increasing flux as much as is feasible above this benchmark is highly desirable.

2. Core design: Much of the well-motivated oscillation physics is at length sales on the meter scale. This motivates a core at or below the meter scale to avoid washing out oscillation physics effects. Determining the absolute flux to high precision, which supports improved nuclear data, motivates thermal power measurements at below the 1% level.

3. Experimental facility: the very small neutrino interaction rate necessitates multi-ton scale experiments. A devoted experimental area capable of hosting 100 ton 1,000 m^3 detectors placed as close as possible to the core is highly motivated. Ideally such a

facility would allow changes in the baseline from a few meters to 20 m. This facility need not be located in-plane with the reactor core but should allow access for large fully assembled equipment.

4. Backgrounds: Ideally a neutrino facility would be located with a minimum of 10 m of water-equivalent overburden to reduce cosmogenic backgrounds. Attention to reducing neutron and gamma backgrounds is secondary, but also important.

The development of the NNS represents a unique opportunity to design a world-leading neutrino facility capable of hosting neutrino experiments to advance our knowledge of neutrino and BSM physics significantly as well as to support the development and calibration of advanced neutrino-based safeguard tools. We recommend that the design process fully engage the neutrino physics community to ensure that this possibility is fully explored.

7.7. Workforce Needs

Achieving these science goals and ensuring that these facilities continue to be a national resource for world-class fundamental neutron and neutrino physics, will require more than just the infrastructure described above. A significant investment in, and expansion of, the current workforce in neutron and neutrino physics at NIST will be needed. Each of the facilities described, the cold endstation, neutron interferometry, the new UCN source, the neutrino program, and the monochromatic beamlines, will require several dedicated scientific staff to run the beamlines and facilities and pursue experiments in collaboration with academic, government, and industry scientists. These facilities will also require significant engineering, radiation safety, and technician support.

7.8. References

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8. Nuclear Methods and Radiochemistry

8.1. Panel

Chair:
L. Raymond Cao – *Ohio State University*

Panel Members:
John Brockman – *University of Missouri*
William Charlton – *University of Texas at Austin*
R. Gregory Downing - *RGD Research*
Zsolt Revay – *Technical University of Munich*

Scribe:
Jamie Weaver – *National Institute of Standards and Technology*

8.2. Glossary of Terms:

Compton imaging: an imaging method that elucidates material structures by inelastic scattering of low-energy gamma rays emitted from an isotope by molecules Inductively coupled plasma mass spectrometry. and other atomic structures.

Digital twin: a virtual model of a physical object

ICP-MS: Inductively coupled plasma mass spectrometry.

ISO: international standards organization

Rabbit tube: pneumatic tubes that transport INAA samples to and from irradiation locations within a nuclear reactor pool.

XRF: X-ray Fluorescence k_0-method – where a universal constant (the k_0) is used to calibrate empirical INAA and PGAA data as opposed to using different calibration constants for each element measured.

8.3. Summary

NIST has an extensive program in neutron analytical methods. The major techniques in the suite of nuclear analytical methods includes Instrumental Neutron Activation Analysis (INAA), Prompt Gamma Neutron Activation Analysis (PGNAA), Neutron Depth Profiling (NDP), and Delayed Neutron Activation Analysis (DNAA). These are key, highly sensitive, multi-element, quantitative analytical methods that are essential to NIST's mission to promote U.S. innovation and competitiveness by providing certified reference materials.

Neutron activation analyses are primary methods, with INAA being a "gold standard" in the certification of standard reference materials required for international commerce. These methods have been used in the certification of Standard Reference Materials (SRMs), development of documentary standards, and/or for measurement services at NIST. SRMs serve as foundational metrology standards for thousands of chemicals and medicines used in our daily life. They play a critical role in calibrating measurement instruments, evaluating test procedures, and ensuring quality control for semiconductor materials, thus enabling the modern electronics-based society.

A future reactor at NIST should preserve and expand upon current neutron analytical methods to sustain and strengthen NIST's leadership as an international metrology institution. The strategic addition of new instrumentation aids in reaching this goal. The requested instruments, detailed below, will also benefit from a new high-intensity, low-energy, positron source for advanced materials studies and additional near-core or beam irradiation locations or facilities for fusion, semiconductor, and quantum sensor studies. The next-generation neutron source must be adaptable so that it can address the "unknown of the unknown" arising over the next 50 or more years.

8.4. Neutron Analytical Methods at NIST

The NIST Standard Reference Materials (SRM) program supports accurate and compatible measurements by providing materials with certified compositions and/or properties. Industry, academia, and governments use SRMs to facilitate commerce and trade and to advance science and technology. They are employed in instrument calibrations and to verify the accuracy of specific measurements, making them a keystone of industrial and regulatory quality assurance programs [1]. Although not a comprehensive list, SRMs play an important role in agriculture, security, manufacturing, transportation, mining, healthcare, energy, and engineering industries [2]. They serve as a primary mechanism for supporting measurement traceability in the United States [2]. They are also crucial to the preservation of cultural heritage, a $500 billion global industry with a projected 4% growth.

NIST certification of a composition or property of an SRM usually requires at least two independent measurement methods [3]. Neutron analytical methods are ideal for independent, high quality, and accurate measurements of composition in a variety of matrixes and chemistries and thus are often employed as one of the measurement methods. The process is quite simple, relying on well-defined physics and requiring minimal chemical processing. For example, dissolution of samples is not required, reducing the possibility of cross-contamination, material loss, or incomplete dissolution. INAA results generally don't depend on the matrix and it is nominally non-destructive. It is also a rather high throughput technique as 1000's of samples can be measured per year. A combination of INAA and PGNAA can provide quantitative elemental composition values for most of the elements in the periodic table. Once produced, SRMs must be monitored for stability for their foreseeable distribution life [4]. Some SRMs, for example the SRM 610 glasses, have been in distribution and monitored by NIST for over 50 years. These measurements are preferably performed by the same methods used for their certification. For over 40 years INAA and PGNAA along with other non-nuclear methods (e.g., ICP-MS) for the certification of standard reference materials SRMs in the United States. In addition, NDP has been used to certify standards for the semiconductor industry. In total, more than 200 currently SRMs have been certified by neutron analytical methods.

In addition to the development and certification of SRMs, the neutron analytical methods facilities at NIST are used to develop and test documentary standards and for measurement services. Measurement services on neutron analytical methods instruments are often categorized as "special tests" which are held to the stringent requirements of NIST quality system for measurement services. The Inter-American Metrology System Quality System Task

Force and the Joint Committee of the Regional Metrology Organizations and the International Bureau of Weights and Measures certify that this quality conforms to the requirements of ISO/IEC 17025, ISO 17034, and ISO 17043. The program also meets the requirements of the International Committee for Weights and Measures Mutual Recognition Arrangement for recognition of national measurement standards. Finally, neutron analytical methods in general are recognized by the Consultative Committee for Amount of Substance Metrology (CCQM) in Chemistry and Biology (a committee of the International Committee for Weights and Measures). This level of recognition is needed for international trade and commerce activities [5].

8.5. Science Drivers

The drivers for advanced neutron analytical methods at a new NIST reactor include:

1. the certification and continued support of the certification of NIST SRMs, creation of standard data sets, and development of documentary standards;
2. providing industry and the general scientific community access to advanced neutron-based irradiation facilities;
3. providing unparalleled measurement services to support of U.S. research and development; and
4. offering exceptional measurement capabilities based on neutron analytical methods to users from across the nation.

The current NIST reactor provides an intense neutron flux for many academic and industrial users. This access should be expanded to meet burgeoning R&D needs into the future. A successful transition to a new reactor requires the continuation and advancement of existing neutron analytical methods techniques with modernized facilities to provide reliable measurement services to meet the nation’s needs. Such services would include, as examples, using NDP to benchmark Li-ion and next generations of battery performance for electric vehicles and personal electronics as well as the development of a circular economy for batteries [6], using PGNAA to gain insight into the long-term durability of materials for our infrastructure (*e.g.*, Cl and H distribution in degrading concrete [7, 8]), and employing INAA to improve environmental and agriculture resilience and vibrancy across all 50 US states and possessions [9].

The new reactor should establish a facility for medical isotope R&D. The medical isotope market is expected to exhibit an annual growth rate of »7% and have a market value of 10 billion USD by 2027 [10]. This market will further expand in future decades as new isotopes emerge for the diagnoses and treatment of health conditions such as heart disease and cancer. Because a new NIST reactor will serve a wide variety of ever evolving research and industrial needs, it will not be optimized for the commercial production of medical isotopes. However, it could be ideal facility to make isotopes for R&D and SRMs. For example, primary standards for medical isotopes are currently needed to ensure accurate measurement and support traceability for regulatory compliance, patient safety, and effective treatment [11]. The Department of Energy is working to increase domestic isotope production [12], however a new NIST facility would not only complement, but also extend those activities. Moreover, an R&D program enabled by a state-of-the-art neutron source at NIST would naturally complement the Brookhaven Isotope Program. At Brookhaven, isotopes are created using an accelerator which typically produces proton-rich isotopes, whereas reactors produce neutron-rich isotopes – both of which are of essential to medical research.

An additional facility that would be unique to the U.S. is one with the ability to irradiate materials for fundamental research and develop testing methods for the radiation resilience and damage induced changes in materials. Lack of knowledge about how radiation damage progresses over long term and from a variety of energy scales/sources (e.g., fusion, fission reactions) presents a barrier to realizing energy independence and advanced travel in or beyond the atmosphere [13, 14]. Most testing facilities use low-brilliance neutron reactor or ion-based irradiation sources, which induce damage that is partially representative of what may be encountered in the above listed scenarios. Radiation-produced defects in diamond and other semiconductor materials form qubits that enable applications in quantum sensing and metrology, quantum communication, quantum computing, and cryptography. A broad spectrum, neutron reactor port/beam with a cryogenic sample environment would also enable studies of defect formation, evolution, and methods of mediation when defects produced are being frozen.

Deep, multi-scale insight into the material and crystal defects and chemical changes produced from the radiation damage could be realized through the establishment of a positron production beamline in addition to the above listed irradiation locations. Such capability is already available in other countries, e.g., Germany [15], but has yet to be established in the U.S. Creation of a high intensity positron beamline will propel the U.S. lead in physical and chemical properties of materials and would be useful for basic science. It will also allow cross-comparison of reactor-based positron results with enhanced reliability of fundamental and applied neutron science research.

Impacts from the inclusion and growth of neutron analytical methods capabilities at a new NIST reactor will include bolstering of the U.S. circular economy, encouragement of growth in aerospace and space exploration sectors, enrichment in U.S. infrastructure resilience, and support of national security and non-proliferation activities. The new facility will also aid in advanced, rapid, and reliable material discovery programs – an area needed for the realization of industrial smart manufacturing (Industry 4.0). Finally, a neutron analytical methods program will facilitate U.S. competitiveness in the energy, medical, agricultural, environmental, and communications sectors through the continued production of Standard Reference Materials, methods, and data sets.

8.6. Requested Capabilities/Instrumentation

The full range of activities under the neutron absorption methods umbrella (Table 1) require that the new NIST reactor be a broad-energy spectrum neutron source that can provide epi-thermal, thermal, and cold neutrons and is capable of supporting associated facilities (e.g., positron station). This range of energies is best delivered through access to in-pool, beam ports, a thermal column, rabbit tubes, and via beamlines. Neutron flux needs will vary based on application but should range from $1x10^{10}$ $cm^{-2}s^{-1}$ for the cold neutron beams to at least $1x10^{15}$ $cm^{-2}s^{-1}$ with optimal thermal-to-fast flux characteristics for INAA and other irradiation applications. An exceptional neutron source that produces a continuous and near-uniform neutron energy, temporal and spatial profile at experiment locations during operation is required to produce the highest-quality data – a highly desirable feature to develop and certify

Standard Reference Materials. Ideally, the neutron field or beam delivered for PGNAA or NDP analyses needs to be uniform in the dimensions of space, energy, and time, and be relatively free of background radiation components that interfere with neutron-analytical experiments, including x-rays, gamma rays, and instrument specific un-desired neutron energies.

INAA and PGNAA are analytical techniques that rely on the measurement of gamma rays emitted from a sample following neutron irradiation. Both techniques are foundational methods for the NIST SRM program. They utilize independent physics from more common analytical methods (ICP-MS, XRF), thus minimizing the possibility of systematic errors during certification. They also provide measurement services on-demand for industry, academia, and other government agency collaborators. Required resources for advancing INAA include access to highly thermalized, epi-thermal, and cold neutrons. At least six rabbit tubes, providing access to a variety of neutron energies and flux characteristics, are needed for the SRM program. These rabbit tubes should possess characteristics of high-flux and uniform neutron fields optimized for thermal and epithermal neutrons. Additionally, one set of rabbit tubes should be able to accommodate smaller-diameter samples which would serve state-of-the-art automated INAA systems. To increase measurement reliability, the flight tubes should be easily replaceable, and access assured by advanced planning for new rabbit tubes and/or easy replacement of the pneumatic tubes and in-core irradiation locations. For measurements of nuclides with short half-life nuclides, transfer times should be fast with minimal cycle time between irradiation location and rabbit-receiving labs for measurements of short half-life nuclides. The rabbit tubes should be actively cooled to enable longer irradiation times. Equally important real-time neutron flux monitors should be included within the irradiation and rabbit stations at multiple locations for quality assurance and control. Finally, with the new reactor design, it will be feasible to adopt the “k_0-method” of standardization of the INAA technique, a procedure already adopted by reactor facilities in Europe, Asia, and South America, which requires high and stable thermal neutron flux and a significant component of epithermal neutrons for resonance activation.

PGNAA has proven invaluable for non-destructive elemental characterization of a wide variety of materials, with an emphasis on low-Z elements, especially H and B, which cannot be easily measured by X-ray methods. Next generation PGNAA instruments should include at least two cold stations: one for SRM measurements and a second for measurement services and method/ instrument development. The cold stations should be optimized for measurement of H and B at extremely low concentration levels (sub-ppm), with a minimum thermal equivalent neutron flux of 10^{10} $cm^{-2}s^{-1}$ and very few fast or epithermal neutrons. The station should be equipped with neutron focusing optics to allow for a broad range of sample sizes (micrometers to meters) that can be easily moved in and out of the beam and replaced by a neutron beam chopper for measurement of decay gamma rays from nuclides with ultra-short half-lives (e.g., ^{20}F, $t_{1/2} = 11$ s). Other features should include a temperature/atmosphere-controlled sample chamber, and an automatic sample changer for high sample throughput. Sufficient space is required for a lead-shielded detector cave housing a standard gamma-ray detector with BGO (bismuth germanium oxide) Compton shield and/or a multi-detector array. Space is required for an adjacent low-background counting station (equipped with multi-detectors) for performing INAA of samples removed from the beam, with the capability of rapid transport of samples from the beam to the INAA counting station. The new neutron facility should also include at least one thermal neutron PGNAA station for SRM measurements. This station should have a minimum thermal flux of $3x10^8$ $cm^{-2}s^{-1}$ and minimum thermal/fast ratio of 2000. Like the cold station, the thermal station requires an automatic sample changer for maximum sample throughput.

The NDP program at NIST has a long history of supporting U.S. industry by providing key contributions to (for example) semiconductor materials development in 1980's and 1990's, nuclear materials resilience in the 2000's, and Li-ion battery materials development and performance benchmarking in the 2010's and 2020's. NDP is different from other neutron analytical methods as it utilizes the energy loss of charged particles produced from neutron analytical methods reactions to provide quantitative depth profiles of select elements within the first 10's to 100's of micrometers from the surface of a material or device.

Table 1: Summary of requested neutron analytical methods capabilities/facilities at the new NIST reactor.

Facility	Nominal Neutron Energy	Minimum Thermal Equivalent Neutron Flux (cm^{-2} s^{-1})	Location	Minimum Number of Locations	Number of Instruments Location(s) or Irradiation Locations	Applications
INAA	Thermal, Epi-thermal	1E12 for beams, 1E13 to 1E15 for rabbit tubes	In or near core (rabbit tubes), port, beamline	6 quick transfer time rabbit tubes, 1 port or beamline	1, 6 receivers* (7 total)	SRMs, Measurement Services, R&D
PGNAA	Cold	1E+13	Beamline	2	1-2 each (2-4 total)	SRMs, Measurement Services, R&D
	Thermal	3E+8	Port	1	1	SRMs, Measurement Services, R&D
NDP	Cold	1E+10	Beamline	2	1-2 each (2-4 total)	SRMs, Measurement Services, R&D
	Epi-thermal	1E+12	Port	1	1	SRMs, Measurement Services, R&D
Thermal Column Irradiation	Thermal	1E12	Thermal column	1	1	Measurement Services, R&D
Medical Isotope R&D Facility	Thermal	1E+13	Flux Trap	1	1	SRMs, R&D
Positron beam Facility	Thermal, positron energy of ~1 keV	>1E+9 moderated positrons	Beamline, Port	1	Min. of 4	Measurement Services, R&D

** A receiver is a location where a rabbit (vessel containing the samples and standards) is placed following it being pneumatically transported through a rabbit tube. The rabbit is moved from the receiver to a detector that is in a separate, low background counting laboratory.*

Elements that can be measured using NDP include He, Li, B, N, Cl, and Na. At least one cold, broad spectrum neutron beamline with a neutron flux no lower than 1×10^{10} $cm^{-2}s^{-1}$ should be provided at the new NIST reactor, as this would provide exceptional capabilities for temporal studies. The instrument should have a clean background (chemical and electrical) with an automated sample changer to maintain current measurement services and certification activities. Inclusion of neutron-focusing optics would substantially improve NDP data quality and reliability. Access to an optimized epi-thermal instrument development beamline or neutron port location could double or triple the list of accessible elements by NDP and open a range of new measurement capabilities to support U.S. R&D activities.

The development of next-generation neutron analytical instruments requires access to two flexible and spacious instrument development cold-neutron end stations with switch-on and off optics for PGNAA and NDP. These beamlines would facilitate the development of next-generation gamma-ray imaging capabilities, such as Compton or "ghost" imaging, NDP time-of-flight, and neutron-induced secondary x-ray emission spectroscopy. All proposed beamline and port stations should be designed to accommodate enhanced sample environments, such as high pressure, magnetic fields, sample temperature, which should be integrated with sample environment services for the entire facility.

A high-intensity, low-energy, nuclear-reactor-based positron irradiation facility is currently only available at FRM-II in Germany [16]. A similar facility should be built at a thermal neutron position. The beamline would produce positrons by employing a cadmium cap to convert neutrons to high-energy gamma-rays, which are then converted to positrons using a platinum target or another conversion metal foil. A magnetic field would be used to extract and guide the positrons to multiple experiment stations. The broad energy range of the positrons would make possible surface texture measurements, coincidence mode doppler broadening experiments, positron annihilation studies, and studies key to fundamental physics along with the investigation of crystal damage and dislocations, and electron density changes in condensed matter. At least four instruments could be supplied from a single port location.

There is great industrial need for a thermal column – specifically for the irradiation of very large samples (up to 5 meters by 5 meters minimum). The column should be adaptable for a sample holder that rotates and can be placed in the facility for long-term irradiation projects. A rabbit irradiation position terminating in the thermal column would enable the precise measurement of radioisotopes at much lower detection limits compared to water mediated neutron fields; specifically due to the much higher thermalization in the thermal column which is typically >10000 thermal/fast compared to roughly 100 thermal/fast elsewhere.

A medical isotope R&D capability could be operated in collaboration with the DOE National Isotope Development Center. This facility would enable the production of small batches of high quality, low-impurity, and relatively short-lived isotopes with high specific radioactivity for R&D and SRMs. These isotopes could be shipped directly to an established US DOE Isotope Production laboratory for processing.

8.7. Auxiliary Facilities

Auxiliary facilities (summarized in Table 2) will be needed to support the analytical neutron analytical methods capabilities. Both radioactive materials labs and non-radioactive material labs are required. Labs for counting of radioactive samples will need to accommodate six or more automated gamma-ray counting systems with at least one lab with low gamma-ray background level maintained for counting of low-level radioactive samples. Additional laboratory space is necessary for sample dissolutions and separation chemistry. Radioactive sample preparation labs (i.e., radiochemistry labs) that include chemical, nanoparticle, and acid/base hoods, gloveboxes, freezers, and other sample preparation equipment and environmental control capabilities will be needed. A separate space will be required for the building, machining, and maintenance of equipment that has become radioactive during use such as 3 – 4 hot cells which will be required for the handling of very radioactive and hard to detect samples or to contain radioactive materials as well as to handle medical radioisotopes. A pneumatic and/or automated radioactive material transfer system between irradiation locations, hot cells, and laboratories will help to meet U.S. Nuclear Regulatory guidelines to conduct experiments that limit doses to humans at *As Low As Reasonably Achievable* (ALARA) levels. Non-radioactive material handling labs should include separate spaces for SRM sample preparation that ensure quality and meet chain-of-handling protocol requirements. Equivalent equipment and space for radioactive materials labs is also needed for both measurement services, research, and SRM development/certification activities. Separate radiochemistry labs and hot cells are needed for the proposed medical isotope research.

Table 2: Summary of requested auxiliary spaces, supporting facilities, and laboratories for a new reactor neutron analytical methods facility.

Name	Designation	Rad or Non-Rad	Number of Spaces	Dedicated or Shared Spaces?	Additional Comments
General Chemistry & Sample Preparation Labs	Lab	Non-rad	4	2 dedicated to Standards work, 2 shared spaces	2: SRM certification 2: Measurement Services & R&D work
Radiochemistry Lab	Lab	Rad	5	Dedicated	2: SRM Research 2: Measurement Services Research 1: Medical Isotopes Lab
Instrument Repair Space	Engineering Space	Rad	1	Shared	-
Clean Room Lab	Lab	Rad and Non-rad	2	Shared	-
Storage/ Management Space	Storage	Rad and Non-rad	2	Dedicated	1: SRM certification 1: Basic Research
Hot Cells	Lab	Rad	3 - 4	Dedicated/Shared	SRM certification, measurement services, medical isotope R&D, basic research
Medical Isotope Research Lab	Lab	Non-rad (target preparation) and Rad	2	Dedicated	1: Target Prep. 1: Isotope testing and quantification
INAA Sample Counting Labs	Lab	Rad	4	Dedicated	1: Low-level (underground), 2: SRM certification 1: Measurement Services

Data reduction and analysis goes hand in hand producing large data files. Therefore, large data sets are inevitable with these new neutron analytical methods facilities. Long-term, stable data storage and processing software will be needed to use, catalog, and process data after it has been collected. Software will be needed that would integrate machine learning and artificial intelligence programs into PGNAA, INAA, and NDP data collection systems so results could be assessed on the fly allowing experimental issues to be rapidly addresses and, reducing the time and resources needed to analyze the data. Modeling and associated computation capabilities are also required.

