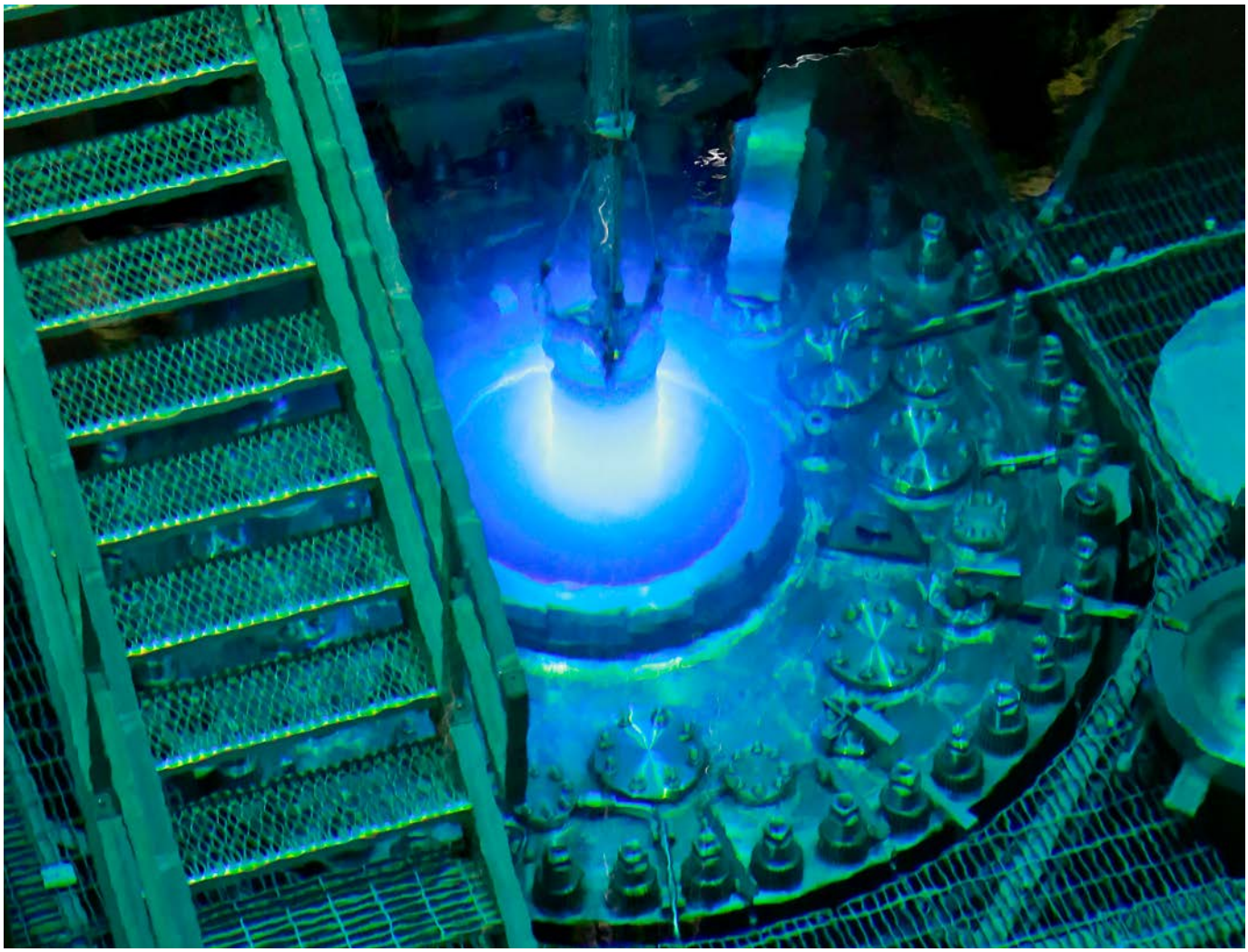
The Scientific Justification for a

U.S. Domestic High-Performance Reactor-Based Research Facility



REPORT OF THE BASIC ENERGY SCIENCES ADVISORY COMMITTEE

U.S. DEPARTMENT OF ENERGY | Office of Science

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The Scientific Justification for a

U.S. Domestic High-Performance Reactor-Based Research Facility

REPORT OF THE BASIC ENERGY SCIENCES ADVISORY COMMITTEE
U.S. Department of Energy/Office of Science/July 2020

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Prepared by the BESAC Subcommittee to Assess the Scientific Justification for a U.S. Domestic High-Performance Reactor-Based Research Facility

U.S. DEPARTMENT OF ENERGY | Office of Science

Department of Energy
Office of Science
Washington, DC 20585

March 3, 2019

Dr. Marc Kastner
Science Philanthropy Alliance
480 S. California Avenue #304
Palo Alto, California 94306

Dear Dr. Kastner:

The U.S. Department of Energy (DOE) has maintained long-term stewardship of neutron capabilities for the Nation. The combination of the Spallation Neutron Source (SNS) and the High Flux Isotope Reactor (HFIR), under the auspices of Basic Energy Sciences (BES) in the Office of Science, has provided the U.S. scientific community with leading neutron capabilities in support of DOE's missions in science, energy, environment, and national security.

To maintain international leadership in neutron science, the 2016 Basic Energy Sciences Advisory Committee (BESAC) Facility Prioritization study acknowledged the critical scientific importance and mission relevance of expanding the SNS with the Proton Power Upgrade (PPU) and the addition of the Second Target Station (STS). Following the report recommendation, BES has worked with Oak Ridge National Laboratory to address the issues identified by the prioritization report, including improvements of the target design, leading to achievement of sustained SNS operation at its full design power of 1.4 MW in 2018.

With the planning process for both the PPU and STS projects under way in 2019, I am writing to seek the input of BESAC on the long-term strategy concerning HFIR, which complements SNS and is among the highest-flux reactor-based sources in the world. With HFIR entering its 6th decade, its long-term future requires careful thought and planning, especially in the context of the U.S. domestic high-performance neutron research facilities.

This charge is also in part informed by the 2018 "Neutrons for the Nation" report, commissioned by the American Physical Society's Panel on Public Affairs, which focuses on the competing goals of reducing nuclear proliferation risk while maintaining intense controlled sources of neutrons for vital scientific and industrial work. The report highlighted the continued need for the U.S. to support its diversity of neutron R&D capabilities, as well as to initiate planning for a new generation of high-performance research reactors.

I am asking BESAC to form a subcommittee to assess the **scientific justification** for a U.S. domestic high-performance reactor-based research facility, taking into account current international plans and existing domestic facility infrastructure. The following questions serve as the framework for the study:

- What is the merit and significance of the science that could be addressed by a high-performance, steady-state reactor, and what is its importance in the overall context of research in materials sciences and related disciplines?
- What are the capabilities of other domestic and international facilities, existing and planned, to address the science opportunities afforded by such a domestic research reactor?
- What are the benefits to other fields of science and technology and to industry of establishing such a capability in the U.S.? In particular, consider applications such as isotope production, materials irradiation, neutron imaging, dark matter research, and neutron activation for trace element analysis.
- What are the strengths and limitations of a steady-state research reactor compared to a pulsed spallation neutron source for science, engineering, and technology? What functions currently performed by research reactors can be assumed by spallation neutron sources?
- Are there feasible upgrade paths for HFIR to provide world-leading capabilities in serving the Office of Science missions well into the future? What can we learn from the experience at the Institut Laue-Langevin?
- Can Low Enriched Uranium (LEU) and High Assay LEU (HALEU) fuels (defined as <20% enriched U-235) replace Highly Enriched Uranium fuels in research reactors while preserving the needed characteristics of neutrons produced by steady-state reactors? What R&D would be needed to support LEU and HALEU fuels development?

In assembling a subcommittee, please consider members from other Office of Science and DOE Federal Advisory Committees, including the Nuclear Science Advisory Committee, the Fusion Energy Science Advisory Committee, the Defense Programs Advisory Committee, and the Nuclear Energy Advisory Committee. We look forward to the results of your review and any recommendations that result from this study.

I would appreciate receiving a written report by July 31, 2020.

Sincerely,

J. Stephen Binkley
Deputy Director for Science Programs
Office of Science

Subcommittee Membership List

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Sue Clark, BESAC/PNNL
Pengcheng Dai, Rice University
Thomas Epps, BESAC/University of Delaware
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October 2020 revision corrected an error on page 1 of the Executive Summary.

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HFIR Refueling: July 2015

The High Flux Isotope Reactor at Oak Ridge National Laboratory is the highest flux reactor-based source of neutrons for research in the United States, and it provides one of the highest steady-state neutron fluxes of any research reactor in the world. Operating at 85 MW, an average fuel cycle for the HFIR generally runs for approximately 26 days—depending on the experiment loading for that cycle—followed by a refueling and maintenance outage for various scheduled calibrations, modifications, repairs, and inspections.

The reactor underwent routine refueling in July 2015, as seen in these photos. While submersed, the spent fuel emits a luminescent blue glow due to Cherenkov radiation, in which shedding electrons move through the water faster than the speed of light in water. Once removed from the reactor, spent fuel is then relocated into an adjacent holding pool for interim storage.

This image shows the removal of a HFIR fuel element from the reactor vessel during defueling operations.

Image credit: Jason Richards/ORNL

Executive Summary

Why neutrons are important. Neutrons are a research tool that scientists and industrial researchers use to probe the properties of materials. As their name suggests, they are neutral (carry no electric charge) and hence do not interact with the electric fields of atoms. Beams of neutrons can thus penetrate deeply into a material without damaging it, and they "scatter" or bounce off the atoms within a material in ways that can reveal its structure and dynamics. Neutrons are also uniquely suited to exploring the magnetic properties of materials. Indeed, whenever an important new material is discovered, its basic structural and magnetic properties will invariably be explored using neutron scattering techniques. In addition, neutron bombardment creates the radioactive isotopes used for medical treatments of cancers and other diseases as well as in a wide range of critical industrial and national security activities.

Where they come from. Neutrons are generated within a nuclear reactor, such as the High Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory and the reactor at the NIST Center for Neutron Research (NCNR) at the National Institute of Standards and Technology, by the process of nuclear fission. Neutrons can also be generated by colliding a beam of high-energy protons with a metallic target to shake loose a pulse of neutrons, such as at the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory. For some types of research, the reactor-based steady flux of neutrons and the spallation-based pulses of neutrons are interchangeable; more often they are complementary, each technique having an advantage in certain areas of research.

The HFIR is a unique resource. It is the world's most intense source of neutrons for research that is widely available to scientists, as well as the only source capable of generating certain critical radioactive isotopes; the only comparable source for isotope production, in Russia, is not available to western scientists. Despite its importance, the HFIR faces a number of current and prospective problems that threaten its continued availability, and which are the reason for this report. These problems include:

- The reactor's age—the HFIR was put into service 55 years ago, and steady exposure of the reactor's steel pressure vessel to neutron bombardment is causing embrittlement of the steel, so that the pressure vessel will have to be replaced (or the reactor shut down) within two to three decades.
- In the short term, the U.S. and other nations are committed by agreements, policy, and precedent to stop using highly-enriched uranium (HEU) fuel for research reactors—inclu-ding the HFIR—as an international security measure against nuclear weapons proliferation. Conversion to low-enriched uranium (LEU) will involve significant changes to the HFIR and, this report argues, should be combined with replace-ment of the pressure vessel.
- Thirdly, demand by both academic and industrial researchers for access to the HFIR and other major U.S. neutron sources (SNS and NCNR) is already as much as three times higher than current facilities can accommodate, meaning that critical research is either not done or delayed for long lengths of time. In addition, national security demand for certain radioactive isotopes produced by the HFIR is more than the reactor can currently supply. During a shutdown of the HFIR to replace the pressure vessel and convert to LEU fuel, it would be possible to add more beamlines that extract neutrons from the reactor and more experiment stations along those beamlines together with enhancement of the instrumentation, plus more isotope production capacity, enabling a significant expansion of neutron-based research. Because of the importance of high-flux neutron research both for fundamental science and for industrial applications, this report argues for such expansion.

The Scientific Case

This report describes a wide variety of important scientific and industrial research for which the intense, steady flux of neutrons generated by a research reactor such as the HFIR is either advantageous or essential.

Neutron Scattering as an Essential Tool for Basic Materials Research

Ever since the discovery of neutrons in the 1930's, neutron scattering has been extremely useful as a means to study the atomic and magnetic structure of materials and their behavior, resulting in a Nobel Prize in 1994

and a steadily growing array of applications. For some areas of research, such as magnetism, neutron scattering has become virtually the only way to investigate many phenomena. More broadly, reactor-based neutron sources such as the HFIR have certain advantages, including more rapid and efficient collection of data.

In solid state materials, neutrons are particularly sensitive to two key constituents of battery materials, hydrogen and lithium, making neutrons an indispensable probe of the nanoscale structure and behavior of advanced batteries. Neutron beams are equally useful in the study of a wide array of other materials, such as advanced and more efficient photovoltaic materials for solar cells and thermoelectric materials that can convert heat into electricity, which may become important for grid-scale energy storage systems. Neutrons are also essential in determining the properties of high temperature superconducting materials which, although not yet fully understood, clearly involve magnetism; and are playing a critical role in the study of novel systems that may have application to quantum information science.

In biology and soft materials such as polymers and thin films, which together constitute a significant fraction of neutron beam research, neutron scattering plays a role that cannot be replicated by any other type of probe. This arises from the high percentage of hydrogen atoms in organic materials, which can be easily mapped by substituting deuterium for hydrogen and contrasting the resulting scattering patterns. Neutron scattering enables the study of molecular structures such as proteins and the organization of biological molecules in organisms. Neutrons have also found application in medicine, through clarifying the mechanisms of disease and the structures of complex biopharmaceuticals and aiding the development of novel nanoscale vehicles for drug delivery and gene therapy. An important future area of research with neutron beams is the biotic/abiotic interface—such as the physical interface between semiconductor technology and biological tissue—where the ability of neutrons to probe both hard and soft condensed matter is likely to be important for designing biosensors and self-assembling biomolecules into useful materials.