8.8. Transition Strategies Suggestions

A vital factor in the success of a new NIST neutron source will include the transition of services and capabilities. The extended closure of the current NIST reactor has provided experience and insight into transition needs. First, it is suggested that DOC provide funding and support the services of smaller, satellite reactor facilities located at U.S. university campuses so that they can absorb the demand for neutron measurement services and aid in the continuation of institutional knowledge and skills. Second, DOC should strategically fund and scope internal staff activities so that they may develop external synergistic activities at these and other high neutron flux institutions several years in advance and during the transition. In preparation for the transition, efforts are needed to increase the network between NIST scientists and staff and associates at other research reactors. This could be achieved by periodic facility working group meetings. Third, there should be a strategic increase in the number of NIST staff to address generational gaps prior to the reactor transition so that instruments and programs have continuous support. Fourth, it is suggested that new and transitioning instruments have a digital twin created and be made to be modifiable and transportable. This will significantly increase confidence in the smooth transition of certification instrumentation from the old neutron source to a new source. Finally, engineering and facilities support (radioactive material focused and non-radioactive material focused) for neutron analytical methods instrument transition/development and exchange of operational experience between NIST and universities should be encouraged and facilitated.

NDP can provide mass percentages to sub-parts-per-million levels for many light elements of industrial significance (lithium, boron, nitrogen, and helium), which is often difficult to assess by INAA and PGNAA and reveal the concentration distribution within the first tens of micrometers from a sample’s surface.

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9. Engineering

9.1. Panel

Chair:
Adrian Brügger – *Columbia University*

Panel Members:
Bjørn Clausen – *Los Alamos National Laboratory*
Thomas Gnäupel-Herold – *National Institute of Standards and Technology*
David Jacobson – *National Institute of Standards and Technology*
Norbert Seifert – *Intel Corporation*
Anton Tremsin – *University of California, Berkeley*
ZhenZhen Yu – *Colorado School of Mines*

Scribe:
Jacob LaManna – *National Institute of Standards and Technology*

9.2. Glossary of Terms

AFM: atomic force microscopy

BEI: Bragg edge imaging, a method to capture deformation and material phase information on structures at the atomic length scale.

DFI: dark field image

High-entropy alloys: solids composed of similar or relatively large proportions of ~ five or more elements, one of which is a metal.

meV: milli electron volt (1/1000th of an electron volt), a commonly used unit of energy.

MeV: mega electron volt (1 million electron volts).

Multi-principal element alloys: another name for high-entropy alloys

nCT: neutron computed tomography; like a CT scan that uses neutrons instead of x rays.

nGI: neutron-grating interferometry, an imaging technique that provides information on structures smaller than the resolution limit.

QNM: quantitative nanomechanical property mapping

SANS: small-angle neutron scattering

Strain: degree of deformation (e.g. in %) of a material due to, e.g., loading.

Stress: force per unit area.

9.3. Summary

Neutron-based research on engineering materials, which includes neutron diffraction and imaging characterization, operates at the core of the mission of the Department of Commerce. Neutron measurements provide unique scientific insights that enable the nation’s businesses to generate new knowledge and value and thus remain at the forefront of their respective fields. Key areas of focus include energy materials, additive manufacturing, aerospace, medical and dental technology, metal-forming and joining, infrastructural materials, and the transition to a decarbonized economy; these areas have a combined portfolio revenue on the order of trillions of dollars. The Engineering Panel recommends reactor capabilities that include both thermal and cold neutron beamlines. The Panel believes the following instruments will meet the engineering research community’s future requirements and specifications for the reactor and accompanying facilities: 1) simultaneous thermal-neutron and X-ray imaging, 2) cold-neutron microscope, 3) cold-neutron-imaging grating interferometer, 4) white-beam stress diffractometer, 5) constant-wavelength stress diffractometer (workhorse), 6) multimodal large sample station, 7) dedicated texture instrument with extensive detector coverage for fast measurements. The proprietary and export-controlled nature of some engineering research necessitates the provision of infrastructure and management systems that can securely store samples and data. Further, the diverse length scales of engineering samples require the future facility to support complex and challenging sample environments with commensurate infrastructure requirements (electrical, chilled water, gas supply and effluent, etc.). Ultimately, the primary goal is to expand neutron measurements from the static domain to the kinetic domain so that measurements of time-dependent processes such as texture evolution, fracture nucleation, phase transformation, and porous media diffusion can be made with a high signal-to-noise ratio. This will require increased flux and brightness.

9.4. Science Cases

The following research areas showcase and motivate the need for engineering materials diffraction and multimodal imaging capabilities at the future NIST reactor. The various research thrusts are motivated by their central importance to US commerce and quantified by the economic revenue generated by each domain.

9.4.1. Energy Materials

Understanding the electrochemical processes in novel battery systems on multiple length scales would transform the development of new technologies in this field. The trifurcation of the battery industry into centimeter-scale cells for mobile devices, ultra-high-performance cells for automotive, aerospace, and defense applications, and low-cost solutions for megawatt-scale electrical-grid-buffering applications will drive innovation of these technologies on various fronts. The challenges inherent in the “greening” of the electrical grids by using natural energy sources, which have highly variable availabilities, and those associated with obtaining relatively scarce elements, such as Li, make innovation in this field absolutely pivotal for the economic and social advancement of the nation.

Electrochemical energy conversion is a complex process that, if not implemented well, can drastically limit the performance and lifetime of energy storage devices. The operation of batteries for energy storage involves kinetics in chemistry, crystal structure, and electrode morphology that occur over length scales ranging from Ångstroms (10^{-10} meters) to centimeters

(10^{-2} meters), as illustrated in Figure 1. The DOE BES's 2017 report titled "Next Generation Electrical Energy Storage" [1] emphasizes that both predictive modeling and advanced characterization methods, including advanced neutron imaging and diffraction techniques, are needed to realize the next generation of energy-storage devices. A fundamental understanding of the irreversible, multi-scale, aging processes in electrochemical cells is key to advancing energy-storage technology, as it will help engineers to manage metal plating and stripping in liquid [2-4] and solid electrolyte batteries [5,6] and control multiscale electrode structures at the anode and cathode to optimize performance [7,8]. Neutron-imaging methods offer length-scale-bridging measurement capabilities that are sensitive to light elements while simultaneously providing the ability to penetrate through metals [9], thereby allowing researchers to see inside devices.

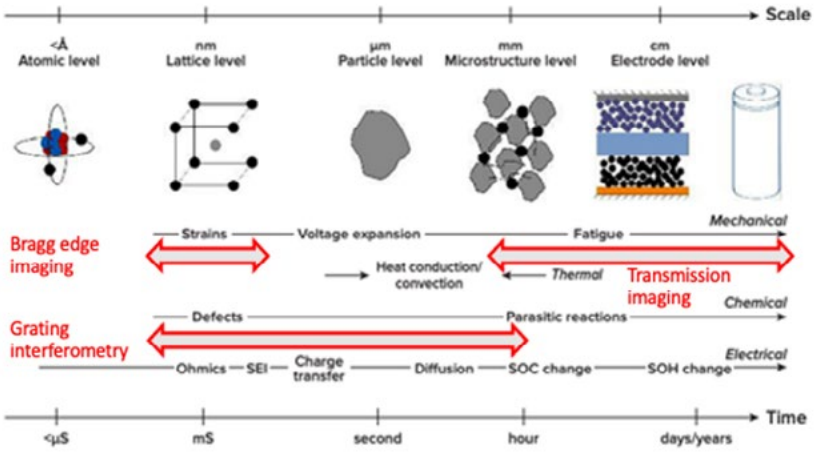

Figure 1. Irreversible processes across time and length scales in electrochemical cells overlaid with Bragg-edge imaging, neutron-grating interferometry, and conventional transmission imaging [1].

The proposed NIST reactor would advance the frontiers of knowledge in energy storage by enabling a suite of neutron-based measurement techniques that can non-destructively characterize these phenomena *in operando* over a full range of cycling conditions and across multiple length and time scales in batteries produced at practical scales, as shown in Figure 1.

The intercalation and deintercalation processes that occur during cycling produce changes in crystal structures that appear as distinct Bragg-edge signatures that affect the contrast measured in imaging data. Such signatures have been observed for both anode and cathode active materials in commercial Li-ion batteries; examples are shown in Figure 3 of Ref. [10] (https://www.sciencedirect.com/science/article/pii/S0167273816000163#f0015). The smaller Bragg peaks seen in this figure result from the strong attenuation of the neutron beam when passing through the commercial cell structure and the hydrocarbon electrolyte solution. More distinct signals may be achieved with cells optimized for imaging experiments and measurements at longer wavelengths. Improving the temporal and spatial resolution of such measurements would enable observation of localized state-of-charge, other inhomogeneities, and crystal structure changes (that may result from aggressive operating conditions) distributed throughout an electrode. Local microstructural changes associated with active material particles, such as pulverization and changes in porous regions due to expansion of high-capacity material, may also be observed using the underlying SANS signal accessed from nGI data [11].

9.4.2. Additive Manufacturing

Over the past decade, Additive Manufacturing (AM) has revolutionized fabrication in industries ranging from aerospace, medical, automotive, construction, to sports, and it has provided the nation with a global competitive advantage and fast response to increasing market demands. The U.S. AM market size was valued at $2.99B in 2021 and is projected to expand at a compound annual growth rate (CAGR) of 18.9% from 2022 to 2030 [12]. AM produces metal parts by selectively melting and solidifying feedstock to build a desired 3D geometry rather than by the more traditional method of removing material from cast or wrought stock [13, 14]. Due to localized cycles of rapid heating and cooling, the constraint of the base plate, and prior material deposits, significant levels of strain and stress arise in the AM parts during fabrication and leave residual stresses in the as-built part [15]. The residual stresses can be large, approaching yield strength, which can result in distortion [14, 16], premature fracture [17], and may affect performance during service. Hence, the performance of the produced parts cannot be derived based upon traditional casting and forming processing routes optimized over centuries. Instead, certification and qualification of AM parts requires a detailed knowledge of the process-structure-property-performance (PSSP) relationships for these new production avenues. Neutron diffraction and neutron imaging provide unique windows into the microstructure of metals, yielding quantitative data on residual stresses, defect concentrations, porosity, phase composition, and morphology, all paramount in determining these PSSP relationships. Moreover, the non-destructive nature of the neutron measurements enables determination of material properties as a function of production steps for a single sample as it evolves, yielding unique guidance and validation data for physics-based processing and constitutive models for the manufacturing processes. Until predictive models capable of determining the PSSP relationships are developed, there is no path forward for the qualification and scalability of AM components in failure-critical applications such as those in the aerospace industry and biomedical implants.

9.4.3. Aerospace

The aerospace and defense industry reported revenues of $741B in 2022 [18] with a positive industry trade balance of $40.6B. Energy efficiency requirements demand high performance and low weight, which pushes the envelope for materials performance and safety. Understanding and predicting materials performance becomes paramount. Advanced studies of PSSP relationships, including those based on neutron-diffraction measurements of residual stresses in components, are advancing both material properties and performance. For example, the complex microstructure of the superalloys used in jet engines provides high-temperature creep strength, and neutron-diffraction measurements were vital in clarifying the underlying high-temperature creep strengthening mechanisms in the γ/γ′ composites. This was achieved by performing *in situ* mechanical loading combined with heating to mimic the operating conditions of the material at temperatures up to 900°C [19]. This also exemplifies the need for advanced multimodal sample environments for materials testing at neutron beamlines and the facility infrastructure to support the power and cooling needs of the ancillary equipment. At the same time, residual-stress management is needed for superalloy turbine parts [20] as well as fuselage components [21], where the penetration power of neutrons allows for studies of full-size structural parts. The part shown in Figure 2 measures 2.5 m by 0.8 m in size, illustrating the need for large accessible sample spaces at engineering neutron diffraction instruments for residual stress measurements.


Figure 2. 7050 aluminum rib support structure for aircraft wing [21].

9.4.4. Welding & Joining, Alloying

Fortune Business Insights reported that the global welding market was valued at $23.75 billion in 2022 and is projected to grow to $34.18 billion by 2030 [22]. A thorough understanding of how residual stresses and far-from-equilibrium phase transformations evolve during welding and joining processes is critical for process optimization, component life prediction, and the development of solutions to mitigate materials property degradation. This is because most welding issues are related to the metallurgical nature, residual stress, and service environment (e.g., H_2, corrosion, elevated temperature, and fatigue).

Neutron diffraction is the only method that can provide 3D maps of the residual strain/stress profiles and phase distributions within weldments of bulk, large-scale engineering components nondestructively. Moreover, it can do so with a reasonable spatial resolution [23] from near-surface depths around 0.2 mm up to bulk measurements of ~100 mm in aluminum or ~25 mm in steel [24]. In recent years, there have been increasing demands to understand the transient behavior of weldments in many materials. One example concerns conventional alloys that are under more demanding service conditions, e.g., transportation of gaseous H_2 using existing steel pipelines for natural gas, steel wind turbine towers experiencing severe fatigue loading, and third-generation solar power plants under higher service temperatures for enhanced power conversion efficiency. Additional examples include newly developed engineering alloys with complex compositions and correspondingly complicated solidification and phase-transformation behavior (e.g., Ni-base superalloys, Generation 3 advanced high-strength steels, refractory alloys, and high-entropy or multi-principal element alloys) used in a variety of manufacturing sectors such as power generation, renewable energy, oil & gas, aerospace, and automotive. Meanwhile, the welding/joining industry has experienced significant technological advancement, which great affects manufacturing and construction industries such as high-energy beams, solid-state joining, hybrid processes, and micro-/nano-joining. This has driven a corresponding demand for improved sample environment capabilities that will make possible *in situ* characterization of materials behavior during rapid heating/cooling, mechanical loading, and exposure to harsh media (e.g., molten salt and gaseous/liquid H_2), all of which simulate relevant service environments, transient welding conditions, and hybrid processes (e.g., arc, laser, or induction heating, and ultrasonic vibration).

9.4.5. Infrastructural Materials

The current U.S. investment deficit on national infrastructure maintenance and construction amounts to $2.95 trillion. A fundamental understanding of the mechanics that degrade U.S. infrastructure is therefore pivotal in delivering scarce funding to the most urgent needs and to ensure that new systems can reliably resist these hazards [25].

9.4.5.1. Metals

Corrosion attacks and substantially degrades the metallic components of the structural and mechanical systems in major infrastructure. Here we take suspension bridges as an unfortunate example, as their reliability represents a critical societal need. The recent collapse of the Polcevera Viaduct (i.e., Morandi Bridge) in Genoa, Italy led to many casualties (43 dead, 16 injured) and a massive economic loss estimated at €784 million ($891 million) [26, 27]. However, the civil engineering community continues to rely on simplistic parametric corrosion models that fail to capture the multiscale mechanics and chemistry at play [28, 29].

To this end, a critical focus remains in trying to understand the residual stresses in structural members caused by material processing, fabrication, defects, and environmental influences such as corrosion. Digital twins are more advanced models that serve as analysis-and-design tools to empower the engineer and scientist to consider complicated stress states, especially in complex structural components and systems. Residual-stress mapping remains the most efficient path to benchmark such digital twins and feed them with residual stress data. Neutrons are the ideal tool with which to measure large metallic parts due to their ability to penetrate centimeters of metallic engineering materials without mechanically perturbing the sample. Progress has been made on understanding the internal mechanics of multi-body wires in suspension bridges using neutron diffraction, but to date we lack the capacity to perform spatially resolved live and *in situ* imaging of the evolution of component degradation, overload, and plastic flow. The latter can only be detected through imaging because plastic deformation is independent of atomic lattice spacing [30, 31]. Current research would be revolutionized by the ability to image live and *in situ* – under load and/or a corrosive environment – the formation of a corrosion front in direct space (nCT), i.e. the strain and phase evolution of the steel, while tracking porosity changes at both the corrosion front as well as at potential fracture sites (nGI).

The abovementioned capabilities could also be used in post-failure forensic investigations of a broad range of structures and components. In particular, engineering-scale structural systems (e.g., civil, aerospace structures) are generally too large to be imaged by traditional X-ray techniques without sectioning. New facilities should allow scientists and investigators to perform holistic, non-destructive characterization of forensic samples to quantify mechanical damage and internal deformation (nCT), residual elastic stresses (BEI), as well as porosity and void nucleation in advance of cracking (nGI). Dynamic data acquisition on the order of seconds or tens of seconds is essential to capture phase transformations and strains adequately as a function of environmental/external stressors.

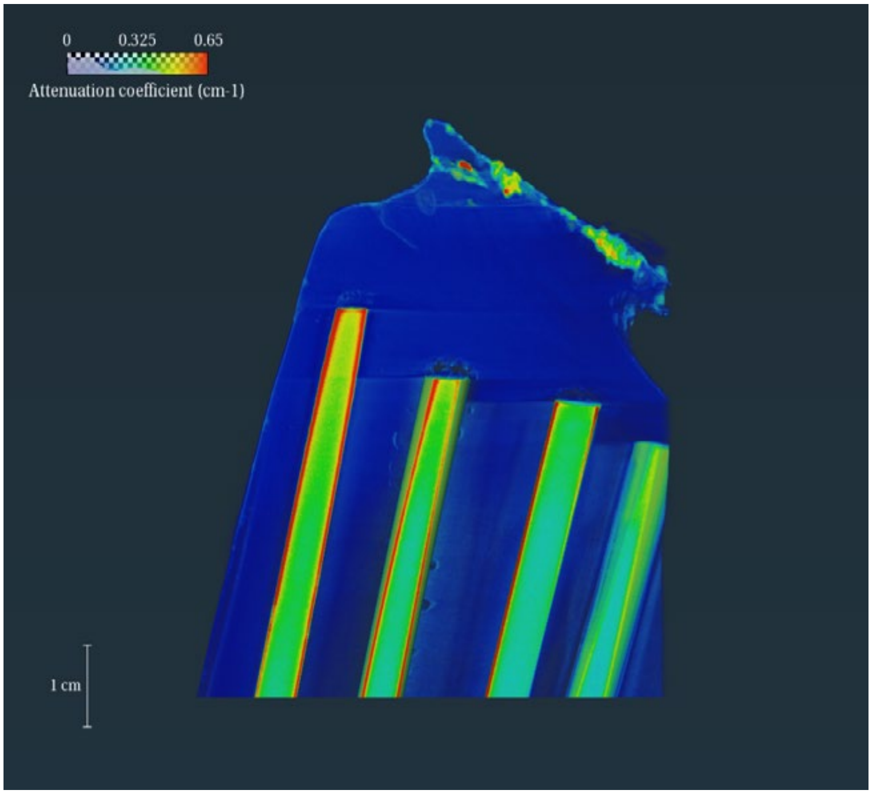

Figure 3. Neutron image of a cable socket from the collapsed Arecibo radio telescope shows arrows indicating voids around the wires caused by cable slippage. Credit: Adrian Brügger, Columbia University.

9.4.5.2. Concrete

As noted by industry and academia, transformative manufacturing is fast emerging as a critical area of development in the United States [31]. Concrete's high strength, flowability during construction, and track record of more than 150 years has led to tens of gigatons being used on an annual basis, requiring over four gigatons of cement powder to be manufactured annually [32]. The global usage of concrete on a volume basis is second only to society's need for water. This hunger for cement leads to massive resource and energy requirements together with emissions associated with the manufacture of cement, amounting to 9% of the total carbon footprint of humanity. Innovation and transformative manufacturing are central to the future of construction materials, where future efforts will focus on sustainability, additive manufacturing, and high-performance systems [33, 34]. The porosity and pore structure of concrete, which ranges from nanometers to millimeters, and the fact that it tends to be in a semi-saturated state makes it well-suited for characterization through SANS [35, 36]. Simultaneous imaging methodologies (dark field imaging, neutron grating interferometry) can be used to study the effects of environmental stressors on the permeability and pore structure of monolithic concrete specimens. This capability will enable the development of new types of high-performance concrete mixes using a materials-driven design methodology to drive, for example, the development of novel concrete AM systems. Neutrons are central for studying transport-dependent processes in concrete due to the aqueous environment found in its pores and associated H_2O molecules.

9.4.5. Hydrogen Embrittlement & Crack Initiation

The three major proposed mechanisms of hydrogen embrittlement (HE) are hydrogen-enhanced decohesion (HEDE), hydrogen-enhanced localized plasticity (HELP), and hydrogen-gas vacancy stabilization mechanism (VM) [37]. In HEDE, hydrogen accumulation at areas of high triaxial stress weakens the Fe-Fe bonds, which leads to premature fracture. In HELP, the presence of hydrogen enhances the mobility of dislocations. In VM, hydrogen is predicted to promote and stabilize the agglomeration of vacancies into pores. Recently, HE researchers have begun to view these mechanisms as being simultaneous and synergistic rather than separate. However, *in situ* measurements that can characterize the lattice structure (through BEI), the pore structure (through nGI), and hydrogen concentration (through contrast radiography) simultaneously during mechanical loading are essential to understand the synergistic action of these mechanisms.

One of the biggest issues with predicting accurate lifetimes of structural materials is determining the stress conditions required for crack initiation. Traditional techniques, such as fatigue-crack-growth-rate measurements, struggle to detect the small crack extensions of a young crack. One suggestion for early crack detection is to use nGI to measure void coalescence, which is often a precursor to crack initiation [38]. The use of nGI to measure the pores (for example, see Fig. 8 in Ref. [38] - https://www.sciencedirect.com/science/article/pii/S0264127517311061 - f0065) measure the strain is precisely the right combination needed to determine the stress conditions required for void coalescence and in turn for the detection of cracks within the timeframe of their initiation and requires a temporal resolution on the order of seconds [39-41].

9.4.6. Energy & Transport Infrastructure

Stress continues to be a key problem in energy and transport infrastructures due to the continuing trend to deploy new, higher strength materials with different properties that challenge existing material models. One example is rails, which, driven by the economics of rail transport, are exposed to higher wheel loads and higher rolling speeds, both of which contribute to an increase in internal stresses (Figure 4, left) that can lead to rail failure. Determining stresses in rails are a prime example of non-destructive stress measurements that cannot be done without neutrons. Another such example is the measurement of weld-induced stresses in safety-critical energy infrastructure parts such as off-shore pipelines (Figure 4, right).

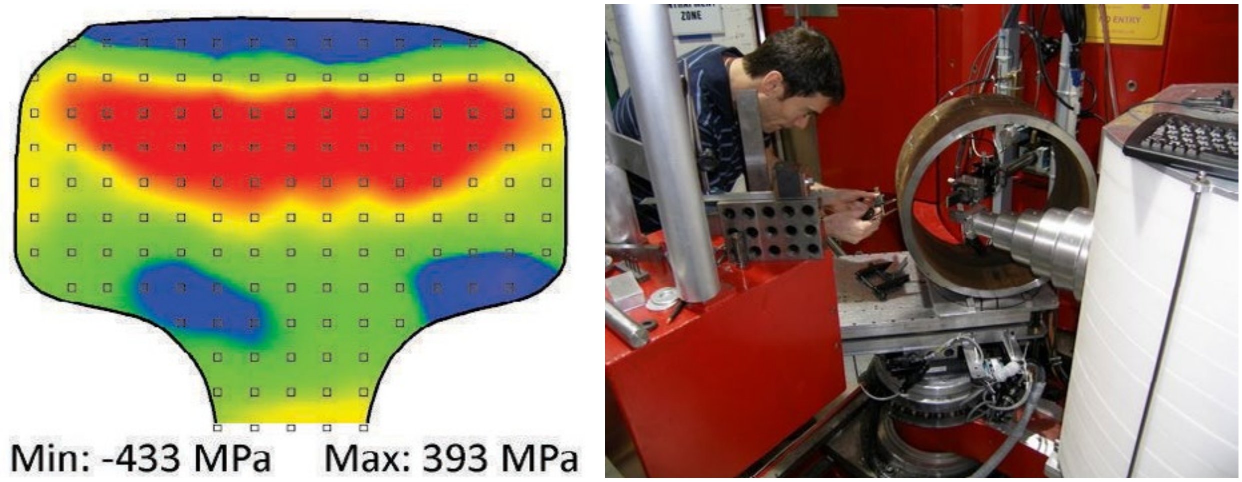

Figure 4. Left: Residual stresses measured with neutrons in a 0.4 m long section of rail [42]. Squares indicate measurement locations. Right: Neutron measurement of residual stresses in an offshore oil pipeline section.

9.4.7. Applied Stress in Structural Materials

Measurements made under applied stress in multi-axial deformation provide vital inputs required for computer modeling of automotive-sheet-metal forming. Industrial forming operations consist of various combinations of bi-axial stretching, shearing, and plane-strain deformation, all of which have their own stress-strain relationships. Also, straining modes often happen in combinations in which the deformation in each straining step depends on the previous straining history. Success in predicting these relationships has been elusive; however, neutron diffraction measurements of multiaxial stress-strain relationships together with innovative straining devices show great potential in meeting this industry need. Moreover, the demand for multiaxial stress-strain data is not expected to decline due to the continuing innovation in alloy development that is driven by lightweighting requirements.

Straining devices for multi-axial deformation require eight-arm actuation with strain levels comparable to industrial forming, i.e. a load capacity (>40 kN) per arm sufficient for testing advanced high-strength steels (AHSS), individual load control and displacement control to facilitate changing the straining mode during testing, sufficient size to allow for digital image correlation equipment, and heating capability for measuring warm-forming properties (Figure 5).

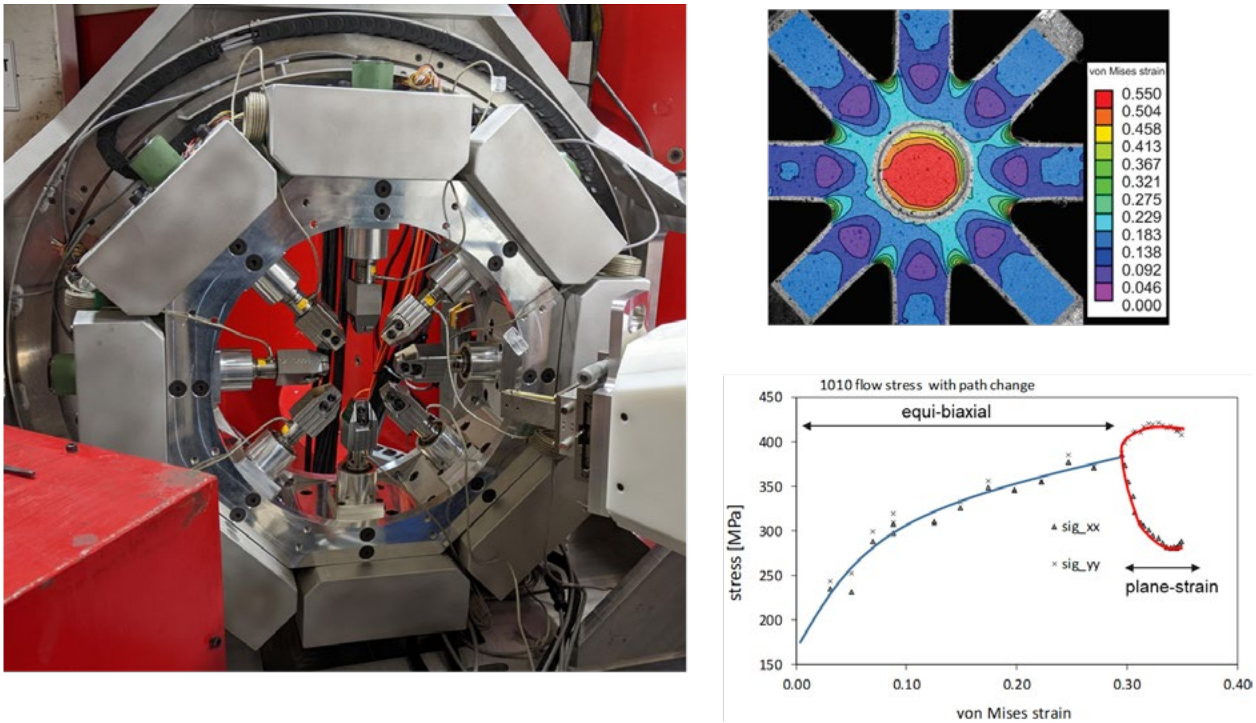

Figure 5. Octo-strain device (NCNR) used for the equi-axial stretching of a ferritic steel (left panel) followed by plane-strain deformation (lower right corner, red). The upper right corner shows the amount of deformation (strain); the area shaded in red is used to measure the acting stress and to correlate it with the strain in the same area measured by digital-image correlation.

9.4.8. Medical & Dental Biomaterials

Implant materials and systems are used to treat, augment, and/or replace dysfunctional tissues and organs [43]. In 2020, the global market for biomaterials exceeded $35 billion dollars and is predicted to reach 47.5 billion by 2025 [44]. Prominent biomedical engineering applications include orthopedic (joint implants, cements, fillers, scaffolds) [45-47], cardiovascular (vascular grafts, valves, pacemakers, stents) [48, 49], ophthalmic (artificial corneas, lenses), dental restorative materials (adhesive resins, resin composites, cements) [50], and implants. Resin composite dental restorations are the most prevalent biomedical intervention in human beings with more than 500 million placed globally every year [51]. The placement of restorations accounts for worldwide annual costs of around $298 billion, which corresponds to a total of 4.6% of all expenditures made in healthcare [52]. According to the American College of Prosthodontics, a large portion of the U.S. population have lost one tooth (~178 million) or all their teeth (~ 40 million) [53]. Dental implants have been used successfully to replace missing teeth. In fact, 3 million Americans currently have dental implants, and this number is increasing by 500,000 every year. In 2019, the market for dental implants in the U.S. and Europe was valued at $1.1 billion and €1.2 billion, respectively [53].

Despite all advancements in the field, the fate and longevity of these restorations are still not fully understood. Even though failure rates are low (2-5%), these correspond to about 275,000 implant failures and about $82.5 million each year [54], which underscores the need for the development and characterization of novel implantable biomaterials. Several established techniques are typically used for the characterization of novel materials in healthcare including light microscopy, electron microscopy, and X-ray based imaging. Neutrons provide strong contrast in this area of study by allowing the imaging of thin adhesive films present in many dental restorations. Further, the interface mechanic of implants and human tissue can be measured; here, BEI provides information on the stress and strain states of the implant material and nGI provides spatially discriminated porosity and defect maps of the human tissue (bone and enamel).

9.4.9. Radiation Damage

The global semiconductor market has been identified as a key industry. Its size exceeded $500 billion in 2021 and is projected to grow at a CAGR of 12.2% annually and reach $1.3 trillion by 2029 [55]. While the radiation-hardened electronic portion of this market amounts to only a few billion dollars [56], market segments with high reliability requirements, including a high degree of robustness with respect to radiation, amount to many tens of billions of dollars and are projected to continue to grow at high CAGRs for the foreseeable future (high-performance computing HPC and automotive markets, for instance). Further, some industries (the military in particular) not only require that electronic devices be designed, manufactured, and assembled domestically, but also that their response to radiation be tested and characterized in the USA.

9.4.9.1. The effect of radiation on semiconductor devices

Radiation effects are defined by the specific device properties and the radiation environment in which the devices are used. Radiation can result in information loss, degradation of device performance and power parameters, and destruction of the device. The spectrum of susceptible devices covers all known semiconductor technologies including quantum bits (qubits), where it is noted that "…reducing or mitigating the impact of ionizing radiation will be critical for realizing fault-tolerant superconducting quantum computers…" [57].

Radiation effects can be divided into single-event effects (SEE), total-dose effects (total ionizing dose (TID) and displacement damage dose (DDD)), and prompt-dose (high dose rate) effects [58]. In the case of SEE, a single particle strike can cause measurable effects in devices, whereas for total-dose mechanisms an accumulation of radiation-induced damage yields measurable effects. Prompt dose refers to damage sustained in environments with very high radiation dose rates [58].

In terms of radiation environments, one differentiates between terrestrial (including flight altitudes), space, and artificial (i.e., anthropogenic sources). For neutrons, the terrestrial and human-made sources are of primary interest. In terrestrial environments, neutrons originate primarily from cosmic rays that interact with earth's atmosphere and undergo nuclear reactions, generating neutrons that penetrate the atmosphere and reach microelectronic systems located at various locations and altitudes (including aircraft) on earth. The flux of neutrons depends on location, where altitude is the by far biggest modulator. The main radiation effects relevant to semiconductors in terrestrial, natural radiation environments are SEE, including single-event transients and upsets, single-event latch-up, as well as single-event burnout and gate rupture in power transistors [59]. In natural radiation environments on earth, neutron energies covering thermal (25 meV) up to several 1000 MeV contribute to SEE [59, 60, 61]. Anthropogenic neutron environments include areas close to nuclear power plants and nuclear detonations. The primary concerns with human-made environments are SEE, TID, DDD, and flux-dependent effects [58]. In these artificial radiation environments, neutron energies from thermal to ~14MeV are dominating the interaction with semiconductor devices [58].

9.4.9.2. The neutron test facility challenge

Currently, there is a distinct lack of neutron sources capable of performing accelerated semiconductor radiation testing for both natural and anthropogenic environments in the USA.

The LANSCE neutron energy spectrum is close to the natural one above a few MeV, and nuclear reactors can cover the thermal part of the natural and anthropogenic energy distributions. Reliable access to LANSCE for neutron radiation testing has been challenging for the commercial semiconductor industry in the USA. Given that the radiation response of modern semiconductor devices in natural radiation environments is dominated by neutron energies above 1 MeV [60, 61], there is still significant value in creating additional capacities of high-flux, low-energy neutron sources for radiation testing. The number of high-power, high-flux nuclear reactors that can be used for accelerated radiation testing purposes is currently not adequate to serve the entire semiconductor industry. Even worse, the need for such facilities is expected to continue to rise as novel markets with high reliability and safety requirements continue to grow at an accelerating pace. Both the defense industry and the manufacturers and vendors of commercial semiconductor devices that serve markets with high reliability and safety standards would benefit from a high-power nuclear reactor.

9.4.10. Crystal Growth

Single crystals are core components of electronic, optical, microwave, and numerous other devices in domains as diverse as medical imaging, security screening, high-energy physics, and space exploration. Key to any viable development of these applications are the yield, reproducibility, and final cost of the material production. The optimization of the latter for the industrial scale has always been challenging [62]. A new crystal material and its growth technique almost always require specific time-consuming optimization as limited knowledge can be inferred from previous developments [63]. *In situ* diagnostics can substantially decrease the process development time and provide guidance for real-time feedback control and optimization of crystal growth. However, most of the time process development is done through many time-consuming trial and error approaches due to the opacity of materials and surrounding furnaces.

Neutron imaging and scattering present unique tools for the *in-situ* characterization of the crystal growth process [64-68]. Neutrons can penetrate the thermal insulation and most materials and thus probe the growth volume through neutron absorption and scattering. These enable direct *in-situ* measurement of the exact location and shape of the interface between the liquid and solid phases, distribution of the elemental composition, the temperature and defect distribution within the material, and other parameters within the growth volume. Thus, *in-situ* neutron imaging provides a new tool with which to guide the development of crystal growth processes for new materials while substantially reducing the cost and time needed to manufacture new materials on an industrial scale.

9.4.11. Cultural Heritage & Archeology

Studies of precious archaeological and cultural heritage objects must be non-destructive, and this substantially limits the techniques that can be employed. In many cases where metals are involved (e.g., bronze statues, metal swords, and coins), conventional techniques such as x-ray or light scattering are unable to penetrate deeply into the sample and thus provide information that is limited to the sample surface [69-71]. Because neutrons have zero electric charge, neutron imaging and scattering methods can probe the bulk properties of samples without damaging the artifact and can quantify the elemental composition and microstructure within large samples with sub-mm spatial resolution. Such information enables a better understanding of the sample manufacturing process, identification of possible past-time alteration/restoration procedures, identification of geographical location and period of sample origin, and even the detection of forgeries. Neutrons can penetrate deep within the bulk of the sample (e.g., up to ~50 mm into steel in comparison with ~0.1mm for laboratory X-ray radiation). As a result, compared to other probes used in non-destructive testing (such as X-rays, electrons, and ions), neutrons provide unmatched non-destructive opportunities for the study of cultural heritage objects.

9.5. Proposed Instruments & Facility Needs

9.5.1. Measurement of Residual and Applied Stress

The primary applications of the existing Diffractometer for Stress and Texture at the NIST Center for Neutron Research are measurements of residual stress on structural engineering components such as welded structures, rails, additively manufactured parts, and other components where structural strength is front and center. Other applications are the measurement of phase fractions, preferred orientation, and multiaxial stresses under applied straining. The current engineering diffractometer is limited by the reactor flux, its truncated beam tube, and by the extremely limited space of the measurement area, which effectively prevents the measurement of large parts that can only be measured by neutron diffraction. Presently, samples are limited to approximately one meter in size. Current operation is based on a small, focusing, multi-wavelength monochromator and an area detector. Monochromator performance is limited by the size of the existing beam tube.

9.5.1.1. Constant Wavelength Instrument

This proposed instrument is based on well-established technologies such as a large, double focusing, multi-wavelength monochromator and a large area detector that can acquire multiple peaks simultaneously. The performance of such a future stress diffractometer would benefit from a new neutron source in the following ways:

- The flux on sample scales proportionally with the increased neutron flux from new source (seeking >10x)
- Additional intensity gains from optimized neutron optical components such as
    - An evacuated (or helium-filled) tube that reduces the absorption of neutrons along the flight path from the reactor to the sample, providing a 5% to15% gain
    - Improved monochromator resolution and beam focusing via optimization, and the largest possible focusing monochromator (given the distances from the reactor to monochromator to sample (seeking >2x). Ideally, we would want to increase the monochromator-to-sample distance to 2.5 meters.
    - A vertically enlarged area detector above and **below** the scattering plane to increase the neutron-scattering count rate. Increasing the height of the neutron beam above the floor would allow for increased detector coverage.

- Much larger workspace is needed for measuring large industrial samples such as pipeline sections (>1 meter), turbine wheels (>1 meter, >500 kg), and aircraft parts.
- Increasing the beam height above the floor is required to measure large parts, including high-capacity multiaxial straining devices.

9.5.1.2. White Beam Instrument

A new reactor could allow for a second instrument station in which a “white” beam diffracts from the sample in all directions with a gauge volume defined by secondary apertures and analyzer crystals with attached simple detectors. This instrument could potentially be located at the same beam tube as the constant wavelength instrument, with the beam attenuated only from passing through the monochromator and the loss of the extracted wavelength band. Analyzer crystals at fixed diffraction angles define the lattice spacings measured. Such a setup would essentially allow an operation like that at spallation neutron sources in that each analyzer measures its own peak. Multiple diffraction peaks would be collected simultaneously, and in orthogonal directions, thus improving data acquisition rates and stress accuracy. The performance of such an instrument is proportional to the number of analyzer crystals along directions in which diffracted intensity is collected. Radiological conditions in this type of measurement are more severe and would require substantially more shielding. A white beam instrument will not necessarily offer faster measurements, but it may give complementary information compared to the fixed wavelength instrument above. This type of instrument would be particularly useful for measurements of applied stress in straining devices (both uniaxial and multiaxial stress) and texture. The continuing need to measure multiaxial stress-strain properties of materials, particularly sheet metals used in the automotive sector, stems from continuing alloy development and short innovation cycles, both of which pose a continuing challenge to model-based needs for materials data.

9.5.2. Neutron Imaging

9.5.2.1. General Instrumentation

Instrumentation needs for neutron imaging would require 4 instrument positions:

1. **Thermal neutron imaging instrument** - optimized for simultaneous neutron and X-ray tomography of thicker samples [72-79].
    a. Applications: Automotive-scale hydrogen fuel cells, commercial-sized Li and Na batteries, degradation processes in concrete, geochemistry, water retention in soils, cultural heritage, additive manufacturing.
2. **Neutron microscope instrument** - using cold neutrons this instrument should be optimized for a neutron microscope based on Wolter optics [80-82].
    a. Water dynamics in hydrogen fuel cells, charge cycling in batteries, rapid crystal growth, bone interactions with medical implants.
3. **Cold neutron imaging instrument** - optimized for wavelength-selective imaging for Bragg-edge and grating-interferometer experiments [83-86].
    a. Applications: Additive manufacturing, hydrogen embrittlement, hierarchical structures, geochemistry, degradation processes in concrete, battery electrode degradation, hydrogen fuel cell catalyst layers.

4. **Fast/Thermal neutron imaging instrument** - optimized for large beam size, ~1 m, for large industrial samples.
   a. Aerospace components, engines, very large active area fuel cells for heavy duty trucks.

9.5.2.2. Facility Location

There are many systems and devices with transient dynamics on the time scale of 1 µs to 1 ms, which can be operated cyclically in synchronization with a detector, and which benefit from the unique penetration and contrast of cold neutrons (fuel injectors, phase change devices, batteries, fuel cells, etc.). Stroboscopic measurements at continuous sources can achieve high temporal resolution. Such measurements require maximum flux to reduce measurement time and improve scientific performance. Consequently, high-flux facilities can be difficult to shield and may require special consideration in terms of location relative to other instruments in the experimental halls. Larger shielded bunkers would allow for maximum flux for imaging while minimizing the background experienced by other experiments.

9.5.3. General Facility Requirements

- High Fluence Rate - Neutron imaging is moving to systems with ever faster dynamics and therefore requires the highest achievable brightness of the reactor, ideally increasing power to 100 MW. The greater intensity will support studies of the charge cycling of Li or Na batteries, drive-cycle testing of fuel cells, *operando* investigations of additive manufacturing, water and salt ingress in concrete corrosion studies, Bragg-edge imaging of welding stress in steels, and far-field interferometry measurements of porosity in metal additive manufactured parts.

- X-ray Facilities - An X-ray imaging laboratory in a workspace that allows activated materials is desired for pre- and post-characterization of neutron imaging samples. Pre-characterization of samples would allow optimization of scans on the neutron instrument for best use of limited time during user experiments or provide enhanced information at higher spatial resolution, e.g., porous structures of transport layers in fuel cells and electrolyzers. Post-characterization could provide nano-XCT on regions of interest identified in simultaneous neutron and X-ray tomography scans, e.g., interfacial transition zone in concrete.

- Beam Line Location - Locating a thermal imaging beamline is a uniquely important decision because the primary method of image formation is based on pinhole optics. This means that the moving parts in the reactor core show up as variations in image intensity at the sample/detector position. This gives rise to shifts of the image in ways that can be difficult or impossible to correct later. This effect at the NCNR NBSR-1 reactor was discussed here in detail (https://doi.org/10.1016/j.nima.2011.01.014). It is possible that this effect will be muted or irrelevant with the new reactor design because the neutron peak brightness occurs in the moderator as opposed to the centerline of the core as it does now. Modeling this effect in the new reactor will be useful in choosing a beamline location. For example: modeling to determine if the effect is mitigated by looking edge-on to the shim arms versus directly at a shim arm. In addition, it is important to provide the instrument control software with an accurate timeline of reactor operation parameters to record as part of the metadata of an experiment. If this is provided as real-time feedback it would allow the data acquisition system to make decisions about vetoing and restarting data acquisition.

- Beam Height - The distance of an imaging beamline from the floor should be much higher than the current value of 105 cm (41.5 inches) for the NIST BT-2 imaging beamline. Preferably equal to or greater than 152 cm in height. This would allow larger engineering-sized samples (like refrigeration systems) to be scanned through beams. For simultaneous neutron and X-ray tomography experiments, it is not possible to translate the sample horizontally across the beam, and this necessitates the vertical orientation.

- Electrical Requirements - Neutron imaging experiments often require large support equipment that have high utility demands, i.e., electricity, chilled water, compressed air, etc. Industrially relevant fuel cell test stands will require air flow at a minimum of 350 lpm (12.3 CFM) @ 690 kPA (100 psi). Instrument chilled water will need to be able to dissipate a minimum of 50 kW. Electrical service is needed at 120 V, 208 V, 240 V, 480 V, with up to 60 A per circuit and room for expansion of electrical service. Domestic water service to supply hydrogen generation and deionized water supply are both required.

- Shielding Requirements - Imaging beams are designed to be high intensity and large in diameter, which results in a lot of neutrons striking samples. Prompt gammas from neutron absorption as well as scattering of fast neutrons and reactor gammas results in high levels of background radiation. For this reason, the location of such a beamline should be chosen to minimize the impact on other instruments. Although in-beam gamma and neutron fluxes are high, they can be lowered using bismuth filter material at a cost of 25 % thermal flux per 5 cm of liquid nitrogen cooled bismuth. For maximum intensity, a neutron-imaging facility should be able to run without any filter material. This requires a marked increase in facility shielding to stop the extra fast neutrons and gammas.

- Computing Requirements - High-speed networking for data transport to onsite high-performance computational resources for real-time data analysis or off-site transfer to users will be necessary. Off-site access for remote experiments and data analysis would increase efficiency. Archival equipment for raw, meta, and analyzed data is also needed.