Polarized neutron beams (which have a uniquely defined spin state) offer the most complete characterization of both atomic and spin structure. That is important for fundamental studies of quantum phases of matter, including materials that exhibit quantum entanglement and that are likely to be essential for practical quantum computing devices. Polarized neutrons can also resolve complex spin structures that are important for understanding magnetism in single crystals and nanostructured materials, areas that may lead to future technological breakthroughs.

Industrial Applications of Neutron Scattering

Neutrons interact with the atomic nuclei in a material rather than its electrons and so easily penetrate dense materials and complex systems. That enables direct observation of an operating internal combustion engine or water flow in a fuel cell. Similarly, the utility of neutrons for probing organic or soft polymer materials has led to their use in optimizing paints and coatings, fabric softeners and adhesives. The pharmaceutical industry has used neutron scattering to understand the effect of drug preparation on stability and shelf life and to optimize drug processing and formulation. The oil and gas industries employ neutron scattering to understand the composition and molecular structures of non-traditional petroleum sources, leading to enhanced oil recovery, and to determine the properties of gas-bearing shale rock formations. Neutron studies have provided useful insights for high-performance turbine blades for the transportation industry, have been used to measure stress in welds in the auto industry, and have proved essential for developing new reactor fuels for the nuclear power industry. One measure of commercial interest is the development of an industrial collaboration to provide technology and expertise in neutron-based measurements to member companies for pre-competitive research at NCNR and to the stationing of industrial staff at that facility for extended periods to gain expertise in neutron-based research techniques. Pre-competitive industrial research proposals for the HFIR are considered on the same basis as university-based proposals; proprietary industrial research is allowed on a full-cost recovery basis.

Fundamental Physics at Reactor and Spallation Neutron Sources

Reactors and spallation sources are unique sources of neutrons and neutrinos (neutral subatomic particles with a mass close to zero that rarely react with normal matter). Both play a key role in fundamental science, enabling scientists to study the constituents of atomic nuclei, to search for new forms of matter, and to

explore the symmetries that govern fundamental laws of physics and the evolution of the universe.

The fission process in reactors such as the HFIR generates a large flux of electron antineutrinos along with neutrons. The neutrons are guided out of the reactor core in beamlines to experimental stations, but the antineutrinos are emitted in all directions, making it desirable to locate experiments as close to the reactor core as possible. The HFIR with its compact but powerful core and regular cycle of operations is an ideal source of electron antineutrinos and has enabled a broad program of studies with those particles as well as with neutrons. Spallation sources such as SNS generate a variety of neutrino types in beamed pulses. Together, these complementary characteristics enable precision experiments such as measurement of neutron lifetimes, which in turn is critical for understanding how the basic elements of matter are formed. Neutrinos, because they interact so weakly, stream freely through the cosmos and have played a key role in the evolution of the universe, yet much about them, including their tiny mass, is still a mystery. Nonetheless, progress is being made: a SNS experiment in 2017, for example, confirmed the characteristics of neutrino-nucleus scattering first predicted theoretically in 1947. A recent HFIR experiment to measure the neutrino spectrum emitted from the reactor core helps understand the properties of neutrinos, as well as providing data for improved modeling of reactor operation. Understanding the properties of neutrons and neutrinos holds the key to some of the most fundamental questions in physics, such as why the universe has matter, and its observed asymmetry in the amounts of matter and antimatter.

A potential upgrade to HFIR provides an opportunity to establish an experimental laboratory close to the reactor dedicated to fundamental physics—in effect moving from opportunistic studies to a strategic research program.

Isotope Production and Materials Irradiation

Since the advent of the nuclear era, the use of radioactive isotopes has brought tremendous benefits to society in a multitude of ways, from expanding our knowledge of the world around us to improving the lives of millions of people through medical diagnoses and treatment. No fewer than 16 Nobel prizes have been awarded in the fields of nuclear chemistry and applied radiochemistry. The use of radioactive isotopes has allowed researchers to answer a myriad of questions about wide-ranging subjects from plant metabolism and ocean currents to the behaviors of ancient peoples and indigenous trade routes. Radiation from such isotopes has also brought immeasurable benefits to industry, allowing the analysis of material densities, inspection of critical systems, and product sterilization. Radioactive tracers have been integral in oil and gas exploration, monitoring fluid flows, and detecting leaks in remote and inaccessible networks. The vast majority of radioactive isotopes used in medicine, industry, and research are produced by irradiating materials with neutrons in nuclear reactors. And because of the HFIR's intense neutron output, it plays a unique role in producing many critical short-lived radioactive isotopes.

In healthcare, for example, radioactivity and radioisotopes have been instrumental in diagnosing and treating disease, improving the lives of millions of people. Ever since the first radioisotope was approved by the U.S. FDA in 1951 for treatment of thyroid cancer, researchers and clinicians have employed numerous additional radioisotopes for both diagnostic and therapeutic applications. While HFIR makes numerous medical isotopes, its high neutron flux is required to produce the first alpha therapeutic approved by the U.S. FDA. Ra-223 is a targeted therapy for symptomatic bone metastases in prostate cancer patients that improves the overall survival with a 30% reduction in mortality.

Californium-252 is used by industry as a small, robust, self-powered, economical source of neutrons for a wide range of applications including energy, homeland security, and agriculture. The isotope is used by the nuclear energy industry to determine the fissile content of nuclear waste; it also provides the source of neutrons needed to start newly constructed nuclear reactors including those on nuclear powered submarines. The mining and minerals industry uses it to measure the amount of sulfur in coal, the ash and stone content of cement, and for oil well logging. Nickel-63 enables gas chromatography detector systems up to 1,000 times more sensitive than those using other types of detectors. Applications of these systems include food and pesticide analysis, forensic toxicology, controlled substances identification and environmental monitoring. In addition, Nickel-63 provides the electron source in ion mobility spectrometry systems that are extensively deployed by the Department of Home-

land Security and the U.S. military for detecting trace amounts of explosives, narcotics, chemical warfare agents and industrial chemicals. Both of these critical isotopes require a high neutron flux for their production and are only available from HFIR and the SM-3 reactor in Russia; the demand for both greatly exceeds the available capacity of these two high-flux reactors.

The heaviest elements on the periodic table—especially those with atomic number 90 through 103—are the ones least well understood. Fundamental research to understand their physical and chemical properties involves very small quantities of trans-plutonium isotopes, which can only be produced by irradiation in HFIR. These isotopes have short half-lives, however, and must be continuously produced. In addition, over the past few years, heavy elements produced at HFIR were used in international collaborations to discover elements 114, 115, 117, and 118. In addition, the HFIR is used to mimic the radiation conditions expected in advanced nuclear power reactors or fusion reactors and thus test structural materials and fuels for such reactors.

Conversion of the HFIR to Low Enriched Uranium Fuel

Since 1978, the U.S. government has worked with civilian research reactors and medical isotope production facilities domestically and internationally to minimize, and, when possible, eliminate weapons-usable nuclear material around the world. The effort has successfully converted 71 reactors from Highly Enriched Uranium (HEU) fuel to Low enriched Uranium (LEU) fuel; 31 other reactors have been shut down.

A concern for conversion of the HFIR was the need for an increased volume of LEU fuel in the reactor to preserve its high flux capability. Ongoing research has identified and tested a fuel based on a uranium-silicon compound that, in combination with changes in the placement of the fuel in the reactor and other adjustments, would preserve the capability of the HFIR. Moreover, sophisticated models of the anticipated neutron fluxes and heat removal have provided strong assurance that the reactor can safely operate at the higher local power densities of the new design. Testing and qualification of the new fuel design is expected to start soon.

This report recommends commissioning a joint feasibility study to explore whether replacement of the HFIR pressure vessel simultaneously with LEU conversion in a coordinated manner could simplify LEU fuel design through modest changes to the vessel and beryllium reflector design, thus reducing long term fuel costs for the refurbished reactor.

The High Flux Isotope Reactor: Status and Plans

Oak Ridge National Laboratory, which operates the HFIR, has developed a preliminary plan to replace the HFIR reactor vessel, upgrade some reactor systems, and improve the neutron source in order to extend the operating life of the facility well beyond 2040. A potential LEU replacement fuel, for which testing is expected to begin soon, could be incorporated into an upgraded or enhanced HFIR reactor core design, potentially allowing a higher reactor power level. These activities could also support the installation of an additional neutron beam guide hall with a new suite of instruments, as well as additional isotope production and irradiation capacity, to capitalize on the enhanced HFIR, which would in turn enable high quality neutron science well into the 21st century. This would go a long way in enabling the United States to recover its world leadership position in this critical area of science and technology.

In parallel, however, this report also recommends that a "scoping study" be undertaken for a new high-flux research reactor optimized for current needs but also incorporating flexibility of configuration to allow for future, unanticipated needs in neutron research and isotope production. Since such a reactor is likely to take several decades to design, construct, and commission, beginning now will ensure the continuing availability of such a critical resource in the U.S.

Recommendations

The subcommittee considered three options:

- Operate HFIR "as is." There are unacceptable issues associated with this option:
  > Consistent with U.S. policy, HFIR has committed to convert to LEU fuel when available, projected to be in 2035. The conversion program has committed to an LEU design and power upgrade that will preserve the capabilities of HEU operation at 85 MW. The conversion will require an extensive shutdown at the time of LEU fuel deployment. Assuming no unforeseen occurrences, the pressure vessel of HFIR is projected to reach end of life about 2060. It should be noted that, given the age and history of HFIR, it is possible that the end of life of the pressure vessel could occur sooner. At best, HFIR will need another very significant shutdown within about 20 years of conversion.

  > While investments in instrumentation in the absence of modifications to the pressure vessel design may add some capability and capacity to HFIR, they will fall far short of meeting the needs of the neutron science community.

RECOMMENDATION: This is the least desirable option. Investment in fuel conversion or instrumentation without replacing the pressure vessel leaves an unacceptable risk of a short life of the reactor.

- Replace the pressure vessel of HFIR, which is the lifetime-limiting component of the reactor. If possible, coordinate this replacement with the conversion of the reactor to LEU fuel so that a single shutdown would accomplish both objectives. Redesign of the pressure vessel could enable:
  > Enhanced capabilities for both in-reactor (isotope production, materials testing, etc.) and beamline work, which would provide an increase in both capability and capacity. Specifically, the new pressure vessel should support larger beam tubes and an improved cold source to enhance neutron scattering capabilities together with improved access for isotope production and materials irradiation. A significant investment should be made in advanced instrumentation for neutron scattering in parallel with infrastructure changes and possible changes in the reactor configuration to reduce dramatically the background for neutron scattering measurements.

  > Modification of the fuel assembly to make it more manufacturable and hence less expensive.

  > The combination of pressure-vessel replacement and conversion may allow a power increase that would restore the flux-trap intensity of the original 100 MW HEU operations and an increase in reflector irradiation site and cold-source capabilities.

RECOMMENDATION: Pursue this approach immediately with the goal that the fuel conversion and pressure vessel replacement be performed during the same shutdown. The significant risk of HFIR failure will be removed, and important capabilities will result.

- Perform a "scoping study" for a green field research reactor optimized to perform neutron studies and isotope production that are uniquely suited to a very high flux reactor such as HFIR. The reactor would be designed to operate on LEU fuel. Reactor and fuel assembly designs should be evaluated to simultaneously optimize reactor performance and fuel assembly manufacturability. Further, the design should, to the extent possible, be optimized for neutron needs as currently understood and for flexibility of configuration to enable future, currently unanticipated, applications.
  > A new research reactor is likely to take several decades from initial design through approval, construction, and commissioning. Beginning the process now will allow time to evaluate options and proceed with planning and approvals in time to ensure continuing availability of a multiply capable high flux research reactor in the U.S.

RECOMMENDATION: Pursue study of a new high-flux reactor in parallel with the shorter term replacement of the pressure vessel and conversion of HFIR to LEU fuel.

Introduction

High-performance reactor-based research facilities have been an essential part of the U.S. scientific and technological enterprise since the mid-1960s. These facilities contribute broadly to our national security, our fundamental and applied science knowledge base, our development of cutting-edge medical treatments, and our technological and industrial competitiveness. The flagship U.S. reactor facility is the High Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory (ORNL). This reactor is stewarded by the U.S. Department of Energy (DOE) under the auspices of Basic Energy of Sciences in the Office of Science.

Operation of HFIR began in 1965 so the facility is 55 years old. It was initially designed primarily for isotope production and materials testing but four beam tubes were included making possible neutron scattering experiments with thermal and cold neutrons. HFIR runs with highly enriched U-235 fuel (HEU) with an enrichment of about 90%. There are two significant issues connected with the continuing operation of HFIR in the current mode. First, there are serious national security concerns about nuclear proliferation associated with the use of HEU. Second, the HFIR pressure vessel has a finite lifetime because of radiation induced embrittlement. This means that the vessel must be replaced by the middle of this century, or sooner if the embrittlement were to accelerate. A third concern is the continuing deficit in facilities for neutron scattering in the United States compared with Western Europe. This shortfall will be partially mitigated by the construction of the second target station at the Spallation Neutron Source (SNS), but it is certain that the available facilities will still fall far short of the national need.

Two recent reports have focused on the HEU conundrum. The first is the 2016 congressionally mandated study by the National Academy of Sciences (NAS), "Reducing the Use of Highly Enriched Uranium in Civilian Research Reactors." This study recommended the conversion as soon as possible of existing U.S. high-performance research reactors to low enriched uranium (LEU) fuel operations as well as the enabling of a new generation of LEU research reactors. Here, LEU is defined as less than 20% U-235. This study was immediately followed by a second study completed in 2018, "Neutrons for the Nation: Discovery and Applications while Minimizing the Risk of Nuclear Proliferation" by the Panel of Public Affairs of the American Physical Society. This report emphasized the critical importance for the U.S. physics enterprise of world class neutron R&D capabilities and explicitly recommended initiating an effort to competitively design and build a new generation of LEU-fueled high-performance research reactors that meet current needs and provide new capabilities.