- Hazardous Gas Requirements - Safe infrastructure to deliver both the supply and exhaust of hazardous/flammable gases should be considered during the reactor facility design phase. This is especially important for the thermal imaging instrument located in the reactor hall. Proper gas evacuation would allow higher hydrogen flow rates for larger, higher performance industrially relevant fuel cells. Other experiments that could produce hazardous gases include CO_2 electrolysis (CO produced), pyrolysis and thermal decomposition, thermal runaway and decomposition of lithium-ion batteries.

9.6. References

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10. Source Characteristics

10.1. Panel

Co-Chairs:
Megan Robertson – University of Houston
Chris Stock – University of Edinburgh

Panelists:
Mark Dadmun – University of Tennessee
Bruce Gaulin – McMaster University
Young-June Kim – University of Toronto
Robert McQueeney – Iowa State University and Ames Laboratory
Bradley Olsen – Massachusetts Institute of Technology
Ian Swainson – International Atomic Energy Agency
John Tranquada – Brookhaven National Laboratory
Klaus Habicht – Helmholtz-Zentrum Berlin

Scribe:
Osman Celiktan – National Institute of Standards and Technology

10.2. Glossary of Terms

Cold neutrons: neutrons with wavelengths between about 0.4 and 4 nanometers.

Thermal neutrons: neutrons with wavelengths between about 0.1 and 0.4 nanometers.

Hot neutrons: neutrons with wavelengths between about 0.04 and 0.1 nanometers

Cold-neutron source: typically a volume of liquid hydrogen (H_2) or deuterium (D_2) that is used to reduce the energies of neutrons from the reactor core to less than about 10 meV.

Isotopes: atoms of an element having the same number of protons but different numbers of neutrons.

HEU: highly enriched uranium 235.

LEU: low-enriched uranium 235.

Light water: Normal water (H_2O) as opposed to heavy water (D_2O).

Spin: a quantum mechanical property of the neutron that allows it to probe magnetism.

ILL: Institut Laue Langevin, a reactor-based neutron research facility located in Grenoble, France.

meV: one thousandth of an electron volt; a unit of energy commonly used by neutron researchers.

MLZ: Maier Leibnitz Zentrum, a reactor-based neutron research facility located in Berlin, Germany.

ORNL: Oak Ridge National Laboratory

SNS: Spallation Neutron Source, a user research facility located at ORNL.

STS: a project to build a second target station at the SNS.

TRIUMF: Canada's national particle accelerator center located in Vancouver, BC.

10.3. Summary

The Source Characteristics Panel strongly supports the NCNR Neutron Source (NNS) pre-conceptual design of the replacement reactor proposed by NIST, which will provide an essential tool for neutron-based materials research in the United States. Indeed, the need for a new U.S. reactor research facility has been highlighted repeatedly in recent years in many reports, including several from the American Physical Society and the National Academy of Sciences. Our report outlines several recommendations regarding the performance, capacity, reliability, and flexibility of the reactor-based neutron source to best meet future U.S. research needs. We recommend that NIST investigate maximum reactor power while balancing considerations related to safety, licensing, and available technology. We strongly recommend the incorporation of a thermal-neutron guide hall to maximize research capacity, and we applaud the preconceptual design in the context of reliability and flexibility.

10.4. National Priorities to be Addressed by Neutron Research

Measurements of materials properties using neutron techniques can provide answers to key scientific questions that have enormous potential to benefit our nation and society [1]. The recently released memorandum "Multi-Agency Research and Development Priorities for the FY 2025 Budget" identifies targeted priorities that include addressing the global climate crisis, achieving better U.S. health outcomes, supporting workforce development, and bolstering industrial innovation, all of which require scientific insights that can be gained through access to enhanced neutron research facilities. The science panels of the "Neutrons for the Future" workshop have each identified future societal impacts of neutron research that are also reflected in the 2018 report entitled "Neutrons for the Nation" published by the American Physical Society [2]. Societal impacts include (i) the development of a more sustainable society (e.g. improved access to food and clean water, mitigation of environmental impacts of plastics, environmental remediation of contaminants in water and air, and climate change and adaption); (ii) advances in medicine (e.g., precision medicine, artificial organs, medical implants, rapid response to emerging pathogens); (iii) advances in energy-efficient technologies (e.g., lightweighting, thermal transport, energy storage, hydrogen economy, efficient catalysts, chemical separations, alternative energy sources, waste remediation, critical materials, industrial decarbonization); (iv) advances in next-generation electronics (e.g., sensors, chips, data storage, human-machine interfaces, bioelectronics, lithography, electronic waste, quantum computing); (v) advances in infrastructure (e.g. cement materials, infrastructure resilience, enhancing U.S. manufacturing); and (vi) other areas (e.g., innovations in space technology, insights in archeology, enhancing forensic science).

10.4.1. Unique Role of the Neutron and the NIST Center for Neutron Research (NCNR)

Neutron techniques offer important advantages over other characterization methods and have enabled numerous materials science discoveries in areas critical to our societal improvement [3]. Several unique properties of the neutron make possible investigations of the structure and dynamics of materials that simply cannot be achieved with other characterization techniques [2]. The fact that neutrons interact differently with isotopes of the same element, particularly in the case of hydrogen and deuterium, allows the study of unique aspects of material structure that cannot be done using other techniques such as x-ray scattering. Because neutrons have no electric charge, they can penetrate deeply into solid materials non-destructively, which enables measurements to be conducted under a wide variety of experimental conditions. The neutron spin can be exploited in polarized neutron scattering techniques to study the structures and dynamics of magnetic materials. A reactor neutron source, such as that at the NCNR, generates an intense, steady flux of neutrons that complements the capabilities of a spallation neutron source, which instead produces a regular stream of neutron pulses. Several new and improved measurement capabilities at the NCNR have become available due to the development of modern, state-of-the-art neutron instrumentation. These include time-resolved and spin-polarized reflectometry on the Chromatic Analysis Neutron Diffractometer or Reflectometer (CANDoR); small-angle neutron scattering on length scales spanning 1 to 2,000 nanometers on the Very Small Angle Neutron Scattering instrument,(vSANS); neutron spectroscopy on times scales approaching 700 nanoseconds on a new Neutron Spin Echo (NSE) spectrometer that is currently under development; advances in Neutron Interference Microscopy/Far Field Neutron Imaging; and time-resolved neutron elastic and inelastic scattering with atomic resolution on millisecond time scales on the Multi-Axis Crystal Spectrometer (MACS) [4]. While there has been a strong development in spallation neutron sources, it has been noted that to reach and support the required capacity of neutron instrumentation, research reactors are needed [2]. Indeed, for the United States to remain competitive in the world-class neutron R&D enterprise, complementary investments in research reactors are essential.

10.4.2. Positive Aspects of the NIST Pre-Conceptual Design in Addressing U.S. Science Priorities

The Source Characteristics Panel notes the following positive aspects of the pre-conceptual design:

- Use of the NIST Gaithersburg site. This allows for ease of transition from the current reactor to the replacement reactor and the possibility of using existing onsite capabilities such as the present cold-neutron guide hall if a greenfield concept is not preferred. Importantly, using the Gaithersburg site retains existing expertise, easing the transition from one source to the next.

- Use of LEU fuel [5][1] to obtain high power performance (Table 1). Using LEU instead of HEU is listed as a key recommendation by the APS [2] to reduce the risk of nuclear proliferation and to achieve the ultimate goal of eliminating HEU in civilian research reactors [6]. This has been a stated policy in the United States since 1978.

- Use of light-water cooling to moderate neutron energies over shorter distances. This leads to a compact core design that is advantageous in terms of obtaining higher power density.

- Use of a heavy-water reflector. This design element opens up substantial space for multiple cold sources and thermal beam tubes.
- Ease of maintenance. Allowing visual access inside the pool vessel and the nine-fuel element design simplifies maintenance of the reactor core. Providing vertical-service access to the cold sources enables ease of maintenance and reliability.
- Allowance for two (or more) liquid deuterium cold sources. This enhances the cold neutron capacity available for high-demand instruments. It also lets each cold source be optimized independently to better target different instruments with differing capabilities.
- Designed for safety, manufacturability, reliability, straightforward maintenance, and consistency with current licensing constraints at the NIST Gaithersburg site.
- Lack of in-core facilities. This simplifies reactor design and functionality.
- Lack of hot source or thermal column. This avoids duplicating the capabilities at other U.S. neutron facilities and recent developments at synchrotron x-ray sources considering the complementarity of different neutron sources and instrumentation at other U.S. facilities [2].

10.5. Panel Recommendations

10.5.1. Recommendation 1: Enhance NNS reactor performance

The NNS pre-conceptual design proposes to replace the current NBSR with a compact 20 MW reactor. The design of this reactor yields a neutron flux 3.5 times higher than that of the NBSR even while converting to LEU fuel. This is impressive, as it appears to be brighter than any current LEU reactor in operation today (Table 1).

Table 1: Major LEU-fueled research reactors with neutron scattering facilities [8, 9]

Reactor	Country	Max Thermal flux (10^{14} cm^{-2}s^{-1})	Power (MW)	Ref.
National Bureau of Standards Reactor (NBSR) at the NCNR	United States	2	20	[8]
NCNR Neutron Source (NNS) Pre-Conceptual Design	United States	5	20	[8]
OPAL	Australia	2	20	[9]
RA-10	Argentina	3	30	[9]
CARR	China	8	60	[9]

The ability to meet growing U.S. science and technology needs increases with increasing reactor capacity. This is achieved by increasing the number of experimental stations served by the reactor and by increasing the neutron brightness/flux at each station. The quality of the source can also affect capacity by minimizing background noise and enabling new experiments with access to wider ranges in length scale, energy, and time. More neutrons on the sample will make possible experiments that require finer spatial resolution, smaller samples, or smaller time slices in time-resolved measurements. Along the same lines, increased neutron intensity will expedite experiments and increase throughput, thereby allowing more users to conduct neutron experiments in any given time period.

The panel recommends that NIST maximize the power of the new reactor for scientific output subject to considerations of safety, licensing, and available technology. Additional gains in neutron flux on sample can be obtained by optimizing the designs of the cold sources and neutron instrumentation, e.g., by including state-of-the-art optics, while enhanced detector efficiencies will boost data rates. Reactor reliability is paramount, and this has been echoed across multiple panels at this workshop. The panel further recommends designing the needed beam ports, cold sources, and other facilities to enable the largest possible suite of instruments. This includes exploring facilities beyond a single story where applicable and scientifically desirable.

10.5.2. Recommendation 2: Increase capacity

A primary motivation for building the NNS is to increase national neutron scattering capacity [10] given the current oversubscription rates of the NCNR and other U.S. neutron facilities in the U.S. In the recent APS report it was noted that reactor sources can serve a larger number of neutron instruments than complementary spallation sources [2]. A reactor source could thus address the huge disparities in instrument availability in the United States, which lags Europe by a factor of 3 and Asia by a factor of 2 [11]. Capacity is determined by several factors: the number of instruments, the source power, and the number of operating days per year. We briefly discuss each of these.

The preconceptual plan includes two cold sources, each with an associated guide hall containing about 20 instruments, making a total of ~ 40 cold neutron instruments. This is an excellent plan that responds to the demand from a major portion of the U.S. user community. In contrast, the plan offers only 8 thermal neutron instruments, located within the reactor confinement building, and this falls well short of the needs of the user community. Therefore, we strongly recommend that NIST consider using 4 of these thermal slots to install appropriately designed beam tubes to transport neutrons to a thermal guide hall, which could provide space for roughly 15 thermal instruments. The extra space would also permit the development of new instrumentation and would facilitate the implementation of extreme sample environments, such as large magnetic fields. In fact, the thermal guide halls at the ILL (Grenoble) and MLZ (Munich) reactors have both been used to develop a variety of instruments for diffraction and spectroscopy. Following the example of the construction and commissioning of the MLZ reactor, the panel also recommends including port access in the confinement building at the initial construction stage, as this would allow future expansion projects, like a thermal guide hall, to be performed without affecting reactor licensing requirements or early-stage commissioning. We note that the NCNR successfully initiated and led a similar type of expansion that significantly increased the capacity of its cold-neutron suite of instruments around 2010-2012.

The capacity of each instrument depends on the brightness of the neutron beam it receives. The initial design concept of the NNS reactor optimizes the core and moderator configuration to boost the cold-neutron flux by a factor of 3.5 relative to that of the existing NBSR facility at the same reactor power. This is very promising. It would be good to evaluate the issues associated with an increased reactor power or, alternatively, to consider how to design a core that would allow for a future power upgrade. There are certainly regulatory and licensing constraints that must be considered; there are also issues of construction and operating costs associated with higher power. Providing a discussion of these issues would be helpful in justifying the eventual conceptual plan.

The initial reactor core design would enable a 40-day operating cycle, which is comparable to that of the NBSR. Another consideration is the number of cycles per year. For example, 6 cycles per year would provide 240 operating days per year. This is contingent on refueling costs and maintenance requirements. Maximizing the number of cycles per year is an obvious preference for users.

10.5.3. Recommendation 3: Design for reliability

A key recommendation of the panel is that reliability be viewed as one of the most important metrics for source design. Meeting scientific needs and the need for capacity and performance cannot be fully realized without reliable operation. For many kinetic experiments, continuous operation over the entire time of the experiment is critical to success, and time-dependent samples that are central to a great deal of the science case cannot be recovered if they are lost due to a reactor outage. The panel has observed, and commends, a clear, strong focus on reliability in the NNS pre-conceptual design, and it offers four detailed suggestions that could further improve reliability.

First, we recommend that the reactor system be designed such that the failure of any one non-critical component does not require shutting down the entire system and/or terminating user operations. The panel observes that cold sources can be designed to operate independently such that if one or both must shut down the reactor does not need to be taken out of service. This requirement would allow the system to operate at half capacity for cold neutron instruments in the event of a cold source failure or with thermal neutrons only. We note that such an independent/decoupled design was advantageous to the recent commissioning of cold sources in research reactors such as OPAL (Sydney) [12].

Second, we recommend the source design explicitly consider ease of repairs and upgrades. It should be possible to perform as many routine and emergency repairs, part replacements, and upgrades as possible without significant disassembly of either the reactor or end stations, thereby minimizing down times. In this respect, the panel strongly endorses the NNS pre-conceptual design for providing vertical access to the cold sources and other reactor components for ease of access and repair. We encourage this strategy be maintained as the NNS design evolves and complexity increases.

Third, the design of the reactor should consider the manufacturability and availability of replacement parts and fuel in detail. It is important that all required parts and fuel elements be easily manufactured and available from multiple suppliers because it is not possible to predict the business conditions for specific suppliers throughout the lifetime of the reactor. It is particularly important to avoid the fuel-supply problems that plagued TRIGA reactors for over 10 years due to a lack of qualified manufacturers, and there must be a high degree of confidence in any proposed “HEU-replacement” fuel on which the replacement reactor is designed. Lead times and potential supply-chain problems should be considered to ensure that parts are rapidly available in case of an unforeseen event.

Fourth, the panel encourages all use cases be tested to assess their effect on reactor reliability as they are considered for inclusion in the final design plan. Use cases that adversely affect reliability should be held to a significantly higher standard for service to the national need. The corollary to this principle is that the system should operate with a larger margin of error than is typical to minimize unanticipated shutdowns.

10.5.4. Recommendation 4: Design for flexibility and future needs

10.5.4.1. Cold-Neutron Source Design

The NNS pre-conceptual design has two identical liquid-deuterium cold-neutron sources (CNS). Liquid deuterium provides the best cold-neutron production of any CNS for high-power reactors. We recommend examining the option of having two different CNS with different spectral characteristics. For example, liquid hydrogen could be used for the second CNS, as it is better suited for “hybrid” experiments that require the ability to cross over from thermal to cold neutron energies. Instruments could then be placed on the CNS most suited to their applications. An alternative suggestion is that NIST consider the “bi-spectral” design implemented at the Berlin reactor for thermal and cold neutrons in the guide hall[13].

The energy spectrum from a liquid-hydrogen CNS changes over a period of days to weeks due to the slow conversion process that takes place from the ortho-spin to the para-spin hydrogen (H2) isomer and the profound difference in the neutron scattering cross sections of the two isomers below about 25 meV. For this reason, we recommend that NIST investigate a catalyst and monitoring system (e.g., Raman spectroscopy) to speed up the conversion process for any liquid-hydrogen CNS. This would increase the performance of the CNS in the early days after a reactor startup and increase its spectral stability. We further recommend that NIST investigate whether a pure para-hydrogen CNS offers any potential advantages in terms of the shape and dimensions of the CNS (cf. the low-dimensional para-hydrogen CNS designs at the ESS and the SNS STS).

Ultimately, the final CNS designs will be determined by the suite of instruments envisioned for the facility. While the current design of two liquid-deuterium CNS may offer maximum flux for instruments under high demand, installing two different cold sources may offer flexibility in terms of future instrument needs that may currently not be anticipated. These factors must be weighed in assessing all these possibilities.

10.5.4.2. Dedicated Port Off the Cold Source – Next Generation Cold and Multiplexed Spectrometer

With increased cold-neutron flux from optimized sources comes the opportunity to create high-intensity cold-neutron instruments that take full advantage of the large angular divergence of cold-neutron beams. Such instruments would need to be located inside the reactor confinement building as close as possible to the biological shield. We note that all large-scale reactor-based facilities such as MLZ (Munich) and the ILL (Grenoble) have incorporated such capacity into upgrades and designs. Examples include Thales (ILL) [14], Panda (MLZ) [15], and notably MACS

(NIST) [16]. These instruments have been transformative in terms of the science they have produced. They have also increased the user base in areas such as energy, environment, and biological sciences, as highlighted in reports by the National Academy of Sciences [4], and have expanded the use of extreme sample environments. This current suite of high-flux cold-neutron instruments also complements existing instrumentation at DOE labs like the SNS and that will be built as part of the STS project at ORNL.

Given the importance of these instruments, we strongly recommend that plans be made to include them in the confinement building during the initial phase of the NNS. We also recommend that they be optimized for geometry and focusing optics where possible by building on the NCNR's experience with the MACS cold neutron spectrometer. Increasing the reactor neutron flux and optimizing the CNS geometry will ensure that next-generation cold-neutron spectroscopy instruments will be available for the general user community and will help to open the field of neutron-based science to new users.

10.5.4.3. Hot-Neutron Source

The NNS pre-conceptual design complements the facilities at ORNL and focuses on thermal and cold neutrons. The Source Characteristics Panel discussed the need for a hot-neutron source within the NNS pre-conceptual design. Short-wavelength (i.e. high-energy) or “hot” neutron sources are used at the MLZ and ILL reactors to provide hot neutrons to two diffractometers (one polarized and the other not) dedicated to single crystal crystallography. The short-wavelength neutrons provided by these sources permit the study of highly absorbing materials, and they simplify the corrections for extinction effects when solving the structure of complex materials. There are no hot sources in the United States, but access to high-energy neutrons for crystallographic studies (TOPAS) and pair distribution analysis (NOMAD) are available at the ORNL SNS facility. Further, crystallography instrumentation is also provided at x-ray synchrotron facilities, and it is not clear from the discussions at this workshop whether hot neutron sources provide capabilities that are competitive with those at existing x-ray facilities and those under development. Perhaps reflecting this was the notable lack of a hot source in a Canadian proposal put forward for a replacement reactor for the NRU facility at Chalk River [17]. The panel also felt that, given the instruments currently available at other large facilities, the scientific case for hot neutrons is not as clear or straightforward as those for cold and thermal spectrometers.

We recommend that NIST study the need for, and the feasibility of including, a hot-neutron source in the NNS given its cost and the availability of high-energy neutrons at spallation sources. We further suggest that NIST investigate the use of the “epithermal neutron tail” from the reactor itself in place of a hot source as well as the possibility of taking advantage of “hot” spots in the reactor core that naturally provide a source of high-energy neutrons without compromising the current compact core design. If a hot source is deemed necessary, it could be included as a separate source located vertically near the reactor core. The panel asks NIST to evaluate this possibility and to research these other possibilities in the context of facilities currently available that use spallation neutrons at ORNL and x-rays at synchrotron sources.

10.5.4.4. Thermal Column

A thermal column provides the ability to perform irradiations on large and irregularly shaped samples, which is useful for metrology and engineering applications. However, a thermal column takes up a large volume in the reactor core at the expense of one or two thermal beam ports and could affect the core design substantially. Because of the impact it will have on the capacity and design of the neutron source, and in particular on the limited number of thermal ports available, the benefit of installing a thermal column should be studied carefully and weighed against the consequences on the goals of the NNS pre-conceptual design. The panel notes the possibility of using existing smaller research reactors for this purpose.

10.5.4.5. Fundamental Physics: Ultra-Cold Neutron Source (UCN) and Neutrino Facility

Ultra-cold neutrons are important to studies of the fundamental physics of neutrons, such as the electric dipole moment. The presence of a non-zero neutron electric dipole moment would imply violation of time-reversal invariance and would have strong implications for the Standard Model of physics and other supersymmetry theories of particle physics. A UCN source would specifically target this problem and could provide new, high-precision, experimental bounds. One of the brightest UCN sources can be created by installing a vertical beam tube in the core, in which neutrons will be slowed down by gravity. However, this would likely strongly affect the core design and the performance of all neutron beamlines. Further study is required to weigh the benefit of an in-core UCN implementation compared to using a cold-neutron guide-hall UCN source. Compromises to the NNS goals stated above must be heavily weighed, in particular the goal of a compact core design. Consequences in terms of licensing and reliability should also be considered. The panel recommends that NIST study the feasibility of such a UCN, balancing benefits, impacts, cost, and risk. The need for a UCN must also be assessed in the context of existing UCN facilities, notably the ongoing developments at TRIUMF's Ultra-Cold Advanced Neutron (TUCAN) source [18] and the UCN source at Los Alamos National Lab discussed in the corresponding Neutron Physics and Neutrino Physics Panel report [19].

One possible use of the research reactor is as a neutrino source. Neutrino detectors could be placed underneath the reactor to study how neutrinos change over varying distances. Creating underground laboratory facilities will require further investigation at the planning stage. We recommend that NIST investigate the feasibility of incorporating underground laboratories to observe neutrino oscillations and their impact on cost. Preliminary discussions appear to point to such a facility having minimal impact on neutron beam lines while also providing the basis for a unique particle-physics facility.

10.5.4.6. Rabbit Facilities and In-Core Irradiation Facilities

The panel discussed the rabbit facilities available at the current NIST reactor. These are used to irradiate small samples (a.k.a "rabbits") in intense neutron fields. The NNS pre-conceptual design lacks such a facility. Similar facilities were also removed from the recently closed Berlin research reactor. We recommend that NIST consider the benefits of including these facilities at the NNS while balancing its desire for a compact core and taking into account licensing issues and existing facilities at research reactors across the US (e.g. the MIT reactor). The effects on the neutron instrumentation and the flux from the compact core design should also be considered carefully. The panel applauds the primary goal of the NNS pre-conceptual design for cold and thermal neutron beams and notes that the design calls for irradiation facilities with negligible detriment to this stated goal. The panel notes that NIST produces standard reference materials (SRMs), de facto international standards on which many neutron-activation-analysis facilities around the world rely. The panel recommends that NIST assess whether this development and service could continue using other US reactors if rabbit facilities were not included in the NNS.

Summary: In conclusion, the panel is very supportive of the NNS proposal because it increases performance and reliability through a compact core design, increases neutron scattering capacity via multiple guide halls, incorporates multiple cold neutron sources that can have different spectral characteristics, and enhances flexibility for neutron scattering instrumentation. The proposal is timely given that the NCNR reactor is over 50 years old and one of the oldest operating civilian research reactors in the world. The proposal is particularly urgent because the NCNR license will expire in 2029 and because of the impending closure of several European neutron sources. The need and urgency of this has been highlighted by an assessment from the National Academy of Sciences [4].

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11. Facilities

11.1. Panel

Chair:
Mark Lumsden – *Oak Ridge National Laboratory*

Panel Members:
Bianca Haberl – *Oak Ridge National Laboratory*
Garrett Granroth – *Oak Ridge National Laboratory*
Marek Jura – *Rutherford Appleton Laboratory*
Daniel Haskel – *Argonne National Laboratory*
Shuo Qian – *Oak Ridge National Laboratory*

Scribe:
Ryan Murphy – *National Institute of Standards and Technology*

11.2. Glossary of Terms

^{3}He cell pumping: A method of polarizing (aligning) helium nuclei.

AFM: Atomic force microscope. A microscopy probe able to resolve spatial features measuring fractions of a nanometer.

ALARA: ALARA is an acronym for “as low as (is) reasonably achievable,” which means making every reasonable effort to maintain exposures to ionizing radiation as far below the dose limits as practical, consistent with the purpose for which the licensed activity is undertaken.

Chopper: A device for converting a continuous neutron beam from a reactor into a series of neutron packets.

Closed-cycle refrigerator: A helium compressor and expansion valve device for producing low temperatures without the use of liquid helium.

CPU: Central processing unit of a computer.

Cryostat: An apparatus used to maintain a constant, low temperature, especially below 0°C, typically using liquid helium.

Density functional theory: A quantum mechanical modeling method used to investigate the electronic structure of materials.

Deuteration: The replacement of some or all the hydrogen atoms in a material with deuterium (heavy hydrogen).

Dewar: A container for cryogenic fluids.

Dilution refrigerator: A cryogenic device used to produce very low temperatures using the heat of mixing of helium-3 and helium-4 isotopes.

Edge computing: A computer environment that permits rapid feedback on the progress of an experiment.

Electrochemistry: A branch of chemistry concerned with chemical changes in response to an applied electric field.

EPICS: A de facto standard instrument control system used at neutron sources and synchrotron light sources.

Flippers: A device used to change the spin (magnetic moment) direction in a neutron beam.

GPU: Graphical processing unit of a computer.

Helium recovery system: An in-house mechanism for recovering and recycling the helium gas that has evaporated from the liquid helium used in low-temperature experiments.

Hot cells: Highly shielded enclosures used for remote handling of radioactive materials.

ILL: Institute Laue Langevin; a high-flux neutron scattering reactor research facility in France.

IR spectroscopy: A method that measures the interaction of infrared (long-wavelength) radiation with matter.

ISIS: The high intensity pulsed neutron source located in Great Britain.

Mass spectroscopy: A technique used to measure the ratio of mass to charge in ions.

Monte Carlo ray tracing: The tracing of a neutron beam through an instrument using repeated random sampling.

Neutron activation analysis: A method for determining concentrations of elements in a material.

Neutron guides (guides): Neutron waveguides used to transport neutrons from a reactor to instruments that are typically located in an adjacent experimental hall.

NMR: Nuclear magnetic resonance; a spectroscopic technique for studying materials using the response of atomic nuclei to a time-varying magnetic field.

Phonon density of states: The number of vibrational (analogous to sound waves) modes per unit frequency range.

Polarized neutrons: A neutron beam in which a unique direction for the neutron spin (magnetic moment) has been selected. Useful for detailed research on magnetic materials.

Rabbit stations: A pneumatic tube system for inserting and retrieving samples from a reactor after irradiation.

Raman spectroscopy: A technique used to determine the nature of vibrational modes in molecules and solids.

Resistivity: A measure of the resistance of a material to the flow of an electric current.

SAXS: Small-angle x-ray scattering. A technique used to probe structural features in materials on length scales larger than interatomic spacings.

Soft matter: A term describing “soft” materials including polymers, liquids, foams, gels, etc.

Specific heat: The amount of heat (energy) that must be supplied to a material to raise its temperature by one unit (typically one degree Kelvin).

Tomography: The imaging of a material by neutrons or x-rays.

UV-vis spectroscopy: Ultraviolet-visible absorption; a technique often used to determine different electrochemical properties.

Velocity selector: A mechanical device used to select a narrow wavelength (energy) band from a neutron beam from a reactor.

WAXS: Wide-angle x-ray scattering. An x-ray technique used to determine structural features on length scales comparable to interatomic spacings.

11.3. Summary

The Accompanying Facilities panel was given a broad scope to consider any activities related to the new neutron source (NNS) that were not captured by the Source Characteristics, Transition Process, and science-area panels. Panel members were joined by multiple staff from the NIST Center for Neutron Research (NCNR) together with representatives from different scientific communities, leading to diverse and passionate discussions. These focused on support space such as labs and shops, sample-environment and computing needs, automation, instrument-development needs, broader facility requirements, and appropriate staffing levels.

Following a discussion of required laboratories and shops, the panel cross-referenced our list with a draft report produced by NCNR staff. Overall, the panel feels that the NCNR list is comprehensive, although it requires prioritization. We identified some larger facilities that require special considerations. First and foremost is the need for deuteration capabilities. The panel feels that this need is essential and has a scientific scope that extends beyond neutron scattering. As such, plans for a National Deuteration Facility should be developed in consultation with representatives from NSF, DOE, and NIH. X-ray scattering is an important complementary characterization tool, and so we believe a sizable, state-of-the-art x-ray facility should be a component of the accompanying facilities. Similarly, an advanced microscopy laboratory should be prioritized with suitable space and specifications to house both electron and optical microscopes.

The ability to establish well-defined environmental conditions of temperature, pressure, magnetic field, etc., around a sample of interest is critical to delivering on the scientific potential of the new reactor. The importance of the sample-environment equipment used for this purpose requires appropriate staffing levels with focused teams devoted to magnets and cryostats, high pressure, high temperature, and soft matter. These areas require space for development, testing, and preparation with appropriate access to the neutron instruments. New sample environments will have implications for facility design. A helium-recovery system will be required, as will plans to mitigate the magnetic-field interference between neutron instruments. Anticipated increases in magnetic-field strength means that the NNS instruments and buildings must be designed to accommodate 30 Tesla fields. High-pressure work will require infrastructure such as gas lines, hydraulics, and lasers on the instruments and a dedicated facility to test pressure cells to failure.

Advances in artificial intelligence / machine learning can enable computer-aided steering or autonomous experiments. NIST should consider this in the NNS planning stages as well as how to provide the needed network and computing infrastructure, automated sample environments and changers, and a carefully designed data acquisition system. The panel identified this as an area where NIST can work collaboratively with the DOE neutron and light sources. We recommend that NIST develop plans for an EPICS-based data acquisition system to leverage the developments at DOE laboratories, including the new Integrated Research Infrastructure (IRI) initiative. Finally, the NNS facility should offer users the option to control experiments remotely.

Advanced methods in data analysis require computing that extends beyond the traditional model of users running code on their own computer. The NNS accompanying facilities will need to provide sufficient network and computing infrastructure to allow routine access to advanced data analysis methods. This will include cloud-based resources, edge computing for real-time analysis and feedback, and access to high-performance computing capabilities as needed. We anticipate the need for scientific workflow tools that will enable analysis across heterogeneous resources. All of this will require adequate staffing to manage the resources, but also staff with expertise in neutron scattering and advanced computing methods and modern software design. There are opportunities for engagement with the DOE supercomputer facilities and for collaborative software developments with the DOE neutron and light sources.

We anticipate that some of the proposed NNS instruments will offer polarized neutron capabilities. These will need appropriate staff and space to support their development and operations. Neutron optics was flagged as a concern for the NNS, as current vendors may not be able to supply the guides needed for the instrument suite, and there is no US-based vendor of high-reflectivity neutron guides. Additionally, we encourage NIST to think carefully about detector needs early in the project, as this may require in-house development. This is another area for potential collaboration with DOE via the ORNL detector development effort.

For a facility of this scale, we encourage NIST to provide appropriate spaces for users to monitor their experiments at the instruments and in locations with easy access to instrument scientists. Collaboration spaces are also an important part of the user experience, as are conference rooms to support virtual meetings with collaborators and spaces for workshops / training activities. We strongly encourage building an on-site guest house and considering methods to simplify user access to the facility.

As a final note, we discussed overall staffing levels. In addition to requiring more staff in the areas mentioned above (sample environments, computing, polarization, optics / detectors), we recommend considering the addition of instrument hall coordinators and a centralized sample management approach. These will be necessary to operate a facility of this size efficiently and safely. We expect that this will increase the staffing per instrument significantly, and we encourage NIST planning on having 9-10 full-time equivalents per instrument.

11.4. Accompanying Facility Suite for New Reactor

The discussion of accompanying facilities was informed by a comparison to other capabilities around the world. In advance of this workshop, the panel assembled capability lists from SNS/HFIR at ORNL, ISIS in the UK, ILL in France, and some relevant information from the Advanced Photon Source at ANL. Rather than list this information, it will be discussed in the following document sections as needed.

11.4.1. Laboratories, Shops, and Workspaces

11.4.1.1. Laboratory Requirements

An extensive number of dedicated laboratory spaces are required to facilitate science across the instrument suites. The panel developed a list of categories and then cross-referenced this list with a previously assembled list from NCNR staff. In general, we feel that the NCNR list is comprehensive. A few minor modifications or additions have been identified. It will also be necessary to prioritize this list at some point in the process.

Below is a high-level description of the laboratory categories that are required. Some types of laboratories will be necessary only in one location, while others will need replicating in the different instrument halls or around specific instruments. Additionally, some laboratories will be needed in versions that do and that do not allow work with radiological materials.

- ***Bulk characterization laboratories:*** There will be various needs to characterize samples and materials before and after irradiation. The NNS should include laboratories for optical characterization, fluids characterization, bio characterization, NMR, Raman spectroscopy, IR, UV-vis including nanodrop UV-vis, magnetic materials characterization, probes for specific heat and resistivity, probes of mechanical properties, and more.
- ***Chemistry laboratories:*** Several laboratories will be required to support user and staff needs for chemistry, synthesis, and electrochemistry. These laboratories will also be required to support other sample preparations such as the polishing and cutting of single crystal samples to make them suitable for specific instruments or sample environments.
- ***Soft matter and biology laboratories:*** Advanced experimentation including high-throughput experimentation, automation, and complex environments will require the placement of laboratories directly at the beamline. Thus, each dedicated soft matter and biology beamline will be best served by their own 'lab around the beamline.'
- ***Sample management laboratories:*** With the large number of potential instruments and increased focus on automation, the NNS facility will handle a significant volume of samples, and this must be centrally managed. Space will be required to store user samples upon arrival (prior to irradiation) and after completion of the experiment (post irradiation). This space must also provide all necessary environmental controls (e.g., glove boxes, cryogenic storage, etc.).
- ***Health physics laboratory:*** This should be a component of a centralized sample-management approach and provide sufficient space for equipment.
- ***Semiconductor and thin film processing laboratories:*** Industry engagement is critical to NIST's mission. Semiconductor irradiation and transmutation programs exist at other neutron sources and should also be offered at the NNS. This will require semiconductor processing capabilities including thin film coating and clean-room facilities. In-house thin-film-coating facilities may also be required for in-house fabrication of neutron optics.
- ***Metrology laboratories:*** Since metrology correlates with NIST's core mission, sufficient laboratory space for work on pre- and post-irradiated samples is required. Careful temperature and floor vibration control is critical in this lab space.

- ***Nuclear and radiochemistry laboratories:*** These need to enable all the anticipated work on rabbit stations, hot cells, counting, neutron activation analysis, radiochemistry, and related areas. They will require rad work, but also excellent shielding, better access to the basement and instruments, possibly through automation and/or dedicated tubes, and may also require some overlap with sample environment spaces if *in situ* irradiation under controlled extremes is desired.

11.4.1.2. Shops and Workspaces

In addition to laboratory space, a select set of shops is also required to support the user program:

- ***Machine shops*** need to be available, and access to quick-turnaround machining is essential. Some shop access should be provided to work on radioactive materials.
- ***A Glass shop*** is needed for ^{3}He cell development and deployment. Specialized skills are required to produce large volume cells.
- ***A 3D printing shop*** is needed to provide resin printing at various scales but could also include techniques like metal additive and printing of B_4C shielding components.
- ***An Electronics shop*** is needed to fabricate and assemble customized boards and electronics components. Data acquisition space with an appropriate test stand is required for integration activities.

Support teams for sample environment, electrical and mechanical, data acquisition, optics, and detectors will require shops and / or workspaces. These can include equipment testing and development and staging spaces for larger instrument components.

- ***Sample environment space:*** Demand for complex sample environments tends to increase with the availability of smaller, brighter neutron beams and the increasing complexity in user science. Significant space is required to develop, assemble, and test new or modified equipment, and space within the instrument halls is required to stage equipment for deployment. More details are provided in the separate sample environment section.
- ***Neutron technology support space:*** Extensive space will be required to support advanced neutron technologies. Support for neutron polarization technologies will require laser space for ^{3}He cell pumping and the development and testing of new polarization components (flippers, guide fields, etc.). Additional lab space will be needed to support efforts aimed at velocity selectors and potentially choppers. Depending on the plans to develop neutron optics and detectors (see section on Optics / Polarization / Detectors below), significant space for in-house development activities may be required.
- A ***"bunker"*** is required to test new pressure cells, velocity selectors, or choppers. New pressure cells can be tested to failure, as the bunker provides safe conditions for testing systems with substantial stored energy.
- ***Engineering laydown or pre-assembly areas*** require large rooms with high ceilings and crane access.
- ***A dedicated loading dock*** would facilitate receipt of larger assemblies.

11.4.2. Facilities with special considerations

We specifically call out the need for a deuteration facility, X-ray laboratory, and a microscopy laboratory, as they require significant space, special requirements, and/or coordination across a broader scientific community.

11.4.2.1. National Deuteration Facility

Deuteration plays a critical role in neutron research by enhancing the contrast and sensitivity of different parts of a sample in scattering experiments. Deuterated samples extend a researcher's ability to probe specific structures and dynamics at the atomic level, making best use of the properties of neutrons. By selectively replacing certain hydrogen atoms in a sample with deuterium, scientists can manipulate the neutron scattering intensities from targeted regions of the sample to obtain valuable insights into the behavior and interactions of complex systems. Deuteration is a crucial requirement in neutron scattering experiments, enabling advances in a wide variety of research fields. The requirement for good access to deuterated samples was clearly mentioned in multiple science panels within the "Neutrons for the Future" workshop. Any new facility must consider the deuteration requirements of experiments at an early stage to allow the capabilities of the facility to develop in time for the start of a user program.

There is clearly a growing demand for deuterated samples across the neutron scattering community. The availability of deuterated samples is often the limiting factor for experiments, and as such the capabilities and capacities of facilities worldwide need to grow to meet this demand.

The need for deuteration extends beyond neutron scattering, as it includes applications in NMR spectroscopy and mass spectrometry. These additional science communities would also benefit from easier access to deuterated materials. In the field of NMR spectroscopy research, existing national facilities like the National High Magnetic Field Laboratory in Tallahassee, FL, the Network for Advanced NMR at the University of Wisconsin, the NMR Facility at the University of Georgia's Complex Carbohydrate Research Center, and the NMR Facility at the University of Connecticut Health Sciences would be key stakeholders in developing a national deuteration strategy.

The panel feels that the establishment of a National Deuteration Facility would be timely. It could be modeled on the very successful ANSTO (Australian Nuclear Science and Technology Organisation) National Deuteration Facility in Australia. The ANSTO lab offers both biological and chemical synthesis routes to deliver the requested deuterated materials, and it serves the neutron scattering, NMR, IR, and Mass Spectroscopy communities. The majority of deuteration facilities across the world operate similar access models, with calls for proposals often linked with neutron scattering experiment proposals. There is an opportunity for a future U.S. National Deuteration Facility to collaborate with the other worldwide facilities, to complement each other's specialist capabilities, and to address the capacity requirements for deuterated materials.

This facility itself could be housed at a National Laboratory such as NIST, ORNL, or NHMFL, or it could be based at a university. Well-equipped chemical and biological labs would be needed, as well as instrumentation and analytical labs to support the facility's activities. The personnel operating and managing the facility will need to have a broad set of science experience and skills in the fields of synthetic chemistry, biological cell culture, and analytical chemistry.

A detailed survey of the user community's needs for specific classes of materials will be required to help specify and plan the lab and staffing requirements of a new U.S. National Deuteration Facility. The panel recommends consulting with The Deuteration Network (https://deuteration.org/) to help with this endeavor.

11.4.2.2. X-ray laboratory

A well-equipped x-ray laboratory housing a suite of instruments dedicated to the offline characterization of samples is an essential characterization capability. This offline capability is critical to ensure high sample quality and/or crystal orientation before neutron experiments are run and to provide additional and complementary information to the user. The laboratory should be equipped with a minimum of a small-angle x-ray scattering instrument, diffractometers for powder and single crystal diffraction, a reflectometer, x-ray imaging / tomography, and a Laue camera for single crystal alignment, and it should include space for future growth. X-ray instruments that mimic the neutron beamline geometry are required to complement, advance, and ensure the highest quality of neutron science.

The x-ray instruments should offer a high degree of automation to facilitate sample changes and accept a variety of sample environments. Computing resources will be needed for data analysis, and the data should be accessible using global data-management tools. Dedicated staff will be required to provide and manage user access, instrument and safety training, technical support, and instrument maintenance. The laboratory should supply bench space for sample preparation, be serviced with power and water utilities required for the x-ray sources, and be large enough to house state-of-the-art equipment with micro-focused beams, rastering capabilities, and high-throughput sample loading. We note that the draft NCNR laboratory list only suggests 1000 square feet, which we feel is insufficient. For reference, the x-ray laboratory at SNS is about 1500 sq. ft., and this does not include a modern SAXS / WAXS instrument. This capability is housed elsewhere at ORNL in a separate laboratory of a similar size. As such, we recommend 2000-3000 sq. ft. be allocated for such a facility.

11.4.2.3. Electron and light microscopy laboratory

Real-space imaging methods are complementary to neutron scattering methods, as they often provide a good initial guess and model validation for the ensemble-averaged structures obtained from neutron scattering methods. The laboratory should house a scanning electron microscope (SEM) equipped with an energy-dispersive spectrometer for real-space characterization of hard-matter structure and chemical composition at the nanoscale. Cryo-TEM is needed for real-space imaging of "frozen" liquid states and soft-matter systems to compare with the ensemble-averaged neutron scattering measurements, further aiding in the interpretation of structure, dynamics, and computational models. A liquid and gas-capable AFM is also critical for characterizing soft and hard surfaces to aid interpretation and sample-quality control in neutron reflectometry. Raman and IR microscopes, which are complementary to neutron methods, are also needed for the real-space mapping of chemical bonding on sample surfaces and bulk. High-resolution, fluorescent confocal imaging microscopes are critical for characterizing complex biologically relevant systems. High-resolution optical imaging microscopes are similarly critical for characterizing engineering samples. As with the x-ray laboratory, we feel that the NCNR draft list has undersized this laboratory. In addition, this space needs to consider vibration isolation and magnetic field interference for the electron microscopes.

11.4.3. Sample Environments

A new facility with a large variety of beamlines distributed across several instrument halls will have extensive requirements for sample environments. This will include the support of current sample environments, adaptation of novel sample environments under development at neutron facilities world-wide, custom development of cutting-edge technology for specific beamlines and applications, as well as entirely new approaches to the application of extreme conditions enabled by advances in neutron instrumentation and automation. This complexity requires adequate staffing levels with dedicated teams focused in the major areas described below.

11.4.3.1. Magnets and Cryostats

One key strength of neutron scattering is its unique ability to explore the structure and dynamics of magnetic materials. As such, applied magnetic fields are a critical sample environment parameter at neutron facilities. Additionally, international focus on understanding quantum phenomena in materials often requires low-temperature measurements. Consequently, workhorse sample environments should include closed-cycle refrigerators (T_{min} ~ 4 K), wet cryostats (T_{min} ~ 1.8 K), and ultra-low-temperature inserts for either cryostats or magnets (T_{min} ~ 300 mK for ^{3}He inserts and T_{min} ~ 50 mK for dilution inserts).

While significant progress has been made in developing "dry" cryostats, these are not ideal for all applications. For example, the cool down time for a dry ^{3}He system can be >18 hours, making it challenging to optimize facility use when rapid transitions between samples and experiments are required. As such, we anticipate that wet cryostats and magnets will still be frequently used. Cost and availability of liquid helium remains a significant concern and, consequently, the NNS must incorporate a centralized helium-recovery and liquefication system. Connections to this system should be available at instruments, in dewar storage locations, and in relevant spaces where equipment is tested and prepared for deployment to beamlines.

The state-of-the-art magnetic field limit for neutron scattering is 15 T for vertical-field split-coil magnets and 18 T for horizontal-field solenoids. The emergence of high-T_C magnets has the potential to push beyond these limits. Consequently, instruments that will use magnetic fields should be designed assuming a higher maximum field (we suggest 30 T) to accommodate future progress in this technology. Experience at the SNS suggests that industry is not interested in designing and fabricating compensated magnets and, therefore, 30 T uncompensated magnets should be assumed for instrument design purposes. This requires consideration of non-magnetic shielding material and appropriate building construction, for example, stainless rebar near the sample position.

The community desire for more and higher magnetic fields needs to be balanced against other instruments that are sensitive to these fields. Examples of the latter include neutron-spin-echo spectrometers and some fundamental-physics experiments. A strategy and policy related to magnetic-field interference between beamlines needs to be devised to optimize facility use and scientific output. One possibility is to consider making one of the two guide halls a zero-applied-field hall. However, this needs to be considered cautiously, as there may only be a small number of instruments with no interest in magnets, and such a decision could significantly constrain scientific output from the facility.

11.4.3.2. High-Pressure

Pressure is a powerful tool with which to tune and control materials properties, structure, and behavior, to obtain new states of matter through non-ambient synthesis conditions, to process biological matter, or to understand how materials withstand extremes. Addressing such scientific problems requires advanced neutron-scattering and imaging techniques together with a variety of high-pressure sample environments at the future NNS.