On March 3, 2019, J. Stephen Binkley, then Deputy Director for Science Programs, Office of Science, DOE, wrote to Dr. Marc Kastner, chair of the Basic Energy Sciences Advisory Committee (BESAC) seeking BESAC's input on the long term strategy for HFIR. Specifically, Dr. Binkley asked BESAC to form a subcommittee to assess the scientific justification for a U.S. high-performance reactor-based research facility (implicitly LEU) taking into account current international plans and existing domestic facility infrastructure. The charge to the committee included six explicit questions:

1. What is the merit and significance of the science that could be addressed by a high-performance, steady-state reactor, and what is its importance in the overall context of materials sciences and related disciplines?
2. What are the capabilities of other domestic and international facilities, existing and planned, to address the science opportunities afforded by such a domestic research reactor?
3. What are the benefits to other fields of science and technology and to industry of establishing such a capability in the U.S.? In particular, consider applications such as isotope production, materials irradiation, neutron imaging, dark matter research, and neutron activation for trace element analysis.
4. What are the strengths and limitations of a steady-state research reactor compared to a pulsed spallation neutron source for science, engineering, and technology? What functions currently performed by research reactors can be assumed by spallation neutron sources?
5. Are there feasible upgrade paths for HFIR to provide world-leading capabilities in serving the Office of Science missions well into the future? What can we learn from the experience at the Institut Laue-Langevin (ILL)?

6. Can Low Enriched Uranium (LEU) and High Assay LEU (HALEU) fuels (defined as <20 % enriched U-235) replace Highly Enriched Uranium fuels in research reactors while preserving the needed characteristics of neutrons produced by steady-state reactors? What R&D would be needed to support LEU and HALEU fuels development?

In response to this charge, BESAC formed a subcommittee with 19 members having expertise covering the complete range of areas impacted by high-performance research reactors. In addition, the chair of BESAC, Marc Kastner, participated in the deliberations of the committee. The formal title of the committee was: "BESAC Subcommittee on the Scientific Justification for a U.S. High-Performance Reactor-Based Research Facility" (HPRBRF).

The committee held a series of meetings exploring all of the issues and opportunities associated with an HPRBRF. The first meeting took place in Berkeley, California on August 19–20, 2019. The meeting laid the groundwork for the study. It included presentations by DOE senior officials giving their perspectives, by Oak Ridge neutron scientific administrators on HFIR and the SNS, by the chairs of the NAS and POPA HEU-LEU committees, by officials from NIST and ILL on their reactor facilities, and finally by European leaders on FRM-II. The second meeting was held on Nov. 14–15 in Washington, D.C. This workshop included a series of talks by outside experts on virtually all of the different important areas of science, technology, and industry where high flux nuclear reactor facilities make important contributions. The final afternoon of this meeting was spent touring and hearing presentations at the NCNR at NIST.

On January 7–8, 2020, the committee had a site visit to ORNL, touring the SNS and HFIR. In addition, there was a series of presentations by ORNL neutron leaders on their plans for the HFIR reactor vessel replacement and upgrade of the facility overall including the neutron scattering instrumentation. In late February, a subset of the committee visited the BR2 reactor in Belgium and the planned Jules Horowitz Reactor in France. A planned site visit to ILL and FRM-II by a second group of subcommittee members in early March was cancelled because of Covid-19.

The final meeting of the committee was held on April 24, 2020. The meeting was originally planned to be held in Washington D.C., but because of Covid-19 was held virtually via Zoom. In advance of this meeting, each of the committee members prepared comprehensive reports on the current and prospective impact of an HPRBRF on important scientific and/or technological issues in their respective areas of expertise. The topics ranged from quantum materials to biology to heavy element chemistry to industrial applications. The committee members made brief presentations on each of these subjects. The committee then finished by producing a set of recommendations for BESAC which appear subsequently in this report.

These individual reports appear in the next section: "The Scientific Case." The breadth and depth of the impact of nuclear reactor-based research is simply remarkable. The individual subjects include solid state physics and quantum materials, soft condensed matter, molecular biology, industrial applications, fundamental physics, isotope production, heavy element production, materials irradiation in general, and fusion materials irradiation in particular. In addition, there are sections on polarized neutron scattering techniques and a comparison of the relative roles of neutrons and synchrotron X-rays in probing condensed matter. There is a comprehensive discussion on the current state of progress on HEU-LEU conversion. These sections are all as comprehensive as possible. We intend this report to be a resource for DOE and for the research nuclear reactor community far into the future.

The report includes brief sections on U.S. neutron facilities HFIR, NCNR, and the SNS. In addition, there are sections on the international research reactor facilities: ILL in France, FRM-II in Germany, BR2 in Belgium, and the planned JHR facility in France. Appendix 1 contains a comprehensive review by ORNL of the history, current status, and their proposed upgrades for HFIR. We are deeply grateful to ORNL for providing us with this strategic plan. Appendix 2 gives a comprehensive discussion of the current state of progress on HEU-LEU conversion. Appendix 3 contains user information from NIST and ORNL which shows that both facilities are vastly oversubscribed. These data show clearly the continuing shortfall in neutron facilities in the United States.

The report concludes with our recommendations to DOE for moving forward and with our overall conclusions.

THE SCIENTIFIC CASE

Researchers Danielle Mai and Yun Jung Yang from Massachusetts Institute of Technology prepare samples for the HFIR neutron beamline CG-3.
Image credit: Genevieve Martin/ORNL

1. Neutron Scattering

1a. SOLID STATE PHYSICS INCLUDING QUANTUM MATERIALS

Neutron scattering has been highly impactful in the field of condensed matter and materials physics for several decades. Soon after the discovery of the neutron in the 1930s, neutron scattering was implemented to study structures, atomic or magnetic, and dynamics. The Nobel prize in Physics in 1994 shared by Shull and Brockhouse attests to that achievement. Over the decades, neutron scattering has evolved to an extent that it has become the only way to study certain problems. Applications of neutron scattering include (but are not limited to):

- The structures and dynamics of hydrogen-containing materials, such as hybrid perovskite photovoltaic materials, metal hydrides, molecules and proteins, and soft materials
- The structure and dynamics of functional materials, such as thermoelectrics, ferroelectrics, metallic glasses, multiferroic materials, photovoltaic materials, and batteries
- Fundamental studies of quantum phases of matter—such as unconventional superconductivity, quantum magnetism, quantum phase transitions, and topological materials—areas that may lead to future technological breakthroughs. (These areas may each lead to future technological breakthroughs.)
- Anything related to magnetism, for which neutron scattering is the go-to technique.

Neutrons are produced either at reactors or by the process of spallation, and the instruments developed at both types of sources are very complementary, spanning wide length and time scales. When combined, they can provide a complete microscopic picture of the static and dynamic attributes of the systems at hand. The proposal to build a high-power research reactor (HPRR) carries certain advantages even when compared to a spallation source. These are: 1) efficient collection of data for parametric studies (focusing on a single feature such as the energy of an excitation at a particular wavevector, as a function of temperature, magnetic field, or other control parameters), and 2) use of neutron spin polarization analysis, including several types of instruments that are difficult to implement at a spallation source. Aside from these unparalleled strengths of an HPRR, linked directly to the continuous and high flux nature of the source, HPRRs are very strong in areas in which spallation sources are more directly competitive. Thus they provide some distinct advantages, as well as an overall increase in capacity for an extremely broad range of applications, which is desperately needed in the United States.

Following are key scientific examples where an HPRR has considerable advantage over spallation neutrons. This list is by no means exhaustive, but highlights the complementary nature of HPRRs and spallation neutron sources.

Applications of neutron scattering at HPRRs

Advantages of HPRRs in the study of unconventional superconductivity

"Unconventional superconductors," such as high-T_c copper oxides, iron-based, and heavy fermion superconductors, share several common characteristics, such as close proximity to a magnetically ordered parent state, very similar phase diagrams as a function of carrier doping, and unusual normal state properties.[1-15] These features are distinctly different from the properties of Al, Sn, or some of the other simple superconductors that can be fully explained by the Bardeen-Cooper-Schrieffer (BCS) theory,[16] in which the superconducting gap is isotropic in space, but orbital effects along with magnetism do not play an important role in the mechanism for superconductivity. Although the underlying mechanism for these so-called "unconventional" superconductors is yet to be established, it is clear that magnetism plays an important role in their anomalous electronic properties and superconductivity.[1] This means that neutron scattering is fundamentally important in sorting out magnetic order and excitations in these materials, as neutron scattering is essentially the only probe that can completely determine the wave vector and energy dependence of the magnetic order and excitations throughout the Brillouin zone.[17,18] Compared with a spallation neutron source, which is excellent in probing magnetic features over large energy and momentum ranges, HPRRs are ideal in studying magnetic and lattice features at a

particular energy/wave vector as a function of temperature/field/pressure and/or other tuning parameters due to its high average neutron beam flux. In addition, neutron polarization analysis, important for conclusively separating the magnetic and lattice contributions, can be much better done at an HPRR. In fact, several types of polarized neutron scattering instruments can only be constructed at an HPRR. These include the neutron Larmor diffractometer, which can be used to very precisely measure lattice parameter variations;[19] the neutron triple-axes spin echo spectrometer,[20] which has extremely good energy resolution (~1 meV) at large energy transfers and large wave vectors; and spherical neutron polarization analysis[21] (i.e. cryopad), which can provide polarization analysis without having to use a guide field near the sample. In the following, some scientific examples are provided to demonstrate the unique capability of an HPRR in studying exotic properties of unconventional superconductors.

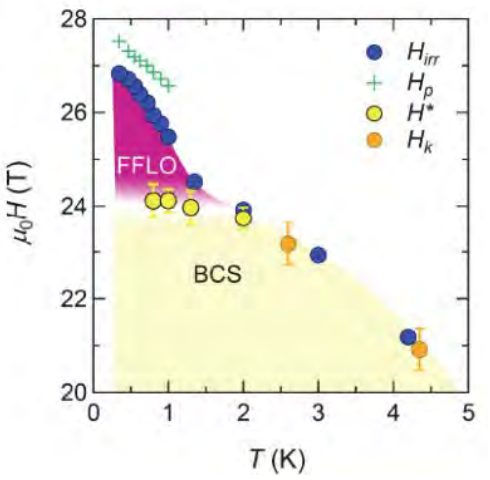


FIGURE 1a.1. High-field phase diagram of FeSe for field parallel to ab-plane. The possible FFLO state is shown in red.

Source: S. Kasahara, Y. Sato, S. Licciardello, M. Culo, S. Arsenijevic, T. Ottenbros, T. Tominaga, J. Boker, E. Eremin, T. Shibauchi, J. Wosnitza, N. E. Hussey, Y. Matsuda, "Evidence for an FFLO state with segmented vortices in the BCS-BEC-crossover superconductor FeSe." *Phys. Rev. Lett.* 124, 107001 (2020).

1. ***Exotic magnetic states in Pauli-limited superconductors.*** In general, static magnetism and superconductivity competes for itinerant electrons below T_c. In some cases, novel static magnetic order appears due to superconductivity, but does not exist without it. These superconductivity-driven pair-density waves (PDW), which are described by a spatially modulated superconducting order parameter, is referred to as a Fulde, Ferrell, Ovchinnikov, and Larkin (FFLO) state.[15] There are several unconventional superconductors which may have FFLOs under a high magnetic field, including $CeCoIn_5$,[22,23] FeSe,[24] and UTe_2.[25] As shown in Figure 1a.1, a possible FFLO state has been identified in FeSe. Such a state can be unambiguously detected by neutron scattering experiments using a high magnetic field, which is much better performed at an HPRR than a spallation neutron source. Neutron polarization analysis can also provide key information concerning the nature of the FFLO state.[15]

2. ***Neutron polarization analysis as a probe of spin-orbit coupling.*** Although unpolarized neutron scattering can identify the presence of magnetic features, it is generally difficult to use unpolarized neutrons to determine conclusively that the feature of interest is indeed magnetic and sort out whether spin excitations are isotropic in spin-space. In many cases, it is extremely important to determine the polarization direction and magnetic anisotropy of the observed magnetic signal, as this information will provide information concerning the strength of spin-orbit coupling in the system. For example, neutron polarization analysis played an indispensible role in determining the magnetic nature of the famous neutron spin resonance in cuprate superconductors.[26] In the case of iron based superconductors, neutron polarization analysis found a strong anisotropic resonance, providing strong evidence that spin-orbit coupling is important for the electronic nematic phase and superconductivity.[27,28] Moreover, the neutron polarization analysis using a cryopad can only be carried out at an HPRR.

3. ***Neutron Larmor diffraction to study accurately changes in lattice parameter.*** X-ray diffraction is commonly used to determine the lattice parameters and structures of solids. However in many cases, X-ray diffraction does not have the accuracy needed to detect tiny changes in lattice parameters of a bulk sample. Neutron Larmor diffraction, which utilizes polarized neutrons to accurately detemine the lattice spacing, can have a Dd/d value on the order of 10^{-6}, and is extremely bulk sensitive. Using this technique, one can accurately determine the tiniest lattice distortions induced by uniaxial pressure needed to de-twin iron pnictides.[29] This technique can also be used to sort out distortions induced by

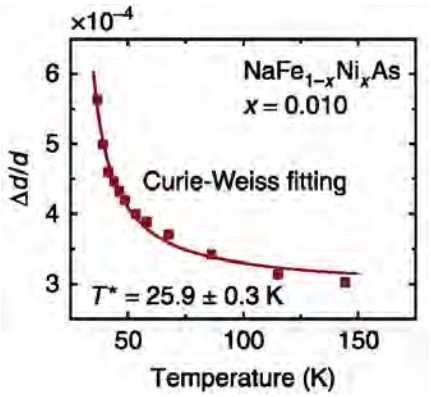


FIGURE 1a.2. Neutron Larmor diffraction can be used to accurately determine the temperature dependence of the lattice distortion of Ni-doped NaFeAs in the paramagnetic tetragonal phase.