NIST has established an excellent high-pressure program for biological materials and soft matter. The pressure cells and accompanying developments will be very useful for future experiments. Smaller, brighter neutron beams should expand the useful range of diamond anvil cells (DACs) to current bio-/soft matter research, a situation analogous and complementary to existing BioSAXS (x ray) capabilities built on DACs.

Existing high-pressure environments based on piston-cylinder devices (e.g., clamped cells) and gas cells will need to be supported. The latter requires infrastructure on the beamline including high-pressure gas lines, access for the gas intensifier, and necessary safety systems. With brighter, smaller beams the higher pressures afforded by opposed anvil devices (i.e., Paris-Edinburgh [P-E] presses and neutron DACs) become accessible. These pressure cells are portable and can be used across instruments, but they can also benefit from use on a dedicated instrument such as extreme-conditions diffractometers optimized for P-E presses (e.g., XtremeD at ILL). Finally, DACs are highly portable and provide the highest pressures possible. Studies on single crystal samples are possible on existing reactor sources, and even higher pressures (through smaller sample requirements) are expected for future sources.

Conducting research using these pressure environments requires significant infrastructure. This includes the requisite workspaces in the instrument halls, spaces where small complex cells can be assembled and loaded, necessary infrastructure on the beamline such as gas lines, hydraulics, optics access, and laser compatibility, and space for development and cell testing.

11.4.3.3. High Temperature

Addressing questions in materials science related to energy, environment, and engineering materials often requires *in situ* studies under high temperature. This includes understanding the mechanisms of novel synthesis pathways, questions about temperature-driven phase transitions, molten salt research, fatigue behavior of engineering materials, etc. High-temperature furnaces need space, equipment, and staff to address these questions. High-temperature research is often coupled with gas-flow experimentation, which requires beamlines to have the necessary gas-handling capabilities, including gas lines, gas input, and gas exhaust. Future use of lasers on beamlines should include laser-heated furnaces. Beyond furnaces, smaller, brighter neutron beams can enable the use of container-less heating devices such as levitators to reach even higher temperatures or more specifically designed conditions. This will require beamline compatibility not just with visible lasers, but also with invisible class IV CO_2 lasers.

11.4.3.4. Multi-extreme environments

at coupled extreme conditions. While x-ray sources have the upper hand for conditions of extreme pressure, reaching into the multiple Mbar range, the power incident on a sample from an intense x-ray beam limits the lowest temperatures that can be simultaneously achieved. Neutron scattering not only has the upper hand for reaching ultra-low temperatures, but it also has superior magnetic contrast. The multi-extreme environment of magnetic fields above 20 Tesla, temperatures down to mK, and pressures into the tens of GPa, will open new frontiers for the discovery of novel magnetic and electronic phenomena and quantum phases to seed new technologies for applications in low-power microelectronics and quantum information sciences.

Another multi-extreme goal is the combination of high-pressure and high temperature, which is needed to address questions in geophysics and for the synthesis of novel materials not accessible under more moderate conditions. The DAC is an excellent tool, as laser-heated DACs give access to Mbar pressures at several thousand K at synchrotron x-ray sources. But many materials of interest include light elements (e.g. H, C, N) in the presence of heavy elements, a situation to which x-rays are not well-suited; by contrast, neutron scattering can excel in these cases and provide unique information. Concepts for laser-heated neutron DACs have been proposed and the future NNS should be prepared to accommodate such capabilities.

Sample environment teams will have to work together to integrate pressure cells, superconducting magnets, and dilution refrigerators as well as class IV lasers for heating to provide an experimental platform for neutron scattering research at multiple extreme conditions. Such integrated capabilities should be portable and shareable between instruments.

11.4.3.5. Soft Matter

Soft-matter neutron experiments require a large diversity of sample environment equipment and support. This includes high/low temperature, high/low pressures, shear/stress measurements, automated sample changers, liquid troughs, solid/liquid cells, chromatographic systems, etc. This diversity is one of the main challenges faced by any sample-environment team supporting the soft-matter user community. These experiments require a high level of parameter stability, reliability, accuracy, control, and flexibility.

The UK’s ISIS neutron and muon facility is an excellent model for how to support soft-matter experiments through a dedicated Soft Matter Sample Environment Team. In fact, many other facilities around the world (including SNS/HFIR at ORNL and the new European Spallation Source in Sweden) are adopting this approach, and this panel recommends that the NNS do so as well.

Along with appropriate staffing, this dedicated team would require significant set-up and lay-down space for a large catalog of equipment. Given the delicate nature and sensitivity of the equipment, this space will need to be close to and have easy access to the instruments.

11.4.3.6. Chemistry on a beamline (gas handling, etc.)

The trend in complex *in situ* experiments has been evident at neutron sources in recent years and is set to continue. Examples include catalytic studies, involving a wide range of hazardous gases, chemical-reaction studies, and depositions of thin-film materials.

To support these experiments the NNS facility will need knowledgeable and trained staff, with chemistry and health-and-safety management experience. The experiments will require access to complex gas-handling equipment capable of flowing a wide range of gases at a range of pressures through the sample positions of various instruments. Facilities should also be able to handle air-sensitive materials under inert atmospheres.

When designing new instruments and sample-preparation labs, consideration should be given to the provision of local gas panels for a range of gases, hazardous-gas monitoring/alarm safety systems, oxygen-depletion monitoring and appropriate fume exhaust systems.

11.4.4. Automation, Data Acquisition, Remote Access

11.4.4.1. Automation

Extended automation is an exciting, new, and developing area for neutron scattering. It can involve synthesizing a sample, performing neutron measurements, and reducing/analyzing the resulting data in one continuous workflow; modifying an acquisition strategy to acquire data more efficiently; and automating high-throughput mail-in experiments. Streamlining the measurement-to-analysis workflow helps to optimize scientific productivity. Sample changers can use different technologies depending on the specifics of the measurements. For example, open sample positions and near-room temperature loading are compatible with robotic changers while low-temperature applications require changers that integrate into a cryostat and are optimized to cool multiple samples rapidly. A different route to consider involves “sample environment changers,” where multiple samples are loaded into separate environments (e.g. furnaces) that are then swapped on and off the instruments by the changers. In addition, software must be developed to enable computer-aided steering of experiments or autonomous experimentation. Recent advances in artificial intelligence/machine learning will expand the potential for this form of automation, and the software (data acquisition, data reduction, and data analysis) needs to be optimized to enable these approaches. Such automation is a current focus of DOE’s Integrated Research Infrastructure (IRI) initiative, and this provides an opportunity for collaboration with the DOE neutron and light sources.

11.4.4.2. Data acquisition

Development of a new neutron source provides an opportunity to review the full software stack, including the data-acquisition system. Today, EPICS is a *de facto* standard and will likely still be the choice for many years to come. Selecting a standard device interface like EPICS can improve efficiency by sharing device drivers across facilities. As the DOE neutron and light sources largely use EPICS, this provides an excellent opportunity for collaboration. Additionally, there is considerable development of the interface layer that sits on top of EPICS, for example BlueSky being developed at Brookhaven National Laboratory. Having a data-acquisition interface that is common to all scattering facilities will help the user community who often visit multiple facilities.

11.4.4.3. Event data collection

The demand for time-resolved measurements is ever increasing. NIST has held a key place in time-resolved rheoSANS that should be maintained going forward. Expansion across all techniques is expected over the next decades especially with the higher-flux sources. Current state-of-the-art time stamping uses a 10 MHz clock. On the time scale of this facility, we envision a 100 MHz clock will be necessary. Though the clock speed limits the ultimate speed of time-resolved measurements for data efficiency, the researcher should be able to choose a sampling rate that makes sense for the speed of their measurement. The new data-acquisition system should be optimized for event data collection for all instruments.

11.4.4.4. Remote Control of experiments

To ensure access to sources during the COVID pandemic, remote-control systems were developed at multiple facilities. These systems enable a broader group of researchers to participate in neutron experiments where some are on site and some participate remotely. Remote access can lower average radiation exposures for local users and staff by minimizing the time personnel need to be near the beam. It can also allow instrument control to be moved to a non-industrial environment, with better lighting, less noise, etc. The system should only allow trained users on the current experiment to control the instrument.

11.4.4.5. Experiment Collaboration Tools

Chat-style tools became more commonplace during the COVID pandemic and have proven to be very useful in coordinating experiments and the subsequent data analysis. At the ORNL neutron scattering facilities, about 250 users per day use the Slack-based communication tool to discuss progress, store notes, and interact with instrument staff. This tool is especially helpful when some collaborators are working far from the facility. Facility ownership of the deployment methodology enables system security to be preserved and archiving of discussions. The ESS has developed their own tool (SciChat) for similar purposes, and it is also being used at PSI. Many individual research groups use Google Docs, Discord, or others. The specific tool-of-the-day should be chosen at the relevant time.

11.4.5. Computing

11.4.5.1. User access to compute

Traditionally, most neutron facilities provide some data-processing software (e.g. DAVE or Mantid) that users must install and operate on their own computer. Driven by the data needs at spallation sources, the SNS at ORNL and the ISIS Facility in the UK have changed this model. ORNL now provides computing resources shared between ~ 250 users on any single day with a total of 1000 cores and 8 TB of memory. The ISIS facility allows users to choose a cloud-based computing resource sized for their specific technique for a dedicated time. They have ~200 simultaneous users per day. The hardware underlying this cloud-based system has ~ 10,000 cores. We anticipate that future users will expect such systems to be available. Applications will require at least CPUs and GPUs, and possibly other heterogeneous processor types. The cloud-based model is currently more attractive as then users do not have to compete for resources, and it separates the user need from the underlying hardware. More heterogeneity in computing type is the trend in computer hardware and software development, and it should leverage various computing hardware transparently.

A challenge facing neutron facilities is that of providing a platform that novice users can quickly learn to access standard workflows while also providing advanced analysis functionality for experienced users. Mantid has attempted to provide a flexible environment where the latter could be implemented, but the interface has been difficult for casual users to understand. Workflow tools and management systems provide the ability to add an interface quickly on top of multiple tools spanning heterogenous platforms. An ORNL Laboratory Directed Research and Development (LDRD) initiative is exploring the use of Galaxy to deploy advanced analysis methods across neutron scattering techniques. In addition, having computational instrument staff to help users with custom workflows was shown to be critical. An example is the Computational Instrument Scientist role that has recently been implemented at ORNL. The use of these workflow tools will be highlighted in several examples associated with other topics below.

11.4.5.2. HPC to help with analysis.

In recent years, high-performance computing (HPC) has become important for understanding neutron scattering results. Density functional theory and molecular dynamics are two techniques that have seen a broad increase across materials science, engineering-relevant materials, biological systems, polymer systems, and quantum materials. Users that are most successful at leveraging these approaches either have access to their own compute cluster or computer resources provided by the facility. Access to larger scale HPC resources can be challenging and requires coordination with the relevant supercomputer centers. At Argonne National Laboratory, 4 PFLP/s are dedicated on the new POLARIS supercomputer, a hybrid CPU/GPU with 44 PFLP/s, to prototype on-demand use by experimental facilities such as the Advanced Photon Source. At ORNL, the DOE NERSC facility is available via proposals managed through the neutron scattering facilities. Expanded models and agreements will be required for future neutron facilities to provide access to more powerful computing resources.

A significant challenge with HPC is that most neutron users lack expertise in using such platforms. Workflow tools have the potential to overcome this limitation. As an initial demonstration, Alex Hexemer at the Advanced Light Source demonstrated the HipGISAX tool that allowed analysis of x-ray grazing incident scattering using the Titan supercomputer at ORNL. More recently an LDRD project at ORNL led by Thomas Maier demonstrated an easy-to-use workflow tool for running DCA++, an advanced modeling software for strongly correlated materials, on the Summit supercomputer for comparison to inelastic neutron scattering data.

Finally, Machine Learning will increasingly be used to perform faster analysis of neutron scattering data and will ultimately be used for experiment steering or automation. Recent examples include using surrogate models to reduce the uncertainty in determining exchange parameters in quantum magnets and the use of density functional theory calculations to train a network that can predict the phonon density of states from knowledge of structure.

11.4.5.3. Fast Compute near the instrument (Edge computing)

Artificially intelligent systems are making neutron measurements more efficient. Clustering algorithms have been used to identify phase transitions in event-based data. Machine Learning has been used to map quasiparticle dispersions more efficiently on triple-axis spectrometers by two groups working at the ILL. A collaboration between NIST and ORNL has demonstrated the automated identification of phase transitions in a more traditional histogram type of acquisition. A project at ORNL has provided a facility for the VENUS imaging beamline that automatically directs the orientations needed to produce optimal tomographs.

Monte Carlo ray tracing has become the standard for instrument design and optimization. These simulations are digital twins of the instrument and have started to be used to quantify multiple scattering and other instrumental effects. These codes are being ported to GPUs that allow them to run at speeds like that of an experiment. This has the potential to enable routine use of digital twins for experiment planning, analyzing complex backgrounds, accounting for instrumental resolution, identifying spurious features, providing training data sets for neural networks, and understanding materials with a mix of scattering processes. For training, these digital twins should have the same interface as the control system. For analysis, there should be sufficient accompanying metadata so that the user only needs to provide the data file they acquired to set up the simulation.

These examples demonstrate things that will become commonplace in the future. These techniques need fast computers near the instrument (edge computing) for real-time operation. These examples also need integration between the acquisition and some amount of analysis. The instrument firewall needs to be designed to ensure security while maintaining flexibility.

11.4.5.4. Data Storage and Management

Neutron data acquired by the instruments should be managed according to FAIR (findable, accessible, interoperable, and reusable) principles. Raw data should be stored with the appropriate metadata, stamped with a DOI (digital object identifier), and provided with instructions on how to analyze it. Furthermore, a method to allow the users to link the results in their publications to the relevant raw data should be provided. A modern data catalog (SciCat at ESS and OnCat at ORNL are two current examples) should be used to allow the user to access their data regardless of where it is stored. Fast network infrastructure is needed to move data quickly between the instrument and associated computers. In addition, connections to national fast networks (ESNet, Internet 2) will allow users to move data to HPC resources as needed. Proprietary access to the beamlines, as sometimes required by industry, should be a consideration in designing the data-management system.

11.4.6. Optics / Polarization / Detectors

Polarized neutron applications are a strength of continuous neutron sources due to the ease of polarizing monochromatic beams. Support for multiple polarization methods is required, including polarizing monochromators, optical components, and ^{3}He transmission cells. The instrument suite for the new facility will significantly increase demand for polarization, requiring appropriate staffing and lab space to develop and deploy new capabilities. Deployment of ^{3}He cells across instruments in multiple halls needs appropriate access to pumping stations, requiring lasers and appropriate power and cooling. *In situ* pumped cells should also be considered where space is available. Additionally, wide angle ^{3}He cells require glass blowing expertise and developing and maintaining this skill set is a challenge faced by all neutron sources today.

Neutron optics pose a project risk as the amount of guide required to support the large number of instruments in two cold guide halls and a thermal guide hall is substantial. There are currently a small number of vendors internationally who can provide these guides, particularly those with higher m-values, and none is in the U.S.. A strategy to mitigate this risk needs to be developed and could include in-house mirror depositing and guide fabrication or building industrial partnerships. Opportunities also exist for collaboration with DOE light sources, which have developed their own deposition systems for fabrication of x-ray multilayer optics. An additional risk is associated with the procurement of pyrolytic graphite (PG) crystals. PG is a commonly used monochromator and multiplexed instruments require many crystals with consistent mosaic spread. The most reliable vendor of such crystals has been Panasonic, but they recently stopped fabrication of PG crystals. The remaining vendor is Momentive, but they tend to produce more variability in mosaic spread. As with guides, a risk mitigation strategy needs to be developed here as well.

Finally, detector needs for the instrument suite should be considered early in the planning stage. A detector group will be necessary, and this may require focused in-house detector development. This is an opportunity for collaboration with the detector development team at the ORNL neutron sources.

11.4.7. Facility Infrastructure and User Space

Infrastructure for specific instruments, including power, water, gas handling and exhaust, etc., should be defined by the science case anticipated. There are, however, some facility-level considerations. Utility trenches should be appropriately sized for both the guide halls and confinement room. These should be at least as large as the trenches in the new NCNR guide hall. A higher beam height (maybe between 60 and 72 inches) will be beneficial for certain instruments and for design of specific sample environments such as split-coil magnets. Adequate crane access and clearance with minimal "dead zones" is essential and this will be a combination of bridge cranes and local instrument cranes. Consideration should be given to a "mezzanine level" in the guide halls where the instrument control hutches could be located. Finally, the facility must design paths for equipment moves between halls and from sample environment workspaces for items like high-field magnets, which must be shared across instruments.

As the new reactor will principally be a user facility, careful thought should be given to user space. In addition to space near the instrument, areas outside the reactor hall / guide halls are required for monitoring experiments and analyzing data. Such spaces, combined with remote experiment capabilities, are important from an ALARA perspective. Space for gathering and socializing is essential for staff and users (a coffee area for example). Conference and meeting rooms of various sizes must be equipped to support virtual and hybrid remote / in-person meetings. Such spaces must also support training and education activities.

We recommend a guest house be built near the NNS facility. For after-hours access, food delivery and/or transportation to local restaurants is important for users without a vehicle. Finally, care should be taken to minimize barriers to site access, and this might require a separate entrance and security boundary for the neutron facility.

11.4.7.1. Staffing

It is important to design buildings and infrastructure with an appropriate staffing model in mind. To staff a large-scale user facility like the NNS properly, there are several areas where we believe staffing levels will need to be increased. These areas include the following:

- **Instrument hall coordinators**: These staff provide 24/7 on-site presence to support users and instrument staff.
- **Sample management staff**: An increased number of neutron instruments and higher throughput complicates the management of samples. Sample receiving, shipping, and disposal is more safely handled by a dedicated group with a sample-management database. This needs to be combined with the necessary staff and resources for radiological calculations and measurements to support sample release or shipment.
- **Sample environment staff**: An increased number of neutron instruments together with the different needs across scientific areas will require sufficient staffing. Dedicated sample environment teams are needed for magnets / cryostats, high pressure, high temperature, and soft matter.

- **Staff for polarization / optics / detector development**: Polarization will be heavily in demand at the NNS facility and will require more staff dedicated to development and deployment. As described above, a strategy must be developed for optics and detector development, which will likely require dedicated staff.

- **Staff for computing**: Managing computing and data storage infrastructure requires dedicated staff. As software for data reduction and analysis will be essential to achieve the full scientific potential of the NNS facility, staff are required to develop and support the software stack across the instrument suite.

We were informed that the current plans were based on a model of 6 FTEs (full time equivalents) per instrument. Based on the need for staffing in the areas listed above together with the expectation of at least 2 instrument scientists and an appropriate number of technicians across the facility, we feel that this number is insufficient. A more reasonable number is 9-10 FTEs per instrument. We encourage NCNR management to reach out to discuss this with colleagues at the European Spallation Source, as they have recently developed a staffing model based on a comparison to other international facilities.

12. Transition Process

12.1. Panel

Chair:
Drew Marquardt – *University of Windsor*

Panel Members:
Stuart Castillo – *University of Windsor*
Ronald Rogge – *Canadian Nuclear Laboratory*
Jamie Schulz – *Australian Nuclear Science & Technology Organization*

Scribe:
Daniel Adler – *National Institute of Standards and Technology*

12.2. Glossary of Terms

ANSTO: Australian Nuclear Science and Technology Organization

Greenfield site: an undeveloped site on which to build a new facility

Guide Hall: A large hall adjacent to a neutron source that typically contains neutron instruments

IPNS: Intense Pulsed-Neutron Source (now closed) located at Argonne National Laboratory. It was the first neutron source to use an accelerator to produce a proton beam directed at a heavy metal target to produce neutrons

LANSCE: The Los Alamos Neutron Science Center; a high-power accelerator that provides neutrons to five research facilities and Los Alamos National Laboratory

NBSR: Acronym for the current National Bureau of Standards Reactor (NBSR)

Neutron guides (guides): Neutron waveguides used to transport neutrons from a reactor to instruments typically located inside a guide hall

NNS: Acronym for the reactor to replace the current National Bureau of Standards Reactor (NBSR)

NRU: Canadian National Research Universal reactor

NSE: A neutron scatting instrument able to probe material dynamics on a range of length and time scales

OPAL: ANSTO's research reactor; OPAL stands for Open-Pool Australian Light Water reactor

SANS: A neutron instrument able to probe material structure on the nanometer (10^{-9} meters) to micrometer (10^{-6} meters) length scale

SNS: The Spallation Neutron Source, the US flagship pulsed neutron source located at Oak Ridge National Laboratory

User facility and user community or base: A scientific research facility that is open to all scientists (user base) and allocates instrument time via a proposal system

12.3. Summary

A transition plan is subject to the location of a future National Institute for Standards and Technology (NIST) Neutron Source (NNS), the Transition Panel thus set out to consider the pros and cons of three site options. The Panel concluded that a site other than the NIST Gaithersburg campus was the least desirable as it most negatively impacted the user experience; retention of key specialized personnel; continuity of scientific, technical, and user-support cultures; and would be a significant impediment to strategic transitioning of personnel and instruments to the NSS. Two options for the NIST Gaithersburg campus were considered: (i) a location shared with the National Bureau of Standards Reactor (NBSR) that would incorporate elements of the NIST Center for Neutron Research (NCNR) such as the existing guide hall, office spaces and associated infrastructure and (ii) a new greenfield site on the campus. While a cost/benefit analysis for both on-site options is advisable, the Panel concluded that any anticipated savings from a shared location with the NBSR would likely be consumed by costs of rework, unanticipated complications and would add challenges for a strategic and orderly transition of personnel and instruments from the NBSR to the NNS, including a reduction of the advantages that could be realized by a 1-2 year period of simultaneous operation of the NBSR and NSS.

> **The Transition Panel recommends locating the NNS at a greenfield location within the NIST Gaithersburg campus. This will facilitate the most effective transition to the NSS while minimizing the impact on the scientific/academic and industry user community, and, at the same time fostering a smooth evolution of the NSS workforce while maintaining strong research and user-support cultures.**

12.4. Overview of options

To contemplate what the transition plan would look like; site selection is a paramount consideration. The panel considered three options for the National Institute for Standards and Technology (NIST) Neutron Source (NNS) and what each meant in terms of managing an effective transition, specifically:

A. Offsite location, which can be anywhere from simply off the current NIST Gaithersburg campus to elsewhere in the USA.

B. Onsite shared, pairing to the existing NIST Center for Neutron Research (NCNR) complex, primarily annex the current guide hall to the NNS and the infrastructure within.

C. Onsite green field, still on the NIST Gaithersburg campus, but fully separated from the NCNR complex.

All three will have licensing implications and the impacts are unknown and warrant further investigation. However, there are many pros and cons of each scenario that can be anticipated and articulated. The pros and cons are broadly summarized in the following tables.

A. Offsite location, which can be anywhere from simply off the current NIST Gaithersburg campus to elsewhere in the USA.	
Pros	**Cons**
• No space constraints and more flexibility with new build. • Potential to address a number of concerns from user community, such as onsite accommodations. • New geographical location could expand the user base by attracting new users based on proximity. • Possibility to identify a welcoming surrounding community.	• Staff retention is more challenging, especially for non-scientific staff. • Continuity of staff culture and effective evolution of staff is difficult to achieve. • Avoiding a *not-in-my-backyard* resistance may lead to remote location that might not support user access accommodations and amenities. • May reduce industrial use if too far from industrial or manufacturing concentration in eastern USA. • No other supporting facilities are currently present on a completely new site. • Simultaneous operation requires doubling all staff requirements (operations, scientists, technical, engineering, security, and user support).

B. Onsite shared, pairing to the existing NCNR complex, primarily annex the current guide hall to the NNS and the infrastructure within.	
Pros	**Cons**
• Retention and effective transitioning of staff (operations, scientists, technical, engineering, security, user support) is easier, especially non-science staff. • Continuity of staff culture and effective evolution of staff. • Potential for some cost savings. • Smoother transition to NNS relative to offsite. • Retain regional user base. • Remains close to the high concentration of industry. • Keeps total footprint relatively small, easier to adhere to 400 m Emergency Planning Zone. • Simultaneous operation of NBSR & NNS permits earlier growth toward long-term goals, e.g., more instruments with new well-trained staff available immediately. • Simultaneous operation allows for strategic relocation of existing instrument to minimize gaps in instrument-beam-days for each instrument. • Continuity of access to complementary NIST labs and facilities. • Numerous regional amenities for users.	• Simultaneous operation of NBSR and NNS may be more challenging when physically connected. • Using existing guide hall and infrastructure could be more difficult and disruptive than expected. (unless it is planned as the second guide hall) • Transition plan needs to factor in subsequent decommissioning activities of the NBSR to minimize ongoing impact to user access and operations. • Challenging to reuse guides if there is simultaneous operations. • Limits options for strategic relocation of existing instruments. • Limits options for future expansion. • Existing facilities require modernization.

C. Onsite green field, still on the NIST Gaithersburg campus, but fully separated from the NCNR complex.	
Pros	**Cons**
• Retention and effective transitioning of staff (operations, scientists, technical, engineering, security, user support) is easier. • Continuity of staff culture and effective evolution of staff. • Potential for some cost savings relative to offsite. • Repurpose current facility space to support new facility. • Smoother transition to NNS relative to offsite and onsite shared. • Retain regional user base. • Remains close to the high concentration of industry. • Simultaneous operation of NBSR & NNS permits earlier growth toward long-term goals, i.e. more instruments with new well-trained staff available immediately. • Simultaneous operation allows for strategic relocation of existing instrument to minimize gaps in instrument-beam-days for each instrument. • Continuity of access to complementary NIST labs and facilities. • Plenty of regional amenities for users. • Strategic reuse of guides where possible.	• Locating adequate space within the campus • Adherence to 400 m Emergency Planning Zone. • Infrastructure will be stretched or possibly insufficient, particularly for simultaneous operation.

12.5. Principles to maintain user experience

The single most import group to minimize disruption for during the transition from the NBSR to the NNS is the neutron scattering community. A detailed overview of the NCNR user community can be secured from the NCNR User Group (NUG). Here we outline the principles sought by users to ensure optimal use of the facility. Maintaining these principles is of the utmost importance during a transition process.

12.5.1. Reliability/availability of neutrons

Users require a facility to be both highly available and reliable to maximize usage. This entails a facility that is highly reliable to ensure neutrons are available for users when they arrive for their experiment. This is primarily due to the cost of travel and the beamtime being scheduled around the availability of the users and often with samples that are degradable.

12.5.2. Expert instrument scientists

Users require instrument scientists that are experts in techniques and can efficiently operate their instruments. Users also require scientific diversity of the team members within the instrument teams to best serve the user community.

12.5.3. Excellent user support systems

User support systems that are efficient, adaptable to the needs of users, utilize a risk-based approach to activities, and supported by an enabling staff culture.

12.5.4. World leading/class instrumentation

Users require world leading/class neutron beam instrumentation and sample environment equipment. Users are continually pushing the boundaries and require instruments with high flux and low background. This requires continual improvement and upgrades to instrumentation.

12.5.5. Access to supporting research infrastructure

Users require access to supporting research infrastructure such as laboratories, workshops, and scientific support equipment such as X-ray instruments, magnetometry capabilities, spectroscopic techniques etc.

12.5.6. Easily accessible and access to amenities

A neutron facility should be located close to regional transport hubs to minimize the time and cost to travel to the neutron facility. Proximity to accommodation options (ideally adjacent and onsite) as well as restaurants and supermarkets.

12.6. Scientific impacts and disruptions during transition process

The transition to a new reactor source can have significant impacts on the science programs of the user community. The potential impacts will depend on various factors, including the capabilities of new reactor source, the transition process, and the readiness of the user community to adapt.

Neutron accessibility is critical to maintain the user experience during the transition from the NBSR to the NNS. There are examples from other user communities that can be looked to as an estimate on the potential disruptive impacts. There is clear evidence from historic domestic transitions such as Argonne's Intense Pulsed Neutron Source (IPNS) to Oak Ridge National Laboratory's (ORNL) Spallation Neutron Source (SNS) and foreign examples that demonstrate the irreparable disruption to the user community when the proper transitions mechanisms are not accounted for, including multi-year gaps in neutron availability.

In Canada, the 2009 National Research Universal (NRU) reactor suffered an unexpected 15-month shutdown due to a vessel leak. When it became apparent that the shutdown would be protracted, mitigation efforts included securing beamtime at other facilities to support planned scientific/academic experiments and industrial work at the NRU. Additionally, support of the Canadian Neutron Beam Centre (CNBC) staff willing to help the non-expert users at those facilities was made available. The outcome was those with near-term beamtime allocations took advantage of the opportunity, and one commercial project was completed. Non-expert user and commercial use then dropped off rapidly with those groups opting to wait. Expert users, however, were already well-connected to the worldwide neutron source community and found their own way. When the shutdown took longer than originally anticipated, the non-expert and commercial users discontinued engagement. Despite mitigation efforts, there was a clear multi-year recovery period after the NRU reactor started up, which was exacerbated by loss of instrument and personnel capacity. The impacts on the scientific output of the 2009 temporary shutdown and the two years post NRU's permanent shutdown in 2018 can are reflected in the 2020 Canadian Institute for Neutron Scattering user surveys [1].

There are clear opportunities for optimization if the NNS reactor operates in parallel with NBSR. The efficiencies of parallel operation are further bolstered by locating the NNS on the current Gaithersburg facility on a greenfield site. Furthermore, if delays in the construction and/or commissioning of the NNS occur, the planned overlap of operations minimizes any gaps in neutron availability for the user community. Further, a planned operation overlap insulates against significant neutron droughts due to delays in new construction and commissioning. When planning the overlapping operations, ample license life and fuel is required to accommodate the transition. Looking at lessons learned from past neutron source transitions such as the High Flux Australian Reactor (HIFAR) to the Open-Pool Australian Light-water (OPAL) reactor in Australia, having the NBSR's license active for years beyond the perceived transition timeline is ideal. Construction consideration is an important factor for parallel operations. Active construction in an occupied space presents challenges and will disrupt the ongoing science in the occupied space. These disruptions could include noise, debris, vibrations, and safety hazards which would be mitigated by a greenfield construction rather than reusing an existing guide hall.

Disruption to users' access to neutrons can be further mitigated by a staggered reactor cycle between the NBSR and the NNS. Under this scenario, the access to functioning neutron instruments would increase much faster as the existing/remaining NCNR instruments and the NNS instruments would run back-to-back. Proper instrument planning and an onsite greenfield location would facilitate an increase in the overall neutron scattering capacity of the facility (NBSR and NNS) at the NNS's first light; truly optimizing the accessibility of neutrons to the NCNR user base (Fig 1). Such an operations model has benefits to personnel transitioning (below).

A smooth scientific transition will also rely on strong coordination with existing domestic neutron sources such as those located at ORNL and to a lesser extent those located at university campuses such as Penn State Breazeale Reactor and the University of Missouri Research Reactor Center. Given the global ecosystem of neutron scattering facilities, it would also be advantageous to form partnerships with international facilities to ensure neutrons for users.

Overall, the impacts on science programs during the transition process will depend on careful planning, resource allocation, and support from stakeholders. When managed effectively, transitions can offer new opportunities and enhance the capabilities of the user community.

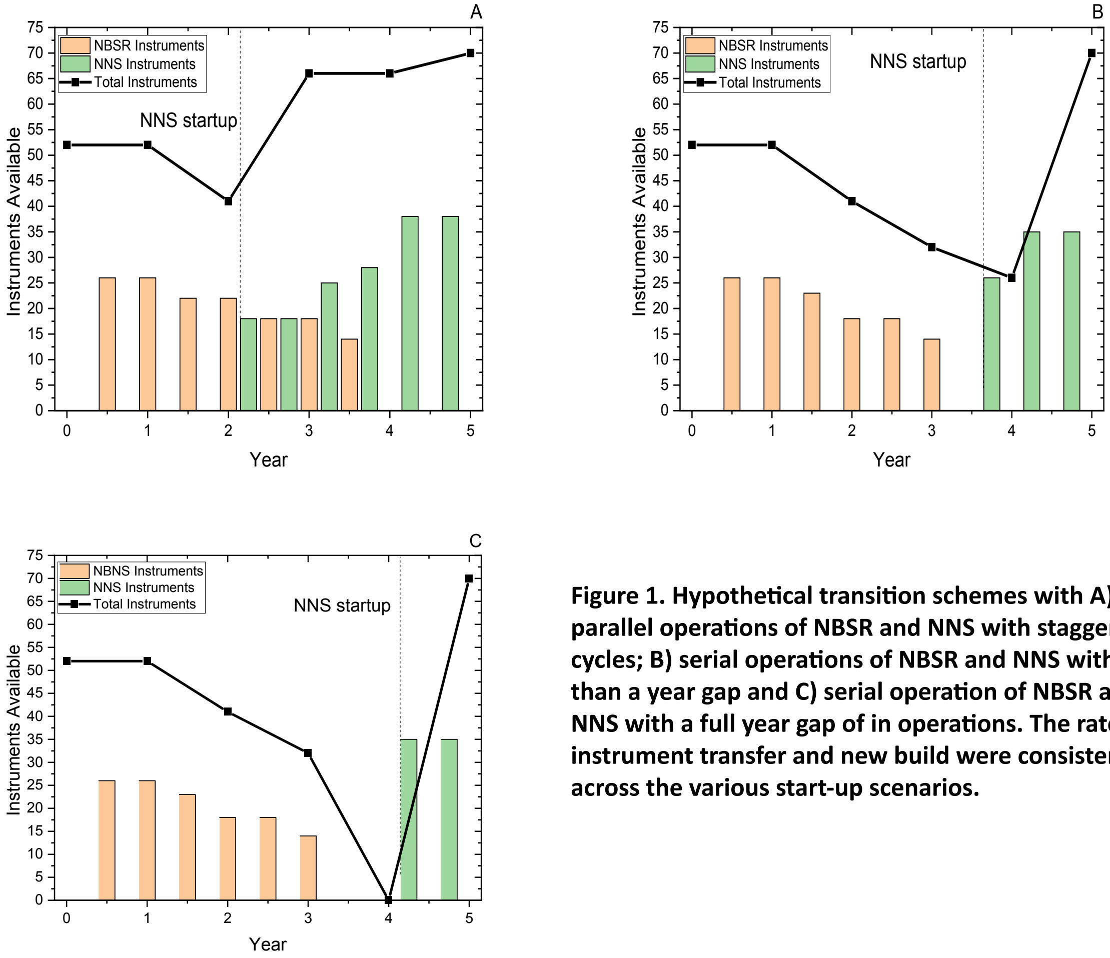

Figure 1. Hypothetical transition schemes with A) parallel operations of NBSR and NNS with staggered cycles; B) serial operations of NBSR and NNS with less than a year gap and C) serial operation of NBSR and NNS with a full year gap of in operations. The rate of instrument transfer and new build were consistent across the various start-up scenarios.

12.7. Principles to maintain facility operations

The current NCNR employs a diverse staff to support its research and operational activities. Some of the key types of staff include scientists, engineers, technicians, administrative staff, safety and facilities staff and a variety of visiting academics of all levels. Understanding the needs of each of these groups is critical to maintain an optimal operation for the facility.

12.7.1. Knowledge transfer

Strategic organization and management of the workforce will ensure that both staff and their expertise are retained, and knowledge is transferred from existing staff to the new staff that are involved with the design, construction and commissioning of the NNS and the new instrument suite. This continuity in the workforce is also critical to ensure that a unified working culture is maintained.

12.7.2. Use of existing and new infrastructure

Strategically manage the instrument suite including planning for which instruments will be transferred from NBSR to NNS and upgraded to ensure that they remain world-class. This is also applicable to new and existing sample environments.

12.7.3. Use of legacy and new workflows

Strategically manage systems and workflow including the early adoption of standardization within the NNS.

Considering these principles will allow facility operations to be more resilient, safe, and efficient, ultimately contributing positively to the user experience.

12.8. Personnel impacts and disruptions during transition process

Impacts on personnel during a transition to the NNS is a multifaceted consideration as different staff groups are affected differently. In all cases however, building the NNS at the NIST Gaithersburg campus with a period of simultaneous operation is strongly favored.

Scientific staff tend to remain attached to the instruments and source and will generally move with the facility. However, scientific staff have established networks that weigh strongly to the NIST Gaithersburg region (see NCNR User Office statistics) for both scientific/academic and industrial users.

Engineering staff experienced with facilities at neutron sources and instrument design are less likely to relocate. Staying at the current NIST campus mitigates the risk of loss of this specialized engineering capability. Moreover, expansion will require more of these engineers; staying on the current campus means the experienced engineers are able to train and support the new engineers and draftspersons.

Support staff such as trades trained and, in some cases, qualified to work in a nuclear environment are also unlikely to relocate. Administrative staff familiar with user facilities are also unlikely to move. Security and emergency response staff are also unlikely to relocate yet are specially trained. If the NNS is built on the current campus, only a moderate increase of these staff is anticipated, while for an offsite greenfield, all of these staff will have to be replicated. Hiring staff is always a challenge, specialized personnel is a greater challenge, particularly the large number required for an entirely new site. A significant number of staff have partners that also work at the NIST Gaithersburg, an offsite greenfield location will have fewer opportunities for the partners of the staff willing to relocate.

The driver for the NNS is to not simply preserve current capacity, but to expand it to meet US demand. A common approach for new builds has been to start with a minimum complement of instruments to address the highest demand and build-up over time. However, simultaneous operation of the NBSR and NNS would allow for strategic and orchestrated build-up in instruments and personnel. This approach makes it possible to provide effective succession planning and mentorship of the new staff required to support the expansion while also allowing current staff to maintain their user community. Years before the NBSR shutdown, new research staff can be used to help the existing user community and learn about the user facility culture preparing them for their roles in the NSS. This also frees up some time of the more senior research staff to continue supporting the community while also providing their expertise toward the design, construction and commissioning of new and transferred instruments at the NSS. The result is a continuity and nurturing of both the research and support personnel cultures. This cannot be practically achieved with an offsite new build.

This is also of critical importance to the operations staff. Such a strategy will require an increase in reactor-based personnel and recruitment considerations should be addressed early. For example, mandated salary caps for operators within government versus private industry is a known issue. Strategic planning of the succession of retiring staff will support training of new operators which takes two years. During the NBSR operation, trainees will benefit from the experience of the current operators before they retire. Some NBSR operators will transition to the NNS and having both groups together during simultaneous operation can help manage staffing requirements. Staggered cycles while running in parallel optimize the training environment for operations personnel.

The difficulties and sometimes negative outcomes of building a new greenfield site can be understood by looking at past cases. It was envisioned that the Spallation Neutron Source (SNS) would reap some benefits of having staff of Argonne's Intense Pulsed Neutron Source (IPNS) ultimately transition to the SNS. The IPNS was used for testing and some training of personnel and the expertise of the IPNS personnel was used to great benefit of the SNS. It was, however, a difficult period for personnel making frequent trips between the two sites. Remaining on the NIST campus will eliminate that challenge and likely result in more effective mentorship and knowledge transfer. A frank review of the IPNS-SNS transition is recommended.

The plan at the Australian Nuclear Science & Technology Organization (ANSTO) was to have the HIFAR reactor operate until the OPAL reactor started up. However, delays in the OPAL reactor construction and the expiration of the HIFAR license resulted in a one-year gap in operation. From the perspective of the neutron beam and reactor operations personnel the impact was not significant and allowed for more time for a transition, but it was not as efficient as planned.

In Canada, the 2009 15-month shutdown of NRU impacted staff. While the shutdown was used to accelerate instrument and ancillary equipment upgrades, catch-up on data analysis, and write publications, after 10-12 months several staff became anxious, resulting in staff loss. The even lower number of staff per instrument (dropped to less than 3), made recovery from the shutdown that much more difficult and put a great deal of pressure on scientific and technical staff. An additional casualty was a newly built instrument that had to be removed for reactor start-up. In the end, this instrument did not get rebuilt as there were not enough staff to support that activity.

The unexpected loss of the Los Alamos Neutron Science Center (LANSCE) general user program resulted in several staff moving to another source, shifts in research focus of remaining staff, and knock-on effects to their established user community. Instruments were shut down and now sit idle. The impact on the broader US user community provided additional insights as to the impact of reductions in capacity.

It is worth noting that the loss of a neutron source that supports a user program does not only result in the disappearance of non-expert and industrial users, but a significant fraction of the facility personnel will choose to instead move to positions not related to neutron scattering for various personal reasons. This amplifies the impact of losing the reactor source on the capacity of both the national and the worldwide neutron scattering community; re-establishing the capability then becomes a one-to-two-decade effort.

Diversity among the neutron user community and neutron source workforce has grown over the past decade and without a doubt will continue in the decades to come. Historically, the neutron science community parallels the predominately white, cis-male, history of physics since before the discovery of the neutron by James Chadwick in 1921. To address historical biases, it is crucial to consider principles of inclusion, diversity, and accessibility at the onset of the design and strategic planning. As this project will develop a neutron source that will be a national user facility for one of the most diverse populations in the world, the facility must be accessible to everyone. Granted, many aspects of diversity and inclusion are a product of the environment's culture, which is directly related to the location of the NNS, but the accessibility in terms of physical accessibility can and should be considered from the beginning. From a "transition process" lens, where the NNS is located relative to NBSR has significant accessibility implications. To maintain accessible access to instruments during the transition, a greenfield construction is critical (e.g., not sharing guide halls).

12.9. Recommended pathways for transitioning to new reactor source

Transitioning to a new reactor source is a complex process that involves several steps and considerations. The transition to a new reactor source is a multifaceted process that requires careful and early planning. Here we outline recommended pathways as well as raise some action items required for making the transition process smooth.

12.9.1. Reactor Location

After assessing the possible scenarios, i) greenfield construction offsite elsewhere in USA, ii) onsite at Gaithersburg adjacent and sharing current facility, and iii) greenfield construction onsite at Gaithersburg, the Transition Process panel recommends the third option of a greenfield construction on the current NIST Gaithersburg campus. The addition of a new greenfield construction onsite at Gaithersburg is the least disruptive transition plan of the possible scenarios. This scenario allows for the simultaneous operation of the NBSR while the construction of the NNS moves forward without contributing to major user interruptions. The specific site of the reactor within the NIST campus depends heavily on zoning laws, environmental considerations, cost benefit analysis considerations and more.

12.9.2. Detailed Profile of User Community

The NCNR facility and NCNR User Group has a strong history of maintaining regular surveys and keeping user statistics on instruments used, science performed, and frequency of users' experimental participation. Once the timelines and milestones are adequately mature, a comprehensive survey of the user community and science should be conducted to assess instrumentation priorities and to inform on the appropriate instruments to be built new and what existing instruments located at the NBSR should be transitioned to the NNS. For the purposes of informing the transition, categorizing users into "Expert" and "Non-expert" or "Heavy" and "Casual" based on usage and output could help identify what part of the user community is a priority to service during transitions [2]. Further, statistics on instrument usage is critical and oversubscribed instruments such small angle neutron scatting (SANS) and neutron spin-echo (NSE) must be dealt with first.

12.9.3. Steps to Minimize Disruptions

The steps summarized below will outline the recommended course of action to minimize disruptions to the neutron user community.

I) Maintenance of a functioning and operating reactor to provide an indispensable service to both the research and industrial community is the utmost important priority of NIST. It is strongly encouraged that the NBSR and NNS have two years of parallel operations with staggered operation cycles. Further, the organized commissioning and decommissioning of instruments in a highly thought-out plan that considers users' needs, industries' needs, and subscription rates of specific instruments is key to sustaining and growing the needs of the users.

II) Maintenance and upkeep of user facilities, labs, and user support while the transition is ongoing is critical to minimize disruption to the user community. This is achieved through simultaneous upkeep of current labs while construction of new user facilities, labs, and amenities occur. The users need access to highly specialized facilities to have successful experiments such as access to deuteration labs, biology labs, NMR and like instruments, sample environment development, general preparatory labs, etc. Without access to these critical facilities the success rate of many experiments sharply declines.

III) Avoiding overlap with planned outages with Oak Ridge National Laboratory and other neutron sources is worth serious consideration when planning critical shutdowns of the NBSR. When such avoidances are not possible, it is critical that NIST partners with international facilities to minimize the downtime of neutrons in the nation. This is obtained through strategic partnerships on the national and international level.

12.9.4. Workforce Planning

The somewhat anecdotal examples above illustrate that extended shutdowns, unplanned or otherwise, can be managed over the period of one year, but as the period goes beyond one year, there are impacts on personnel with corresponding impacts on instrument capacity, and to the particularly sensitive non-expert and industrial user communities. The panel recommends that these and other cases be studied to see if there are lessons to learn that can help mitigate these impacts on personnel and workflow.