Source: W. Wang, Y. Song, C. Cao, K.-F. Tseng, T. Keller, Y. Li, L. W. Harriger, W. Tian, S. Chi, R. Yu, A. H. Nevidomskyy, P. Dai, "Local orthorhombic lattice distortions in the paramagnetic tetragonal phase of superconducting NaFe1−xNixAs." *Nature Communications* 9, 3128 (2018).

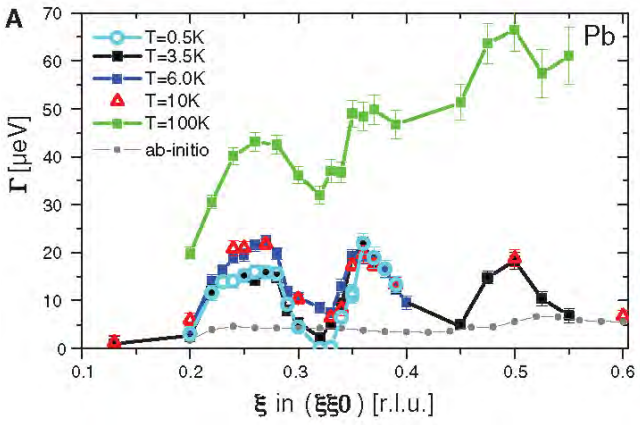


FIGURE 1a.3. Linewidths of transverse acoustic phonons along q = (ξ,ξ,0) in Pb.

Source: P. Aynajian, T. Keller, L. Boeri, S. M. Shapiro, K. Habicht, B. Keimer, "Energy gaps and Kohn anomalies in elemental superconductors." *Science* 319, 1509-1512 (2008).

an electronic nematic phase as in the paramagnetic tetragonal state of an iron based superconductor, and its connection with lattice distortions is shown in Figure 1a.2.[30] The neutron Larmor diffraction is very difficult to implement at a spallation neutron source, but is readily available in spectrometers at an HPRR.

4. ***Neutron Spin echo investigation of lattice and magnetic excitations.*** Typically, the instrumental energy resolution of a neutron spectrometer is inversely proportional to the energy of the excitations one wants to probe. This is understandable because in order to probe large excitation energies one needs higher incident beam energy, which inevitably gives poor instrumental energy resolution. However, by combining neutron spin echo with a triple-axis spectrometer, one can measure the intrinsic linewidth of elementary lattice and magnetic excitations with an energy resolution in the meV region over a broad range of momentum and energy transfers. These measurements can provide unique information that is not possible with any other technique. For example, the momentum and temperature dependence of the lifetimes of acoustic phonons in the BCS superconductor lead (Pb) have been measured, and new information obtained in these measurements suggests that many-body correlations beyond the standard BCS theory[31] are present. The instrument can also be used to study magnon lifetime in classical antiferromagnets and ferromagnets.[32]

5. ***Instantaneous spin-spin correlation function of a system.*** The spin-spin correlation function measured by neutron scattering by integrating over a wide range of energy excitations can provide important information on the nature of the spin interactions. This is widely used to test different theoretical models proposed in cuprate superconductors.[33,34]

More generally, measurements of the instantaneous spin-spin correlations in varied physical systems provide a direct measurement of the static wave vector dependent susceptibility (Q); the latter in turn is often directly amenable to theory. Such measurements, carried out with very high momentum resolution, are essential in characterizing the static critical behavior in second order magnetic phase transitions.

This technique is particularly powerful in one- and two-dimensional magnetic systems. In those cases, by arranging the scattering experiment such that the outgoing neutron is exactly perpendicular to the chain or plane the energy integration is essentially exact. It is just in those situations that one often has first principles' calculations of the spin-spin correlation functions from statistical physical models, perhaps the most famous being the work of Chakravarty, Halperin and Nelson on the two dimensional Heisenberg model. These types of experiments can be done straightforwardly

with a steady state source and would be much more difficult to realize with adequate signal strength with a pulsed spallation source.

A more exotic example is the instantaneous correlations in physical systems with static random fields. In that case, the static susceptibility has two components, a simple dynamic Lorentzian arising from the thermal fluctuations and a perfectly elastic Lorentzian squared contribution arising from the random field fluctuations. As the temperature is lowered from high to low temperatures there is a progressive crossover from a Lorentzian to a Lorentzian squared lineshape in (Q) as the disorder evolves from being dominated by thermal fluctuations to random field fluctuations. Observation of such delicate changes in line-shape require both high Q-resolution and very high counting statistics. So far, such experiments have only been realizable with steady state sources.

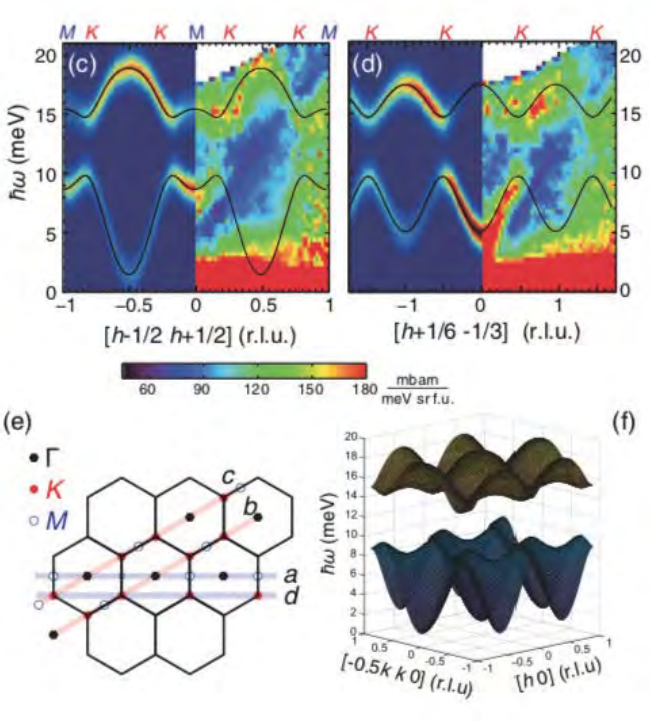


FIGURE 1a.4. Experimental (top, right panels) and calculated (top, left panels) neutron data for CrI3: the band gap at Dirac points along different cuts (bottom left)

Source: L. B. Chen, J. H. Chung, B. Gao, T. Chen, M. B. Stone, A. I. Kolesnikov, Q. Z. Huang, P. C. Dai, "Topological Spin Excitations in Honeycomb Ferromagnet CrI3." *Physical Review X* 8, 041028 (2018).

Advantages of HPRRs in studying topological quantum materials and two-dimensional (2D) van der Waals materials

The development of the next-generation quantum information systems requires the exploration of a variety of novel materials with enhanced quantum coherence. Topology[35,36] and strong correlations are two of the foundational concepts in modern condensed matter physics, but they rarely coexist in the same system and therefore are not often investigated experimentally. The role of spin in topologically-protected states has implications on both our fundamental understanding of material properties and on the technological applications of certain materials. While most topological materials known so far have strong spin-orbit coupling, they can generally be understood within a Landau Fermi liquid picture and density functional theory (DFT) with weak electron-electron correlations (weak U).[36,37] As electron correlations increase, magnetic interactions in topological materials start to become important, and one can ask whether spin waves in topological magnetic materials can play a similar role as electrons in topological insulators. Magnetic topological materials may be relevant for dissipationless transport of spin information, and important for quantum computation.[38-41] Since neutrons are sensitive to the magnetic moment of the system and can directly probe spin excitations, neutron scattering will play an important role in determining topological magnetic properties of the system. Compared with time of flight chopper spectrometers at a spallation neutron source, triple-axis spectrometers at an HPRR can play a unique role in determining the temperature, magnetic field, and pressure dependence of the spin excitations at a particular wave vector and energy. In the following, we list several examples where an HPRR can play an important role in determining the magnetic properties of the system.

1. ***Topological spin excitation in 2D honeycomb lattice van der Waals ferromagnets.*** For magnetically ordered 2D honeycomb lattice materials, spin waves (magnons) can behave like electrons in 2D graphene and form topologically protected edge states. In graphene, the conduction and valence electronic bands touch at Dirac points (the six corners of the hexagonal Brillouin zone). Adding spin-orbit coupling opens a bulk gap at the Dirac points, making the system an insulator except at the perimeter where conducting edge channels with certain fixed spin and momentum orientation appear.[42] In the presence of a spin-or-

bit-coupling-induced next-nearest-neighbor Dzyaloshinskii-Moriya (DM) interaction that breaks inversion symmetry of the lattice, a gap can open in the magnon spectra at the Dirac points[43] and the system may exhibit topological magnon edge modes. In contrast to the electronic spin, where dissipation can be large due to Ohmic heating, topological magnons have no charge and so in principle can propagate for a long time without dissipation.[41] Consequently on the surface of a topological magnetic material, the magnons neither leak into the sample interior nor back-scatter, making them potentially useful for dissipationless spintronic devices. Recently, spin waves in a 2D honeycomb lattice ferromagnet, CrI_3, were found to have a gap near the Dirac point, suggesting that spin waves in CrI_3 may host topological magnons. If the magnon gap indeed arises from the next-nearest-neighbor DM interaction, an in-plane magnetic field should rotate the ferromagnetic moment direction from the c-axis to the in-plane direction. This should cancel the DM interaction and therefore close the Dirac magnon gap. An inelastic neutron scattering experiment under a magnetic field is much better done at a triple axis spectrometer at an HPRR. This is because background scattering from a magnet can overwhelm the magnetic signal in a time-of-flight spectrometer at a spallation neutron source.

2. Candidate Kitaev Quantum Spin Liquid (QSL) materials. A QSL is a state of matter in which the spins of unpaired electrons in a solid are quantum entangled, but do not show magnetic order in the zero-temperature limit.[44] Because such a state may be important to the microscopic origin of high-T_c superconductivity[2] and useful for quantum computation,[40] experimental realization of a QSL is a long-sought goal in modern condensed matter physics. Models supporting QSLs for 2D spin-½ Kagome, triangular, honeycomb, and 3D pyrochlore lattice systems indicate that all QSLs share the presence of deconfined spinons, elementary excitations from the entangled ground state which carry spin S = ½ and thus are fractionalized quasiparticles, fundamentally different from the S = 1 spin waves in conventional 3D ordered magnets.[44] In particular, honeycomb and hyper-honeycomb lattice magnetic materials are of interest because a QSL can arise from the exactly solvable Kitaev model with S=½ Ising spins on a honeycomb lattice.[40] Neutron scattering studies of spin excitations in α-$RuCl_3$, performed at both spallation neutron source (SNS) and High-Flux-Isotope Reactor (HFIR), have identified this material to be a candidate material near a Kitaev's QSL.[45-48] Time-of-flight spectroscopy at the SNS has shown that, unlike conventional ordered magnets which have sharp signatures of their excitations in momentum and energy, -$RuCl_3$ has a broad inelastic signature at relatively high energies, coexisting with the (conventional) lower energy sharp signatures.[46] This broad spectral response is expected for fractionalized quasi-particles, since a single neutron creates two (or more) quasi-particles, and the neutron's energy and momentum conservation is under constrained. This type of broad response is typically called a "continuum of scattering" and its connection to fractionalization hints that -$RuCl_3$ is nearby a QSL. However, what is truly remarkable in this material is that the sharp (conventional) excitations *disappear* when a magnetic field is applied in the plane of the honeycomb layers, while the continuum remains.[47] This strongly suggests that the magnetic field has induced a QSL phase by removing the long range magnetic order. In further support of the QSL scenario, triple axis spectroscopy at HFIR was used to understand the magnetic field dependence of the conventional excitations (and their disappearance), to identify the range of applied fields necessary for the QSL to exist.[48] Commensurate with the expectation that -$RuCl_3$ really does display the required quantum many-body state, there are currently efforts to produce device-like structures with this material, by coupling a monolayer of -$RuCl_3$ with graphene.[49,50] The ability to probe extremely low sample masses with neutrons, requiring the extreme flux and focusing capabilities offered at HPRRs, will become essential for probing these next-generation QSL materials and devices. Although the detection of the fractionalized excitations and their unique transport properties is sufficient to show there is a Kitaev QSL in -$RuCl_3$, new techniques are needed to validate older candidate materials, such as Herbertsmithite, as other types of QSLs. Innovations in neutron scattering, such as the use of entangled beams of neutrons, currently being pursued at spin echo spectrometers at HPRRs,[51] may finally yield direct

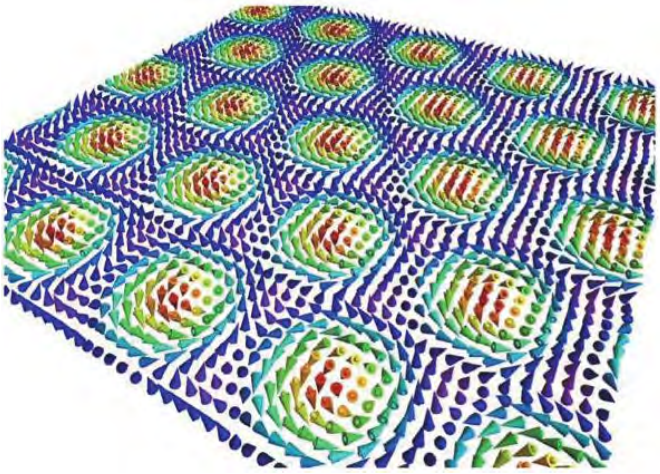


FIGURE 1a.5. An image of the magnetic skyrmion lattice as seen by small angle neutron scattering. After forming a stable, triangular lattice of skyrmions, magnetic field can rearrange them into a square pattern.