Detailed workforce planning is required to manage the transition from design, construction, commissioning, and transfer to full operations of the NNS while continuing to operate the NBSR in parallel. The workforce plan should strategically ensure that existing staff and new staff are transitioned to the NSS. For all employee groups it will be beneficial to make use of mechanisms such as financial incentives, emeritus appointments, and planned retraining to retain staff over an extended transitional period that all start well before the start-up of the NNS. Indeed, the benefits of training through mentorship and active work during NBSR operation has a greater impact with a period of simultaneous operation. Regardless of staff involved, this approach most effectively supports the strategic transition of existing instruments and their user groups to the NNS, resulting in a nearly seamless transition. Consideration should be given to incentivize staff to remain at the NBSR that are likely to leave/retire at the shutdown of the NBSR.

Expansion of scientific staff to the total operating capacity of both the NBSR and NNS during the simultaneous operation period is required to offset personnel burnout. NNS-only staff need to start early on such that they gain experience from pre-existing staff, learn what it takes to support users, be part of the instrument design, and aid in transfer of instruments to the NNS from the NBSR.

12.10. Summary

The Transition Panel examined various site options for the future NNS to ensure that proper consideration to different scenarios were examined. The Transition Panel recommends locating the NNS at a greenfield site within the NIST Gaithersburg campus for the most effective transition, minimizing disruption to users and ensuring a smooth evolution of the NNS workforce while maintaining essential strong research and user-support environments.

Table 1: Comparison of three independent considerations: (I) Greenfield construction offsite elsewhere in USA, (II) Onsite at Gaithersburg adjacent and sharing current facility, and (III) Greenfield construction onsite at Gaithersburg. (✔) Represents a desirable/acceptable outcome, (!?) represents an unknown outcome for a specific outcome at the present time and, (✖) represents an outcome in which a consideration would be less than desirable/unsatisfactory.

Consideration	Greenfield construction offsite elsewhere in USA	Onsite at Gaithersburg adjacent and sharing current facility	Greenfield construction onsite at Gaithersburg
Reliability/availability of neutrons	✔	✖	✔
Expert instrument scientists and user support	✖	✔	✔
World Leading/Class Instrument	✖	✖	✔
Access to supporting research infrastructure	✖	✔	✔
Easily accessible and access to amenities	!?	✔	✔
Knowledge Transfer	✖	✔	✔
Use of existing and new infrastructure	✖	✔	✔
Use of legacy and new workflows	✔	✖	✔

12.11. References

[1] CINS membership survey – (Aug 2020) Results from the 2020 CINS membership survey. http://cins.ca/wp/wp-content/uploads/2020/12/cins-cni-survey-2020-report.pdf

[2] Danish inspired approach: Daniel Banks and Thad A. Harroun. 2019. Seventy years of scientific impact using neutron beams at the Chalk River Laboratories. FACETS. 4(1): 507-530. https://doi.org/10.1139/facets-2019-0003

Appendix A

Charge to Breakout Groups

Science-based breakout groups

1) Scientific and technical drivers for future neutron-based research. Include the expected impact of neutron measurements on science and technology and their ability to address emerging national priorities.
2) The ability of the current plans for the reactor and cold source(s) to provide industrial, academic, and government researchers with the necessary tools and infrastructure to address the identified national priorities - what changes would you like to see?
3) The characteristics of the instrumentation and facilities (including *e.g.* sample environments) needed to address the identified national priorities. Identify any technological and instrument developments that are required in the early stages of construction to effectively address national scientific and technological priorities.

Reactor breakout group

1) The ability of the current plans for the reactor and cold source(s) to provide industrial, academic, and government researchers with the necessary tools and infrastructure to address national priorities - what changes would you like to see?

Accompanying Facilities breakout group

1) The characteristics of the facilities (including labs, sample environments, IT, shops *etc*.) required to provide industrial, academic, and government researchers with the necessary tools and infrastructure to impact science and technology.
2) Identify any technological and instrument developments required in the early stages of the project to address to effectively address emerging national priorities.

Transition breakout group

1) Describe the considerations and steps required to minimize disruptions to the user community during the transition from the current facility to a future one.

Appendix B: Workshop Agenda

PROGRAM	WEDNESDAY OCT 18	THURSDAY OCT 19	FRIDAY OCT 20
08:00-09:00	**BREAKFAST** ***(Invited Attendees Only)***	**BREAKFAST** ***(Invited Attendees Only)***	**BREAKFAST** ***(Invited Attendees Only)***
09:00-09:15	**Welcoming Remarks**	**Preliminary Panel Presentations**	**Final Panel Presentations**
09:15-10:00	**Plenary I:** “Neutrons for the Nation” *Norm Wagner (UDel)*		
10:00-10:30	**** COFFEE BREAK ****	**** COFFEE BREAK ****	**** COFFEE BREAK****
10:30-11:00	**Plenary II:** “Economic Impact of Neutrons” *Amanda Walsh (RTI)*	**Preliminary Panel Presentations**	**Final Panel Presentations**
11:00-11:30	**Plenary III:** “Pre-Conceptual Design of New NIST Reactor’’ *Dagistan Sahin (NIST)*		
11:30-12:00	**Charge to Workshop Panels and Attendees** *Dan Neumann (NIST)*		
12:00-13:00	**LUNCH** ***(Invited Attendees Only)***	**LUNCH** ***(Invited Attendees Only)***	**END OF WORKSHOP**
13:00-15:30	**Breakout Sessions**	**Breakout Sessions**	
15:30-16:00	**** COFFEE BREAK ****	**** COFFEE BREAK ****	
16:00-18:00	**Breakout Sessions**	**Breakout Sessions**	
18:30	**DINNER** ***(Invited Attendees Only)***	**DINNER** ***(Invited Attendees Only)***	

Appendix C

A New Neutron Source for NIST and the Nation

The mission of the NCNR is to "Assure the availability of neutron measurement capabilities to meet the needs of U.S. researchers from industry, academia, and other government agencies.". The NBSR reactor at NIST first went critical in 1967. In the 55+ years since the facility has undergone multiple source, facility, and instrument upgrades to remain at the forefront of neutron research. In 1985 the NBSR was relicensed to double power (from 10 MW to 20 MW). NIST broke ground on a major cold neutron research facility in 1987 which led to a rapidly increasing demand from the research community as state-of-the-art cold neutron instruments came online throughout the 1990s. The performance also improved significantly from upgrades to the cold neutron source (CNS) in 1995 and 2002.

In 2011, the cold neutron experimental area was nearly doubled, allowing the installation of five new beamlines serving seven additional instruments, and a small liquid hydrogen (LH_2) CNS was dedicated to the MACS instrument. Each improvement led systematically to an increased demand beyond available capacity from the scientific community. Since 1985, the number of participants in neutron research at the NCNR soared from a few hundred to nearly three thousand, leading to nearly 350 publications each year. This trend is expected to continue as NIST is currently preparing for the installation of a liquid deuterium (LD_2) CNS which will provide significant gains in the cold neutron spectrum below 5 meV and more than compensate for eventual conversion to low enrichment uranium (LEU). Concurrently, the three oldest cold neutron beamlines at the facility will be renewed and upgraded.

This impressive growth has occurred because neutron measurements play a key role in the discovery and development of new materials, advancing technologies that promise to improve the quality of life for all Americans. These areas include biopharmaceuticals, drug delivery systems, personal care products, advanced polymers, energy conversion and storage technologies, chemical production, and separation, advanced data storage systems, quantum information technologies, dissipation-free electronics, and advanced engineering materials such as those produced through additive manufacturing. In the era of big data, AI, and combinatorial materials synthesis, neutron scattering is a leading tool for guiding the design, discovery, and characterization of new materials. It is therefore not surprising that despite continual performance upgrades, the requested-to-available neutron beam time has increased to nearly 3.

Overarchingly, the aging reactor requires longer outages and larger reactor maintenance expenditures to maintain safe and reliable operations. Some reactor components are not easily replaceable or serviceable, or they depend on obsolete technology.

Therefore, the central question of how NIST can best provide a source of neutrons into the future must be addressed. A 2018 assessment of the NCNR by the National Academies of Sciences, Engineering, and Medicine [1] recognized that

> "*Loss of this facility would have a strongly negative impact on neutron science within the United States and the scientific disciplines that the NCNR serves*."

Furthermore,

> "*NCNR should commission a detailed assessment of the current facility and begin the conceptual design of a new reactor*." The American Physical Society in their 2018 report [2] entitled "*Neutrons for the Nation*" recommended:
>
> "*The United States should initiate an effort to competitively design and build a new generation of LEU-fueled* [*low-enriched uranium*] *high-performance research reactors that would satisfy all needs presently met by current HEU-fueled [high-enriched uranium*] *U.S. high-performance research reactors and provide new capabilities*."

Other recent reports that highlight the important contributions of neutron scattering and imaging techniques to a broad range of scientific disciplines and technology have been published by the U.S. Department of Energy (2020) [3] and the Swiss Academies (2021) [4].

Prior to these recommendations, a NIST study on future options for neutrons at NIST was already underway. This study concluded that keeping the existing reactor operational is undesirable not only because of the long-term uncertainty in the condition of the reactor vessel and thermal shield but more importantly because it could not allow any further expansion of the neutron beams. A rehabilitated reactor would address the issue of aging management and may expand user facilities. However, the many unknowns involved with removing and replacing the reactor vessel and thermal shield, and the long downtime required make this option less desirable. The overall conclusion was that a replacement reactor is the best option to ensure a reliable neutron source at NIST over the long term.

A new reactor located at NIST can be constructed while the current one continues to operate and would take advantage of the infrastructure and personnel in place at the NCNR with a proven track record of running a world-class and cost-effective neutron science facility.
In anticipation of the need to plan for its replacement, NIST assembled a NIST/NCNR - Brookhaven National Laboratory (BNL) collaborative group to define top-level functions and requirements and to develop a pre-conceptual design of a replacement reactor and neutron scattering facilities.

Foremost, the reactor operation must be safe, reliable, and efficient with a high availability and built on a time scale that minimizes disruption to US neutron research. The current global nuclear policy also mandates the use of "low-enriched" uranium as the reactor fuel. The design should promote straightforward maintenance, accessibility to serviceable components, and upgradability. A ground-up reconfiguration incorporating lessons learned from the design and facility layout of the NCNR and other installations around the world allow significant performance upgrades over the present facility. Importantly, these gains can be realized with a reactor design including established safety analysis models and construction solutions which are key to an efficient regulatory review, licensing, and construction process.

An appealing option that satisfies these combined conditions is a forced-cooled reactor core in a pool with a heavy water reflector surrounding a compact core for optimum neutron delivery. The emphasis is on increasing both facility capacity and performance through optimized beam extraction, neutron optics, state-of-the-art instrumentation, and signal-to-noise enhancements which have the potential to produce order-of-magnitude gains. Note that increasing the reactor power is less cost-effective, complicates the licensing process, and increases the scale and challenges associated with core heat extraction while only generating gains that scale linearly. As such, the present concept (dubbed the NIST Neutron Source, or NNS) (Fig.1) would operate at 20 MW with a compact, light water-cooled LEU fuel array surrounded by a heavy water-reflector tank containing two (vertically-introduced) LD_2 CNSs and beam tube penetrations. Tangential beam arrangements mitigate fast neutron and gamma contamination and twin CNSs in vertical thimbles greatly facilitate serviceability and upgradability over the present horizontal thimble arrangement of the current reactor (Fig. 2).

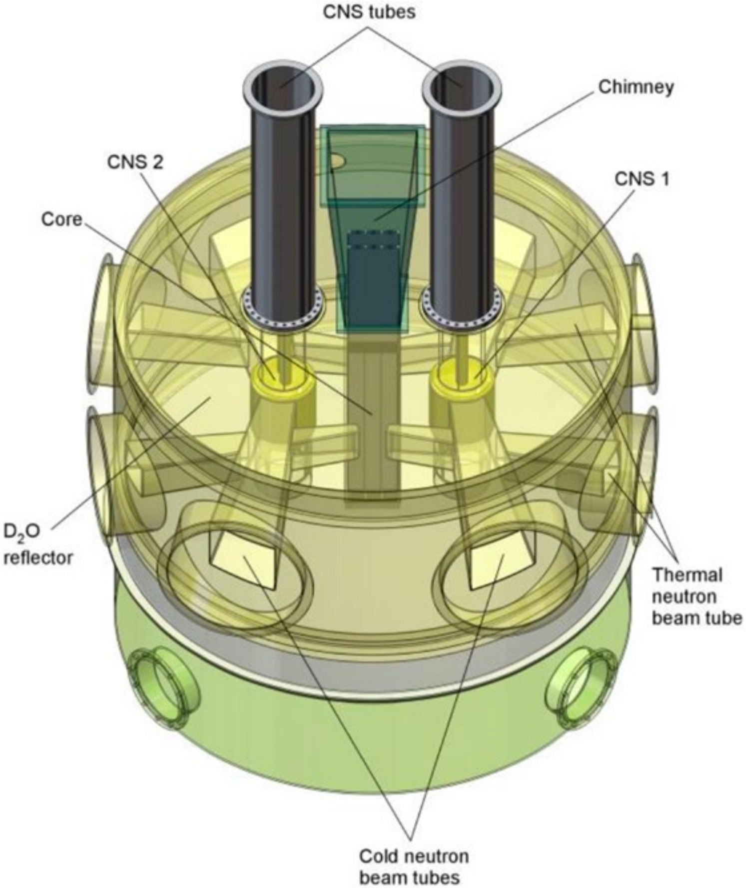

Figure 1. Isometric view of the present concepts of the NNS core (with two LD2 CNSs) and the reactor building.

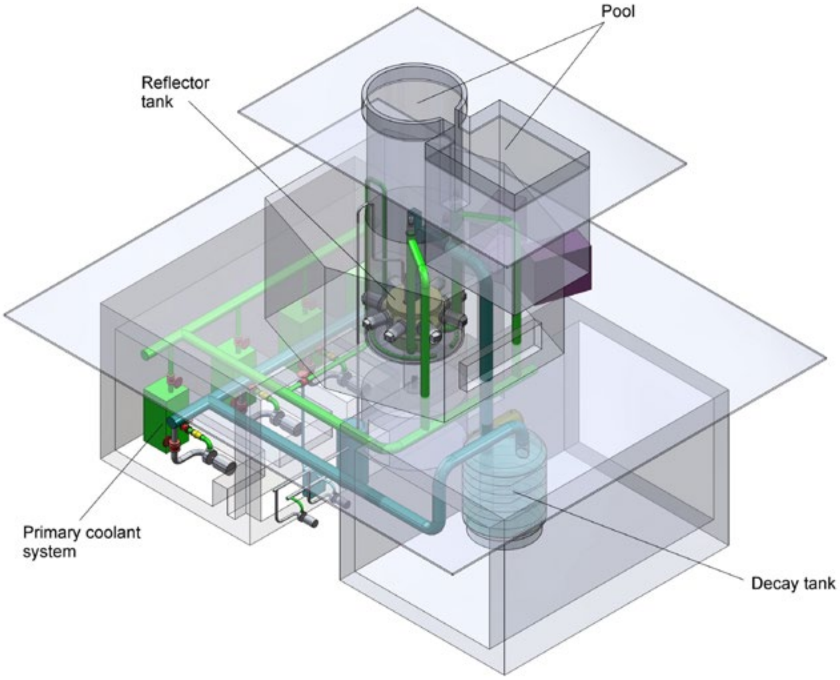

Figure 2. The present concept of the reactor building.

An initial facility layout concept extracting cold neutron beams in opposing directions from each CNS, with thermal beams in an approximately perpendicular direction is illustrated in Figure 3. From initial studies up to perhaps 50 cold and thermal neutron instruments could be accommodated with high-performance, low-background cold neutron guides, with additional end-positions provided by benders on side locations at multiple levels from tall guides, together with monochromatic beam positions.

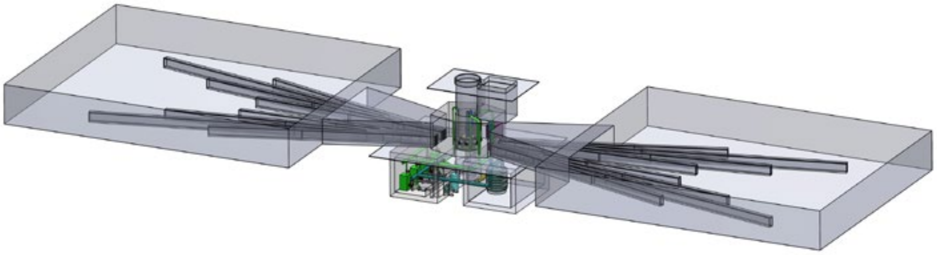

Figure 3. Conceptual facility layout with opposing cold neutron guide halls shown with 16 cold neutron guides viewing two CNSs. The reactor block is at the center. Thermal beams (not shown) emerge approximately perpendicular to the cold neutron beams.

The under-moderated compact core eliminates the compromises of the sparse NBSR fuel assembly array allowing the NNS CNS to be placed in, and thermal beams extracted from, regions much closer to the thermal flux peak in the D_2O reflector (peak unperturbed$_1$ thermal flux of 5.3×10^{14} $cm^{-2}s^{-1}$.) that are unencumbered by fuel assemblies. (Unperturbed flux is assessed with the bare core and D_2O reflector without the beam penetrations and cold neutron sources. Conversely perturbed flux is assessed with these features introduced.) This is illustrated in Figure 4. Despite comparable simulated perturbed thermal flux peaks of about 3.55×10^{14} $cm^{-2}s^{-1}$ (NBSR) and 3.63×10^{14} $cm^{-2}s^{-1}$ (NNS), simulations based on an LD_2 CNS design predict a cold neutron (< 5 meV) brightness 3.5 times greater for the NNS than currently available at the NCNR. Factoring in solid angle and illumination improvements of the cold neutron guide array yields an order of magnitude increase in transmittable cold neutron current is achievable at the same reactor power.

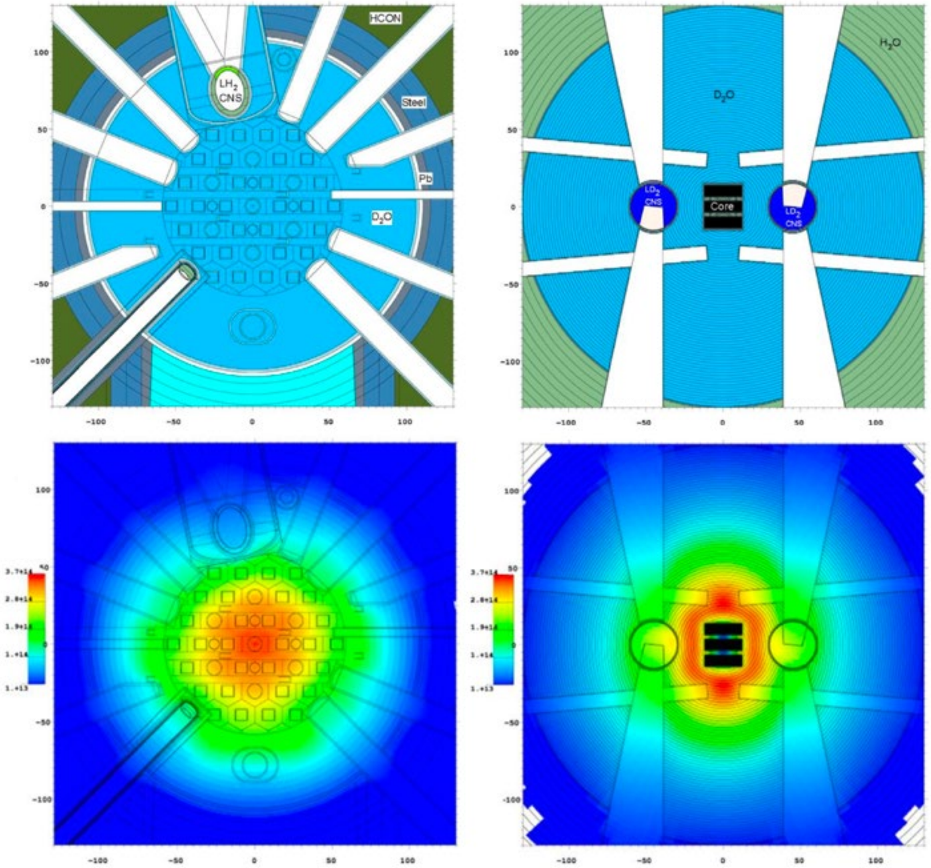

Figure 4. Top row: MCNP models for the current (left) and NNS (right) shown on the same spatial scales. Bottom row: Thermal neutron flux (< 300 meV) shown on the same spatial scales and normalized to the same intensity scale for ease of comparison. The horizontal and vertical scales are in cm.

Additional brightness gains are possible from moderate increases in the CNS vessel diameter and further intensity and signal-to-noise gains are achievable at the instruments with instrument-optimized neutron optics unlocking areas of research previously restricted by time and data quality constraints. Radiation heat load simulations confirm that the CNSs can be placed as close to the fuel as shown.

At initial startup (commissioning), the NNS would deliver measurement capabilities comparable to those of the existing NBSR neutron source by operating, at a minimum, one cold source delivering cold neutrons to one of the guide halls. Once both guide halls are fully operational, the facility would provide new measurement opportunities and substantially increase the neutron measurement capacity for the nation.

References

[1] *An Assessment of the Center for Neutron Research at the National Institute of Standards and Technology: Fiscal Year 2018*, The National Academies Press, Washington, DC, 2018. https://nap.nationalacademies.org/catalog/25282/an-assessment-of-the-center-for-neutron-research-at-the-national-institute-of-standards-and-technology

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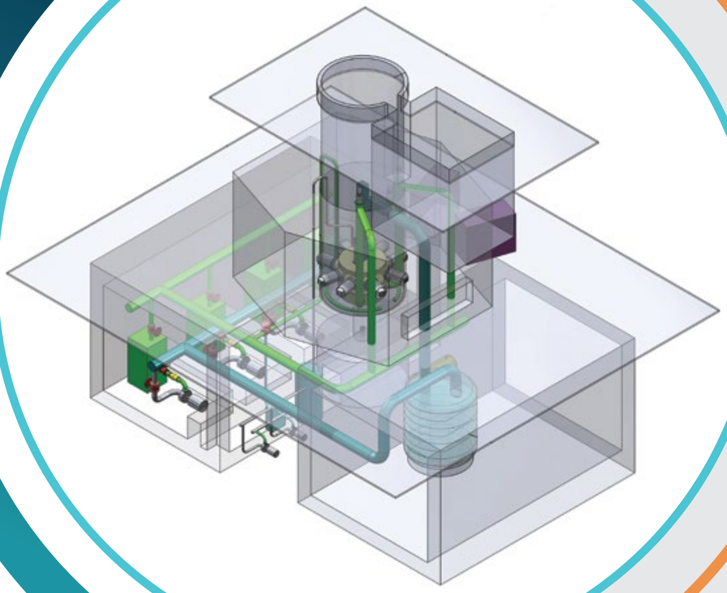

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