Source: T. Nakajima, H. Oike, A. Kikkawa, E. P. Gilbert, N. Booth, K. Kakurai, Y. Taguchi, Y. Tokura, F. Kagawa, T.-h. Arima, "Skyrmion lattice structural transition in MnSi." *Science Advances* 3, e1602562 (2017).

evidence of the long-range spin entanglement, the defining feature of a QSL. Further into the future, for quantum information science applications it will be important to control QSL dynamics in a functional setting, which is likely to be one of the important frontiers for neutron reflectometry and INS from small (thin film) samples.

3. ***Skyrmion materials.*** Magnetic skyrmions, particle-like spin textures (Figure 1a.5),[52] are of interest due to their topological properties and potential for use in high density, low dissipation information storage applications. SANS studies, most efficiently carried out at HPRRs for the very long length-scales involved (5 to 100 nm), have been critical in the development of this research area. Their topological nature influences electronic motion, as well as ensures that they are protected against local perturbations. From the application standpoint, skyrmions are ideal magnetic "bits", since they cannot be easily destroyed, and can be moved/manipulated using low energy-cost electrical or spin currents. The original identification of skyrmions in a material was in MnSi, using a SANS instrument at an HPRR (FRM II).[53] SANS continues to be of utmost importance in identifying the presence of skyrmions in the bulk of new materials, but has also been successfully used recently on thin film samples, which are relevant for technological applications.[54] Compared to complementary techniques such as Lorentz TEM, an advantage of neutrons is the ability to give access to a greater breadth of sample environments,[55] allowing in-situ studies of skyrmion dynamics,[56] or a determination of how the skyrmion phases are modified under pressure.[57] Furthermore, spin polarized neutrons can be used to detect the detailed spin configurations within the skyrmions, which are invisible to other techniques.[55]

Advantages of HPRR in studying functional materials

Inelastic neutron scattering is unparalleled as a comprehensive probe of lattice dynamics. Due to the energy and momentum transfer ranges for thermal and cold neutrons, phonon dispersions can be tracked throughout multiple Brillouin zones, which has proven essential for studying thermal conductivity in thermoelectrics. Meanwhile, extremely high resolution measurements have been useful in identifying the role of hydrogen dynamics in new photovoltaic materials.

1. ***Thermoelectrics.*** Thermoelectrics are materials that can be used to convert a thermal gradient into electricity, and vice versa, and are of interest in increasing overall efficiencies of processes that produce significant heat waste.[58] For a material to function well in this regard, it must have high electrical conductivity while maintaining low thermal conductivity. In order to optimize this, it is essential to understand how to limit lattice thermal conductivity by preventing coherent phonon transport. Using broad surveys of the phonon dispersions, obtained from time of flight chopper spectrometers at the SNS, combined with a detailed temperature dependence of certain key features from a triple-axis spectrometer at HFIR, researchers have been able to identify a large anharmonic phonon coupling in PbTe,[59] which is one of the most popular thermoelectrics used in the temperature range of 400 to 800 K. This anharmonic coupling limits the ability for phonons to propagate. Triple-axis spectrometer data obtained at HFIR was used to investigate the temperature dependence of the anharmonicity in detail, which was crucial for understanding its microscopic origin. This is a prime example of the complementarity of the two types of inelastic neutron scattering measurements which are often used in conjunction.

Both types can be carried out at HPRR sources, but chopper spectrometers (survey instruments) are well-suited to spallation sources, while triple-axes spectrometers are much more efficient at a continuous high flux source such as an HPRR.

2. ***Hybrid perovskite semiconductors.*** The organic-inorganic hybrid perovskites emerged in 2009 as unexpectedly efficient semiconducting materials for photovoltaic and solid state lighting applications. These materials, exemplified by $CH_3NH_3PbX_3$ and $CH(NH_2)_2PbX_3$ (X = Br, I), consist of an inorganic anionic framework (e.g. PbX_3) with organic molecules as the cations (e.g. methylammonium, $CH_3NH_3^+$ or formamidinium, $CH(NH_2)_2^+$). Despite their unoptimized nature, which is epitomized by the ability to easily and cheaply spin coat their films for devices, they have "out of the gate" solar conversion efficiencies rivaling the best known photovoltaics on the market (e.g. silicon). The converse of this effect is high efficiency light emission, and thus the hybrid perovskites are also being investigated as solid state lighting components. The role of the dynamics of the organic cations in the high efficiency of these materials has been under intense scrutiny, and neutron scattering has played a key role in elucidating these effects. Neutrons, being highly sensitive to hydrogen, are an ideal probe of the bulk structural and dynamic properties of the organic cations. The wide range of relaxation timescales involved require high resolution *and* high bandwidth quasi-elastic neutron scattering (QENS), achievable with a combination of cold neutron chopper spectrometers and backscattering instruments. The combination of the Disk Chopper Spectrometer (DCS) and High Flux Backscattering Spectrometer (HFBS) at the NIST Center for Neutron Research have proven to be exceptionally well suited to these studies, having recently produced two important results in this field: the cation dynamics in $CH_3NH_3PbI_3$ were analyzed in terms of their "jump" symmetries, leading to an improved understanding of the long lifetimes of carrier recombination.[60] Meanwhile, re-orientational transitions of the cations in $CH(NH_2)_2PbBr_3$ were shown to correlate with the steady state photoconductivity of this material[61] providing the first direct link between the functional property of interest and the cation dynamics. Given the intense interest in these materials for energy applications, it is expected that neutron scattering studies of the cation dynamics in hybrid perovskites will continue to play a pivotal role. Reactor-based backscatterers have the advantage that they are more flexible in their data collection strategies, offering the ability to quickly scan the temperature dependence in a fixed energy-window, for example, to produce high quality information on the dynamics across the multiple phase transitions known in these materials.

3. ***Battery materials.*** Neutron reflectometry (NR) and SANS studies of the microscopic structures of layered battery thin film structures continue to play an essential and unique role in advancing a fundamental understanding of such systems and in the development of related technological applications. The fact that neutrons are particularly sensitive to two key constituents of battery materials, namely hydrogen and lithium, make NR and SANS studies of such thin film layered battery systems an indispensable probe of their nanoscale structure and behavior. An example is a recent SANS study that investigated electrolytes based on zinc and lithium salts, showing that they hold promise for constructing batteries with high efficiency, lower toxicity, and intrinsic safety.[62] NR and SANS instruments have advantages at HPRRs, if they are designed so that a wide range of neutron energies can be used simultaneously. SANS instruments can simultaneously use 10% or more wavelength range, making the continuous flux of an HPRR highly advantageous. Meanwhile, development of NR instrumentation which can make full use of a white beam has been undertaken at NIST (CANDOR). Making use of the continuous, white beam from a HPRR, this instrument produces over an order of magnitude better signal to noise compared to previous monochromatic NR instruments.

Advantages of HPRRs in studying the structure of materials

Understanding structure-property relationships are of utmost importance in designing compounds or materials for specific purposes, whether the applications are proteins, high temperature superconductors, or anything in between. Neutron diffraction has been an indispensable tool in structural studies, as it is highly

complementary to X-ray diffraction due to its sensitivity to hydrogen, deuterium, and oxygen. HPRRs have played an essential role in structural studies, providing "workhorse" instrumentation for neutron powder diffraction.

1. Hydrogen-containing materials. Neutron scattering is able to differentiate between hydrogen and its other isotopes, such as deuterium, due to the different scattering absorption and incoherent cross-sections. One of the earliest works on hydrogen containing systems was that of Nobel Laureate Cliff Shull on the hydrogenated lattice of palladium. Using neutron-diffraction measurements on powdered samples at a reactor predating HFBR, it was shown that both hydrogen and deuterium atoms in β-phase Pd-H and Pd-D were located in the octahedral positions of the palladium lattice. It was also determined that although the vibrational amplitudes of hydrogen and deuterium were similar to those observed in other compounds, the total neutron-scattering cross-section for hydrogen in this system was abnormally low, indicating that the protons were more nearly free than in other hydrogen compounds.[63] The advantage of detecting hydrogen via neutrons over other techniques is particularly important to obtaining accurate crystal structures of hydrogenated systems. While X-ray diffraction can reveal the formation of metal-hydride phases, the position of the hydrogen atoms can only be indirectly inferred from the measurement. The difficulty in locating hydrogen atoms renders the structure determination very difficult along with the type of bonding and the nature of metal-hydrogen bonds. However, with neutron scattering, the location of hydrogen can be identified. This is due to the fact that neutrons are scattered by the nucleus, and both light and heavy elements can scatter neutrons equally well.[64] Due to this strength, neutron scattering has infiltrated the field of protein crystallography, traditionally an X-ray diffraction stronghold. Neutron diffraction provides an experimental way to directly locate hydrogen atoms in proteins, a technique complimentary to ultra-high-resolution X-ray diffraction. Three different types of neutron diffractometers for biological macromolecules have been constructed in Japan, France, and the United States, and they have been used to determine the crystal structures of proteins. Results relating to hydrogen positions and hydration patterns in proteins include the geometrical details of hydrogen bonds, H/D exchange in proteins and oligonucleotides, the role of hydrogen atoms in enzymatic activity and thermostability, and the dynamical behavior of hydration structures. Combined with advancements in deuterating proteins, growing large single crystals, and the use of cryogenic techniques, neutron scattering offers new capabilities to deciphering biological systems. Neutron protein crystallography helps in the identification of all the hydrogen atoms in biological macromolecules and has helped to establish hydration patterns in proteins. More recently, technical innovations involving the development of the neutron imaging plate have made it possible to shorten the long amount of time required to collect a full diffraction data set. These instrumental improvements have been applied to Laue diffractometry (see Figure 1a.6), as well as to more conventional data collection techniques, such as those using monochromatized neutron beams,[65,66] well suited at HPRRs.

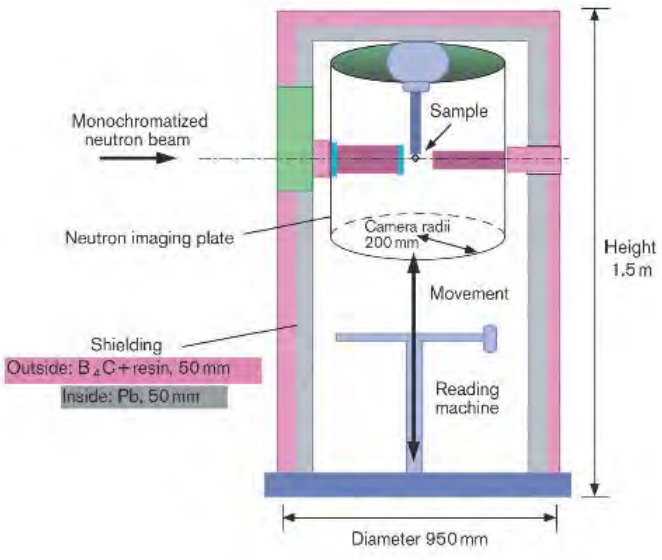


FIGURE 1a.6. The BIX-3 diffractometer, equipped with a neutron image plate, is dedicated to protein crystallography using a monochromatized neutron beam source (installed at the JAERI reactor, Japan).

Source: N. Niimura, "Neutrons expand the field of structural biology." *Current Opinion in Structural Biology* 9, 602-608 (1999).

2. Oxygen positions in cuprate and nickelate superconductors. Neutrons are particularly vital to the study of oxygen-containing compounds. Neutron spectroscopy has been instrumental in understanding strongly correlated electron systems ranging from cuprates, nickelates, manganites and cobaltites. One example where neutron scattering has made significant contributions is the cuprate superconductor $YBa_2Cu_3O_{7-y}$. Compared to all the elements in the system, oxygen has nearly the same coherent scattering lengths as the other elements in this compound and provides an unambiguous method for locating the oxygen atomic positions and determining the site occupancies. From the neutron diffraction analysis, the correct structure with the right oxygen positions were reported soon after this system was discovered. The crystal structure of the single-phase stoichiometric high-temperature superconductor in the Y-Ba-Cu-O system was determined using high-resolution neutron powder diffraction. This compound has an orthorhombic structure with space group Pmmm with buckled CuO_2 layers.[67] Oxygen ordering and the orthorhombic-to-tetragonal phase transition in YBCO became a very important issue soon after the discovery of this system. In situ neutron powder diffraction measurements showed that the orthorhombic-to-tetragonal phase transition near 700°C in a pure oxygen atmosphere is an order-disorder transition in which the disordering of oxygen atoms into a normally vacant site destroys the one-dimensional Cu-O chains present in the room-temperature orthorhombic structure.

The tetragonal structure has a partially occupied, nearly octahedral Cu-O arrangement, in contrast to the orthorhombic structure that has one-dimensional Cu-O chains. For both structures, the oxygen stoichiometry decreases monotonically with increasing temperature. It was found that the transition temperature depended on the oxygen partial pressure and occurred when the stoichiometry was near $YBa_2Cu_3O_{6.5}$. Furthermore, suppression of the superconducting transition temperature in tetragonal $YBa_2Cu_3O_{7-x}$ was linked to the disorder of oxygen atoms which destroys the one-dimensional chains or from the absence of Cu^{3+} ions.[68] The structural properties of oxygen-deficient $YBa_2Cu_3O_{7-\delta}$ have been determined by neutron powder diffraction

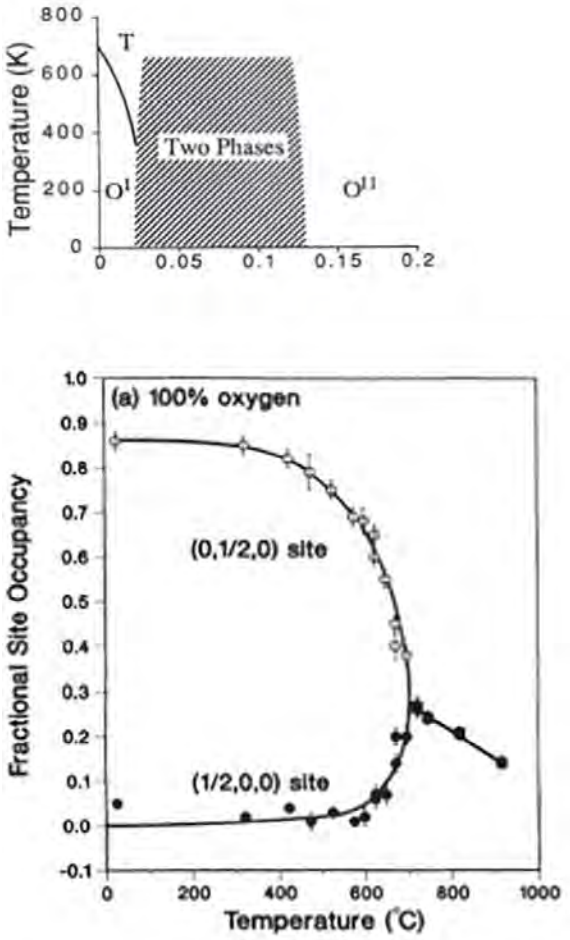


FIGURE 1a.7. Results from Refs. 69 and 70 using pulsed neutron diffraction from IPNS. These experiments were among the first to accurately determine the structure of $YBa_2Cu_3O_7$.

for $0.07<\delta<0.91$ (see **Figure 1a.7**). It was known at the time that superconductivity disappeared at the orthorhombic-to-tetragonal transition that occurred near $\delta=0.65$. By following oxygen across the transition, it was determined that the superconducting behavior could be controlled by charge transfer between the conducting two-dimensional CuO_2 planes and the CuO_x chains, which acted as reservoirs of charge. None of this work could have been done by X-rays at that time.[69]

Oxygen defects were also important in nickelates such as $La_2NiO_{4+\delta}$. Using standard crystallographic techniques of neutron powder diffraction data, it was shown that the excess oxygen in $La2NiO_{4+\delta}$ was incorporated as an interstitial oxygen defect. The defect was located with high accuracy in the orthorhombic *Fmmm* structure, which provided a favorable coordination to four La atoms but required

four nearby oxygen atoms to be displaced from their normal positions. The defect concentration determined from structural refinement agreed well with the overall oxygen stoichiometry determined by hydrogen reduction. For intermediate oxygen contents (δ 0.07), the system phase-separated with different defect concentrations. Structural data suggested that the nearly stoichiometric phase, 0<δ<0.02, incorporated excess oxygen by forming a different defect. $La_2NiO_{4+\delta}$ exhibited very similar behavior to superconducting $La_2CuO_{4+\delta}$, suggesting that the oxygen defect structures were the same in both systems.[70]

3. Local structure. 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 local structure analysis spread beyond disordered systems to highly ordered systems, with improved intensity and resolution. One class of materials where the local structure analysis has made important contributions is the relaxor ferroelectrics, which are at the border of order with disorder. Relaxor ferroelectrics exemplify a class of functional materials where interplay between disorder and phase instability results in inhomogeneous polar nanoregions (PNRs). The direct observation of the formation of PNRs in $Pb(Mg_{1/3}Nb_{2/3})O_3$ using the neutron pair distribution function analysis over the temperature range from 1,000 to 15 K demonstrated the existence of local polarization and the formation of medium-range PNRs with local rhombohedral order. The volume fraction of the PNRs was estimated as a function of temperature which steadily increased from 0% to a maximum of 30% as the temperature decreased from 650 to 15 K. Below T~200 K, the PNRs freeze into the spin-glass-like state.[71] Elastic diffuse scattering studies on $Pb(Mg_{1/3}Nb_{2/3})O_3$ revealed interesting features related to the polar nanoregions (see Figure 1a.8). The intensity distribution measured near the (100) Bragg peak in the (hk0) scattering plane assumed the shape of a butterfly with extended intensity in the (110) and (1-10) directions. The temperature dependence of the diffuse scattering showed that both the size of the polar nanoregions and the integrated diffuse intensity increase with cooling even for temperatures below the Curie

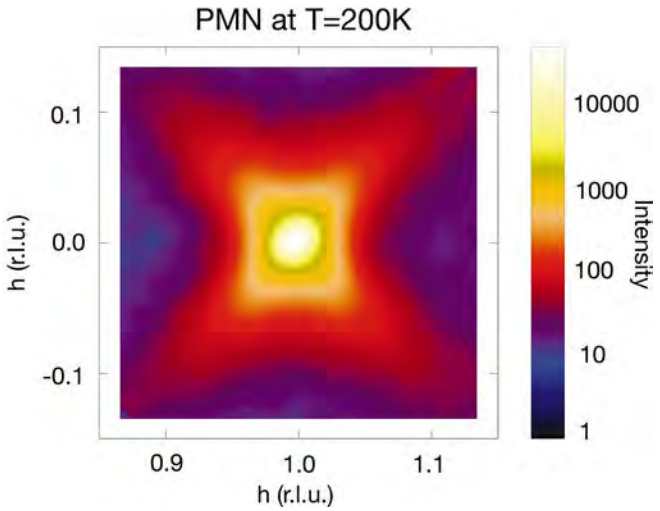


FIGURE 1a.8. Neutron elastic diffuse scattering intensity at an HRPP on a relaxor ferroelectric (from Ref. 73)

Source: M. E. Manley, J. W. Lynn, D. L. Abernathy, E. D. Specht, O. Delaire, A. R. Bishop, R. Sahul, J. D. Budai, "Phonon localization drives polar nanoregions in a relaxor ferroelectric." *Nature Communications* 5, 3683 (2014)

temperature T_C~213K.[72] Using neutron scattering, it was additionally shown that phonon localization drives polar nanoregions in relaxor ferroelectrics. Ferroelectric phonon localization drives PNRs in relaxor ferroelectric PMN-30%P. At the frequency of a preexisting resonance mode, nanoregions of standing ferroelectric phonons develop with a coherence length equal to one wavelength and the PNR size. It was determined that the size and shape of PNRs was not dictated by complex structural details, but by phonon resonance wave vectors.[73]

Another exemplary system in which local lattice distortions were instrumental in understanding the competing mechanisms and strong correlation effects was the perovskite manganites. The discovery of colossal magnetoresistance, CMR, in the 90s led to considerable research to understand the competing spin, charge and lattice interactions, and the role of the static Jahn-Teller distortions. It was found that over certain ranges of composition, a transition from a paramagnetic insulator to a ferromagnetic metal occurred as a function of temperature and magnetic field. While the connection between ferromagnetism and electrical conduction was initially explained in terms of the double exchange mechanism, theoretical work pointed at the time to lattice involvement in the mechanism, possibly via polaron formation. Thus the manganites have become the canonical system for understanding polarons. Soon after, through

neutron scattering experiments and the pair-density-function (PDF) analysis, it was demonstrated that the *local* structure in this system was quite distinct from that suggested by the crystallographic structure. It was shown that the Jahn-Teller distortion was locally present in the metallic as well as insulating phases, suggesting a direct link between the distortions and the polarons. Through the local structure analysis, it was also reported for the first time that the metallic state was not homogeneous, which led to a completely new picture of the metallic phase (see Figure 1a.9).[74]

Finally, a very early example of charge ordering confirmation by neutron scattering was in magnetite Fe_3O_4 below the Verwey transition. Verwey initially discovered that magnetite undergoes a sharp, first order transition on cooling below 120 K at which the resistivity of magnetite increases sharply by 2 orders of magnitude, and the structure distorts from cubic symmetry. He hypothesized that this effect was to charge ordering of the Fe^{2+} and Fe^{3+} states on the B sites in alternating layers, but was unable to confirm it. The charge ordering was determined to show a pronounced [001] modulation, consistent with the gap that opens at the Verwey transition, although other structural modulations might be present as well.[75]

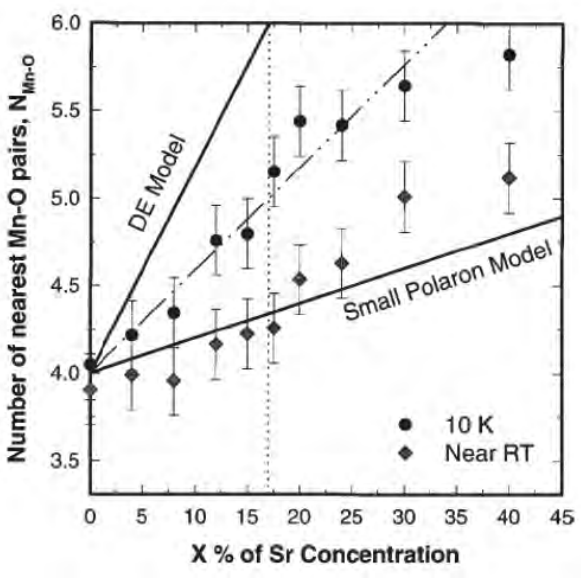


FIGURE 1a.9. The composition dependence of the Jahn-Teller polarons in CMR material, $La_{1-x}Sr_xMnO_3$ determined from pulsed neutron diffraction and the pair density function analysis from data collected at IPNS.

Source: D. Louca, T. Egami, E. L. Brosha, H. Röder, A. R. Bishop, "Local Jahn-Teller distortion in La1-xSrxMnO3 observed by pulsed neutron diffraction." *Physical Review* B 56, R8475-R8478 (1997).

Summary

HPRRs play an important role in solid state physics and chemistry, and the examples above illustrate that the applications range from the fundamental (quantum spin entangled states and unconventional superconductors) to the practical (magnetic storage, thermoelectrics, and photovoltaics). In the realm of the solid state, neutron scattering excels at probing lattice structure, particularly with regards to hydrogen and oxygen positions, lattice dynamics, and all aspects of magnetism. The primary advantages of HPRRs over spallation sources is the efficient collection of data over a targeted range of energy, and momentum space as a function of another control variable (such as temperature, magnetic field, or other parameters), as well as the use of spin polarization techniques. However, new instrument design concepts for HPRRs are always in the works, so that techniques can be improved dramatically and make excellent use of the continuous, high flux beams and in some cases can outperform comparable instrumentation at spallation sources. Thus, HPRRs and spallation sources can sometimes produce comparable efficiencies for the same types of measurements, depending on instrument design. This means that HPRRs not only offer complementary strengths to spallation sources, but also help to address the general oversubscription problem for neutron instrumentation in the U.S.

1b. SOFT MATTER

Soft matter research is one of the largest areas of investigation using neutron scattering instrumentation, and represents—along with biosciences—the soft 'half' of neutron scattering users. Key techniques used include small-angle neutron scattering (SANS), ultra-small angle neutron scattering (USANS), neutron reflectometry (NR), neutron spin echo (NSE), and the emerging method, offspecular neutron reflectometry (similar to grazing incidence scattering). There are other techniques used as well, however the majority of experi-

ments in soft matter rely on SANS and NR, for which soft condensed matter research represents at least half of the experimental volume.

Currently, the vast majority of neutron scattering experiments in the United States are performed at HFIR, SNS, and NIST. University-based research reactors do not make a substantial contribution to the total available experimental time for the neutron scattering community. This focus at Oak Ridge and NIST is due to the fact that the larger sources have the required flux and beam quality to perform experiments in a substantially shorter period of time, and they offer instruments with a better range of momentum space for the most popular soft matter-related experimental techniques. In the case of many smaller reactor sources, state-of-the-art instruments adaptable to effective soft matter research studies do not exist.

The Unique Role of Neutrons in Soft Matter

Neutron scattering methods play a unique role in soft matter research that cannot easily be replicated by any other category of experiment. There are three primary advantages that neutrons offer for this type of research. First, soft condensed matter tends to have a very high percentage of hydrogen within its structures, as it is predominantly based on organic molecules. This feature allows control of scattering contrast through the use of readily accessible H/D isotopic labeling, enabling many experimental designs that could not easily be achieved using other methods, such as:

- examination of chain confirmations in polymer melts and solutions[1]
- bi-continuous microemulsions[2]
- block copolymer diffusion experiments[3]
- contrast matching for structure determination[4]
- partial structure factor analysis[5]
- solvent and additive partitioning in nanoscale structures,[6] and
- the determination of hydration numbers.[7]

Furthermore, the fact that many soft matter systems (micelles, vesicles, coacervates, biohybrid systems, and gels) also exist in media with a substantial water content makes them ideal for this type of H/D contrast by simply varying the concentration of D_2O within the water. This type of contrast variation provides extremely strong scattering contrast, enabling complex behavior such as self-assembly at air-water interfaces, ordering in polymer thin films, and concerted polymer dynamics to be readily accessed in a manner not easily accomplished *via* other techniques.

Second, neutrons are considered 'non-destructive' as there is typically no radiation damage to exposed soft matter samples. This makes them the probe of choice for materials that may show substantial damage or degradation when exposed to X-rays or electrons, including many micellar systems, gels, and biological-synthetic hybrid systems.

Third, the relatively large penetration depth of neutrons facilitates the *in-situ* and *in-operando* investigation of soft matter systems to uniquely probe time-dependent and path-dependent processes, such as the operation of fuel cell and battery membranes, mechanical deformation, or ordering dynamics in external fields. [8,9,10,11]

Priorities in Soft Matter Research

In soft condensed matter research, the main priority is access to high quality neutron sources that can support world-class instruments, such as SANS,USANS, NR, and NSE, on which researchers can conduct experiments. The differences in source characteristics between spallation and reactor sources tend to be of secondary importance for soft condensed matter research, and the time/pulse structure of a spallation source offers relatively little advantage for most soft condensed matter studies. Conversely, the continuous-flux structure of a reactor source is highly beneficial for the rapidly emerging, high-resolution NSE approaches that can bridge the gap between soft matter and biophysics (e.g., measurement of membrane bending constants [cell membrane mimics] at air/water interfaces),[12] and it is also ideal for low-Q (USANS)-type studies. Overall however, the key characteristic is maximizing the intensity of the scattered beam, while maintaining the necessary momentum and energy resolution required for the experimental design.

The Current Role of Reactor Sources

Currently, reactor sources provide a large fraction of the available neutron time on the key instruments used in soft matter research. The reactor sources at HFIR and NIST, but particularly HFIR, provide a high flux of neutrons enabling soft condensed matter scattering experiments to be performed faster than other neutron sources in the United States. These high-flux reactor sources therefore form a critical part of the nation's current neutron scattering infrastructure. The loss of either of the two reactor sources would critically compromise the technological

capability of the community if it were not replaced by a new source that provided an equal or superior experimental throughput. Given the large number of instruments of interest to the soft matter community, particularly SANS, supported at both of the nation's largest neutron scattering reactor sources, it is difficult to imagine that the research community would continue successfully if either of these sources were to cease operation.

Current instruments are already over-subscribed often by a factor of up to 3, making it difficult for academic and industrial research efforts that rely on neutron scattering or that focus on the development of neutron techniques. For instance, soft matter M.S. and Ph.D. theses are becoming increasingly dependent on neutron scattering information, as hierarchical structure determination and processing-dependent behavior become critical factors in next-generation soft materials design.

With respect to industry, there are several key areas in which neutron scattering has led to transformative advances, and the importance of these techniques is evidenced by the 13 major corporations that are members of the nSOFT consortium. Impacts include improved transportation fuels,[13] improved polymer processing,[14] and a better understanding of energy resource development.[15] Perhaps more good proposals are denied beam time than are granted.

Future Needs of the Soft Matter Community

Research in the soft matter community is limited by the number of high-quality instruments that are operated in the United States. While the community has several needs with respect to sample environments, data analysis tools, and the specific range of momentum and energy space to be probed, the main limit is accessibility to beam time on world-class instruments. Currently, reactor sources support a critical fraction of such instruments. Continued development and expansion of this instrumental suite on new or existing sources is the most important need of the community. Due to their ability to support a large number of instruments and provide for high scattered-beam intensity in the right momentum range with cold neutrons, reactor sources play an irreplaceable role in providing these neutrons.

Some methods, such as NSE and offspecular neutron reflectometry, will also benefit from improved flux, allowing a wider range of samples to be studied as well as faster acquisition times, which will increase the number of experiments that can be run on the instrument. These methods would benefit from next-generation reactor designs. ■

BOX: Polymer Micelles

Until recently, a major unanswered question in colloid and soft matter science was how polymer micelles relax and how molecules might exchange between them. Using the unique capabilities of neutron scattering, Lodge, Bates and coworkers devised a clever experiment where they prepared a blend of purely deuterated and purely hydrogenated micelles in a mixed aqueous solvent. If chains interdiffuse between micelles, contrast will decrease until it reaches the match point which was set to be equivalent to a random distribution of chains. By using time-resolved neutron scattering, the investigators were then able to extract the rate of interdiffusion and show how it depended upon the chemical structure and thermodynamic interactions of the system. This study illustrates the critical role that reactor sources play in soft matter where they enable this type of experiment over long times with high intensity scattering.

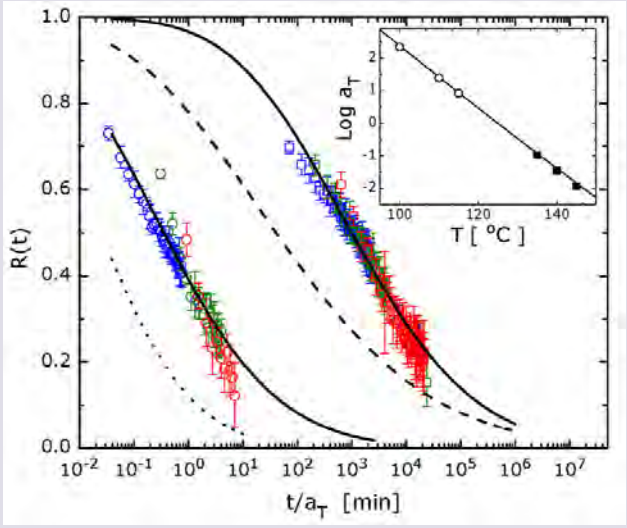


FIGURE A. Time decay of scattered intensity from blends of deuterated and hydrogenated micelles
Source: Choi, Lodge, and Bates PRL 2010, 104, 047802

1c. BIOLOGY

Neutron scattering has found application in a broad range of biological and biology-related research.[1] A diagram of the current major application spaces for neutrons in biological research is shown in Figure 1c.1. The primary biological application of neutron scattering is in basic science, particularly structural biology,[2] or the study of the molecular structures and organization of biological molecules in organisms, with the goal of establishing the relationship between structure and biological function.[3] Structural biology research with neutrons includes:

- examination of protein structure, particularly the chemical mechanism of enzyme active sites;
- examination of the organization and dynamics of the bilayer lipid membranes that separate cells from their environment and enclose subcellular structures such as organelles;
- examination of the association of membrane proteins with bilayer lipid membranes; and
- examination of the organization of large molecular assemblies.

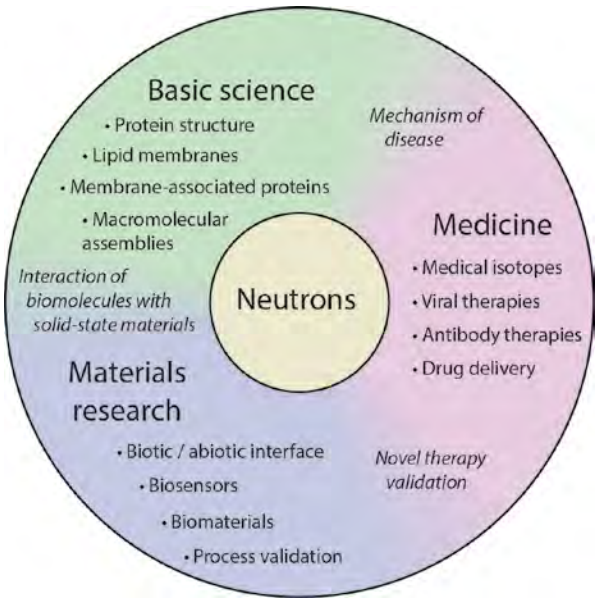


FIGURE 1c.1. Application space of scattering neutrons from biological materials. Applications at the intersections of basic science, materials research, and medicine are italicized.
Source: David Hoogerheide/NIST

Also, neutrons have found important applications in medicine, including in elucidating the mechanisms of disease, assaying biopharmaceutical formulations, and facilitating the development of novel nanoscale vehicles for drug delivery and gene therapy. Finally, neutron scattering is often useful in probing the interaction of biomolecules with solid-state materials, from designing biosensors and self-assembling biomolecules into useful materials to reducing biofouling.

Why Neutrons in Biology?

Four features of the interaction of neutrons with biological matter account for the widespread application of neutron scattering to the study of biological systems. Each of these features stems from the fundamental fact that in the sample material, neutrons scatter from the atomic nuclei, rather than from the electrons.

- First, neutrons are highly sensitive to hydrogen atoms, which account for a large fraction of the atoms in biomolecules.
- Second, neutrons are sensitive to nuclear isotopes. Thus the scattering properties of a biomaterial can be completely transformed (*e.g.*, by isotopic substitution of deuterium for hydrogen) while having only a small effect on the biochemistry. Often this substitution is simply and effectively performed on the aqueous medium of the sample by exchanging water for heavy water, though it also can be done on the macromolecular portion of the sample.
- Third, because neutrons do not disrupt binding electrons, beam damage from neutron scattering experiments is extremely limited.
- Finally, 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 simple theoretical treatments, small contributions from systematic errors in data analysis, and a wide range of neutron-compatible materials for sample 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. On the other hand, the weak scattering of neutrons from biological materials increases the required sample size or data collection times, limiting both the applicability and accessibility of the technique to the broader structural biology community, and highlighting the importance of high-flux neutron sources.

TABLE 1c.1
Suite of Neutron Scattering Techniques for Probing Biological Materials

TECHNIQUE	SAMPLE FORM	LENGTH (TIME) SCALE	INFORMATION
Small angle neutron scattering (SANS)	Solubilized	1 nm – 10,000 nm	Structure
Neutron reflectometry (NR)	Thin film	1 nm – 1,000 nm	Structure
Neutron macromolecular crystallography (NMX)	Crystallized	0.1 nm resolution	Atomic structure
Neutron spin echo (NSE)	Solubilized	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

Major Techniques

Neutron scattering in biology utilizes four major techniques or classes of techniques (see Table 1c.1). *Small angle neutron scattering* (SANS) is perhaps the most widely used, particularly for low-resolution (≈10 Å) analysis of structures associated with solvated biomolecules and biomolecular assemblies. SANS is both analogous to, and complementary to, small angle X-ray scattering and is often deployed in conjunction with other structural techniques such as NMR spectroscopy or electron microscopy to probe large macromolecular assemblies.[4] *Neutron reflectometry* (NR) is used to provide low-resolution structural analysis of biological molecules and assemblies at the interfaces between solid, liquid, and air phases[5,6] and is highly complementary to other interfacial techniques such as scanning force microscopy, as well as electrical and optical methods.[7] NR studies benefit from the penetration of neutrons through materials such as single-crystal silicon, enabling the fabrication of samples with large areas while using relatively small liquid volumes. *Neutron macromolecular crystallography* (NMX) is analogous to X-ray crystallography and yields atomic resolution structural information, such as of the active sites of enzymes where the position of hydrogen atoms is important for enzymatic function.[8] Finally, a range of *dynamics* techniques, including *neutron spin echo spectroscopy* and *inelastic neutron scattering* can probe a range of time scales from 0.01 to 1000 ns, similar to that accessible by molecular dynamics simulations.[9] These techniques are used to probe collective motions in lipid bilayers[10] as well as the motions of protein sidechains and the dynamics of water at biomolecule surfaces.[11]

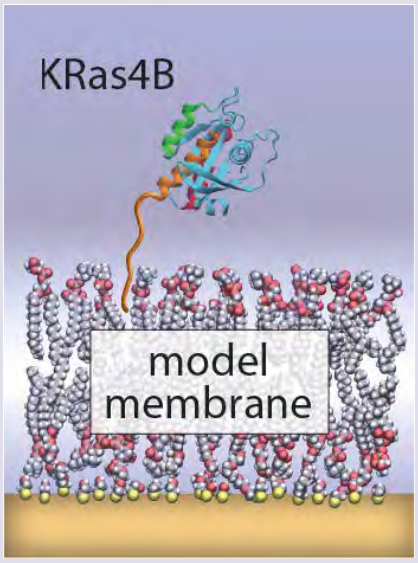
Future Opportunities and Requirements

In the future, neutron scattering is likely to continue to be a crucial component of biological research in three major areas:

1. **Structural biology.** In structural biology, due to its unbiased sampling of distributions of structural conformations, neutron scattering will be particularly important in studying proteins and protein complexes with high disorder that are invisible in crystallographic techniques and difficult to assemble from electron microscopy images.
2. **Biopharmaceuticals.** In recent years, there has been a sharp increase in the economic footprint of biopharmaceuticals.[12] Unlike small molecule pharmaceuticals, biopharmaceuticals are structured on the nanometer scale and are thus readily probed by neutron scattering techniques. As a recent example of the importance of neutron scattering, Amgen acknowledged the "valuable impact" of SANS measurements to probe the stability of formulations of the first oncolytic virus therapy approved by the FDA (**https://www.nist.gov/industry-impacts/cancer-therapy-formulations**).
3. **Biotic/abiotic interface.** Finally, development and characterization of the biotic/abiotic interface (*i.e.*, the physical interface between semiconductor technology and biological tissue) will require a probe that interrogates both hard and soft condensed matter materials and is likely to be an important application for neutron scattering in biology. [13]

BOX: Membrane-Associated Proteins

Membrane-associated proteins are proteins that are embedded in, or transiently interact with, the lipid membranes that define the boundaries of cells and their compartments. As a result of their strategic location, membrane-associated proteins play an outsized role in how cells process and respond to their environment and thus constitute a large fraction of drug targets. Their confinement to the crowded two-dimensional membrane surface, however, limits the number of these proteins found in cells and makes them difficult to study by conventional solution-based biochemical and biophysical techniques in which their natural membrane environment is not present. An important contemporary example is the KRas4B GTPase ("KRas") protein, a small, membrane-bound molecular switch that controls cell growth and division. Certain mutations of KRas inhibit its switching function, leading to cell proliferation and cancers of the lungs, pancreas, and colon for which no effective treatments are currently known. A critical step in the activity of KRas—and a potential target for therapeutic drugs—is the binding of the Raf effector protein; however, development of such an inhibitor for KRas has been hampered by the lack of a structural model for membrane-bound KRas. Recently, researchers in a collaboration involving the NIST Center for Neutron Research, Carnegie Mellon University, and the National Cancer Institute's RAS Initiative performed a combination of neutron reflectivity, nuclear magnetic resonance, and protein footprinting measurements that, together with molecular simulations, elucidated the structure and dynamics of KRas at a membrane surface. The researchers found the KRas adopts an ensemble of molecular conformations in which the body of the protein, attached to the membrane via a flexible tether, dynamically explores the space above the membrane, with only brief excursions to the membrane surface (see Figure).



The flexibility of this protein allows it to efficiently find and bind to the larger Raf protein; when this occurs, KRas is locked into a single conformational state. This mechanistic insight, enabled by neutron scattering, may prove critical to guiding the development of small-molecule or biopharmaceutical therapeutics inhibitors for Ras-driven cancers.

Realization of these opportunities will rely on a robust response to the challenges facing researchers interested in neutron scattering for the biological sciences. The most significant obstacles are slow measurement speeds and the lack of automation in sample handling and data analysis. Biological samples (and soft matter samples generally) have a limited lifetime, even with appropriate sample handling and refrigeration equipment. Protein samples are particularly sensitive to experimental conditions and handling protocols, and may lose functionality on the hours-long time scales of a conventional neutron scattering measurement. Because effect sizes are small for biological samples, multiple independent measurements are often desired for accurate uncertainty estimation. Similarly, biological samples are complex, with many components in the sample and its aqueous environment, and therefore they benefit from the multiple measurements required for parametric mapping. Precious samples, such as virus-based drug formulations, are available only in small sample volumes or at dilute concentrations. High capacity and sample throughput, for which high-flux sources with efficient detectors are a fundamental requirement, are thus essential for biological samples.

A promising recent development in this area is the construction of wide-band energy-dispersive detectors for SANS and NR instruments at reactor sources.[14] These combine energy discrimination (the primary efficiency advantage of pulsed-source measurements) with the uninterrupted flow of neutrons from a continuous source, increasing measurement speeds over conventional instrumentation by well over an order of magnitude.

In addition to the technical requirements for neutron sources and instrumentation, biological research requires an appropriate level of infrastructure and staffing support. Due to the limited neutron scattering resources in the United States, and the traditional role

of neutron scattering in the physical rather than the biological sciences, academic researchers and their trainees are unlikely to be familiar with both biological science and neutron scattering techniques. As a result, neutron beamline scientists are highly involved in both technical and scientific levels at the conception, execution, analysis, and final publication of neutron experiments for biological samples. In turn, this situation limits the number of research groups that can be supported at existing facilities. As a result, the rate of technique and instrumentation development for biological measurements—particularly automation of sample preparation, sample handling, and data analysis—has not kept pace with the growth of biological research applications. To achieve a self-sustaining research environment for biology akin to that for hard condensed matter, multi-pronged investment in neutron facilities, instrumentation, and both technical and scientific staff commensurate to the needs of the biological research community, will be required. ■

1d. POLARIZED NEUTRONS

In synchrotron X-ray and optical spectroscopy and imaging, polarized beams are widely employed to enhance the specificity and quality of data. Polarized neutron beams offer analogous benefits over unpolarized neutrons, but are not widely utilized. However, with the advent of more powerful neutron sources and more efficient means of delivering and analyzing polarized neutrons, there are opportunities for transformational impacts on a wide range of science through polarized neutron scattering.

Unpolarized neutrons can detect magnetic structure because neutron diffraction is a self-interference effect that survives averaging over the incident neutron spin state. But more specific information can be obtained by controlling and analyzing the incident and scattered neutron spin state respectively. Not only does this allow systematic separation of magnetic and nuclear scattering, but in spherical neutron polarimetry, each Bragg peak yields a second rank tensor that describes the rotation of the incident neutron spin state during diffraction. Polarized neutron diffraction and reflectometry can thus uniquely resolve the complex non-collinear spin structures that are important for understanding topological and multiferroic magnetism in single crystals and nanostructured materials. Also, by essentially solving the phase problem, polarized neutron reflectometry can be used to determine complex bio-membrane structures through first principles inversion.

Neutron spectroscopy brings into view collective quasi-particles with energies from micro-eV to eV, including phonons and magnons. However, we are increasingly interested in materials where magnons and phonons hybridize, or where quasi-particles are topological and can only be created in multiples. For the most interesting experiments, no theory is yet available to help understand the superposition of various particles' contributions to the unpolarized neutron scattering intensity. Polarized neutrons can systematically separate into separate channels the vibrational component and each magnetic component of multiple or composite quasi-particles. Polarized neutrons may be the only way to convincingly isolate the subtle features of continuum scattering from Majorana quasi-particles in a Kitaev spin liquid from phonon scattering.

Polarized neutrons offer the ultimate in energy and momentum resolution. Spin echo techniques familiar from nuclear magnetic resonance can be exploited to access temporal or spatial correlations from the atomic to the 100 nanosecond or the micrometer scales respectively while employing a neutron bandwidth 5–6 orders of magnitude greater than conventional scattering methods. Spin echo methods provide a unique window on dynamic phenomena in soft and biological materials, and on glassy and critical phenomena in hard condensed matter.

While entanglement is the key resource of quantum materials and the basis for quantum computing, a direct experimental probe of entanglement within a quantum material has not been reported. Conventional polarized beam methods utilize product states of a plane wave and a spinor wave function. However, using methods from neutron interferometry that were previously used to probe the fundamental tenets of quantum mechanics, it is possible to form a spin-path entangled neutron beam. Probing whether the entanglement built into the incident beam is sustained during interaction with the sample might be the basis for a transformative probe of quantum entanglement in materials.

Polarized neutrons offer unique capabilities with growing impacts on the full range of materials-based sciences

Recent developments in incident beam polarization techniques and wide angle polarized analysis indicate great scientific potential. Fully spin resolved diffraction resolves non-coplanar spin structures that are important for topological materials. Some examples follow.

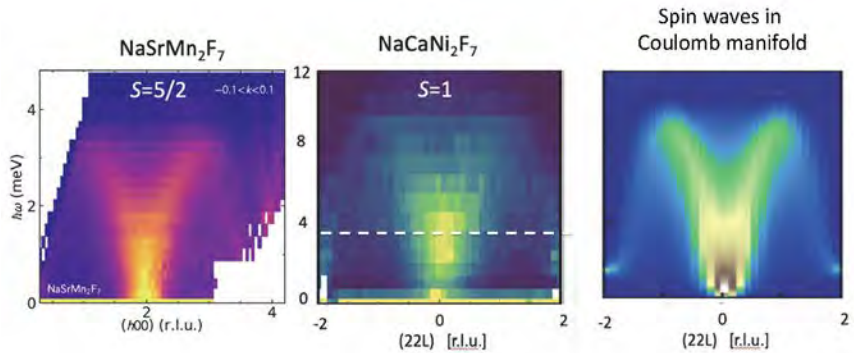
Some additional advantages of polarized neutrons include:

- Larmor labeling methods can extend neutron scattering to regimes of energy and momentum resolution inaccessible with other methods.
- Use of the neutron in "quantum sensing" methods could provide transformative access to quantum entanglement.

In view of these advantages, when developing new sources and instrumentation, polarized neutrons should be the default. Facility level investments may facilitate access to polarized neutrons (dedicated polarized guides that do not lose half the neutrons).

Polarized neutron beams can be generated and employed at both spallation and reactor sources. However, the extra layer of spin selectivity and the greater complexity of the subsequent measurements necessitates optimized instrumentation at the optimal high flux neutron source. The three-source strategy (short and long pulse target stations and HFIR steady state) for neutrons puts ORNL in a unique position to exploit polarized neutrons in the materials sciences. Fully polarized triple axis spectroscopy was first demonstrated at the HFIR facility, the highest flux neutron scattering facility in the world. An emphasis on science with intense polarized neutrons could be a scientifically productive focus at a revamped HFIR.

For example, one may consider a facility level provision of fully polarized neutron beam guides based on polarizing super-mirror guide sections. Bifurcating an unpolarized guide into two guides with opposite polarization may be an effective way to provide multiple high flux spin polarized end stations. Some uses of polarized neutrons, including for spherical polarimetry, larmor labeling, and entangled scattering, appear harder to combine with parallelized detection systems. For these the higher time-averaged beam flux of a reactor facility will be essential to achieve adequate data rates. However, massively parallel detection systems inevitably deliver higher data rates and should be the ultimate goal so that continued development of wide angle neutron spin analysis will be important to realize the scientific potential of polarized neutrons. ■



Experimental Exploration:

- Find other disorder free realization of spin-1 pyrochlore
- Does non-magnetic doping produce spin-½ like degrees of freedom?
- Examine Zeeman splitting of the gap-like excitation

FIGURE 1d.1. Dipolar Spin-Ice State in $Ho_2Ti_2O_7$ Haldane-like Effect in Spin-1 Pyrochlore?
Sources: (left) Scheie, et al. (2019); (middle) Plumb, et al. (2019); (right) Shu, et al. (2019)

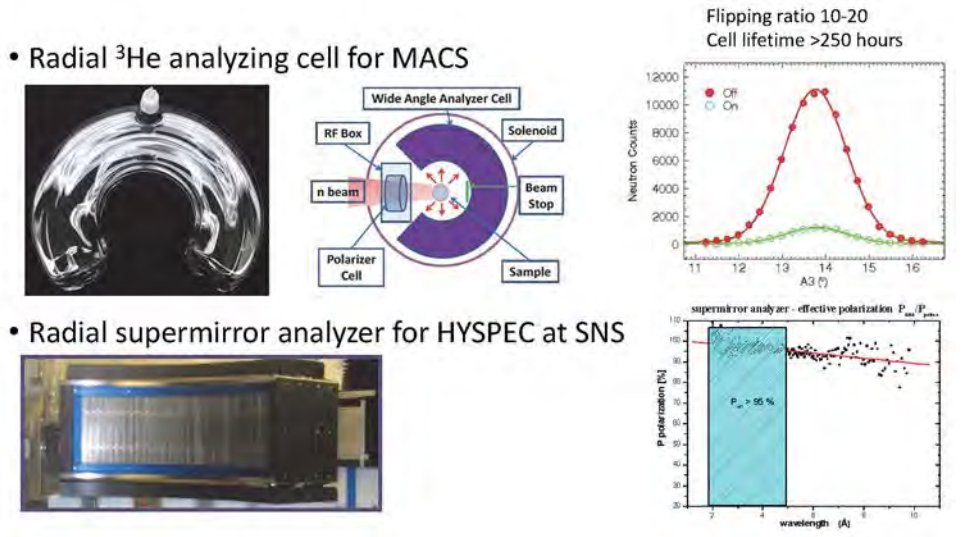


FIGURE 1d.2. Wide Angle Polarization Analysis
Source: Collin Broholm, private communication

1e. SYNCHROTRON X-RAYS VS. NEUTRONS

Elastic and inelastic neutron scattering has been a critical part of experimental condensed matter physics since the 1950s. Initially that stemmed from the unique capability of neutrons to reveal the precise way in which moments order in particular magnetic materials (even if the order is complex); also because of neutrons' ability to probe phonons, magnons, and other excitations of matter over a broad range of momentum. Over the decades since the first neutron scattering facilities were constructed, there has been tremendous progress in probing similar properties of matter using X-rays. This progress has been achieved[1] mainly due to the development of synchrotron X-ray sources and advances in the instrumentation used to interpret synchrotron X-ray scattering.

As we explain below, however, X-ray scattering is very far from being a drop-in replacement for neutrons in studies of magnetic materials. The two techniques have instead developed a complementary relationship, with one technique often filling holes in what can be explored with the other. Neutron scattering is still the technique of choice for studies of the magnetic properties of materials, and is increasingly important for studies of soft matter, including biological matter.

Neutrons couple to matter through their strong interactions with atomic nuclei and through the interactions of the neutron spin with magnetic fields created by orbital or spin moments in a material. X-rays couple to matter mainly through the interaction of the light wave's electric field with charged electrons in the material. Because the two coupling mechanisms are unrelated and uncorrelated, the trends in the coupling strengths of the two-probes across materials classes are quite different. X-rays couple strongly to materials with a high-density of electrons per volume (*i.e.* heavy materials), whereas neutrons couple most strongly to materials with large nuclear cross sections and/or large densities of unpaired electron spins or large orbital angular momentum density. In general, the sensitivity of X-rays to magnetism is weaker than that of neutrons.

Synchrotron X-ray scattering opens up a number of possibilities not available in neutron scattering. Most important, perhaps, is the possibility of achieving element specificity by taking advantages of resonances. Resonant X-ray scattering (REXS) and diffraction can easily identify which atoms or ions in a compound are most responsible for particular structural features, or if inelastic (RIXS), a particular excitation. It can also detect diffraction patterns associated with different types of electronic order, including not only magnetism but also charge and orbital order.

In a very typical and important example, the resonance that is exploited in studies of transition metal oxides is between a metal ion-core *p*-level and a metal valence *d*-level. These transitions are in the soft X-ray range for 3d metals, in the tender X-ray range for 4d metals, and in the hard X-ray range for 5d metals. By tuning an X-ray source to a transition energy associated with a particular metallic cation, the contributions of different metals to structural, magnetic, or

other electronic features in a compound or artificial superlattice can be distinguished. (See box on Oxide Heterojunction Magnetism.)

Other important possibilities are opened up by taking advantage of the pulsed and coherent character of modern high flux synchrotron X-ray beams. Using X-ray pulses and borrowing *pulse-probe* techniques from optics, it is possible to examine how the atomic scale electronic degrees of freedom of complex materials equilibrate after being excited by an X-ray or another beam. Taking advantage of X-ray coherence, X-ray photo-correlation spectroscopy (XPCS) can provide unique information on the slow dynamics of glassy materials. Coherent beams can also be easily focused down to their diffraction limit, adding spatial resolution to X-ray scattering experiments.

Modern X-ray sources (particularly the X-ray free electron laser) are sufficiently intense to enable some studies that are simply impossible with neutrons (e.g., studies of thin films of Van der Waals materials down to the monolayer limit). Thanks to increases in available beam intensity and improved energy resolution, inelastic X-ray scattering can even be the technique of choice for studying phonons in crystals, a task normally accomplished using neutron scattering. The advantage of X-rays is that measurements can be successfully carried out in samples that are too small to generate detectable inelastic neutron scattering signals.

In one interesting recent example, Dimitri Reznik and collaborators[2] were able to use beamlines at RIKEN and at APS to measure the temperature dependence of acoustic phonon dispersion in small crystals of Fe-based superconductors that have nematic phase transitions. This important measurement took excellent advantage of steadily improving beamline characteristics and instrumentational flexibility to achieve an important scientific result.

X-ray scattering can also be the only option available in some materials in which unusual nuclear physics details make it difficult to use standard neutron scattering techniques. One important example is compounds containing iridium, which are difficult to explore using neutron scattering because the most common iridium isotope has a large cross section for neutron absorption.

X-rays also have important limitations compared to neutrons, especially in probing magnetism and biological or soft condensed matter. In biological matter, the role of light elements like hydrogen, which are nearly invisible in

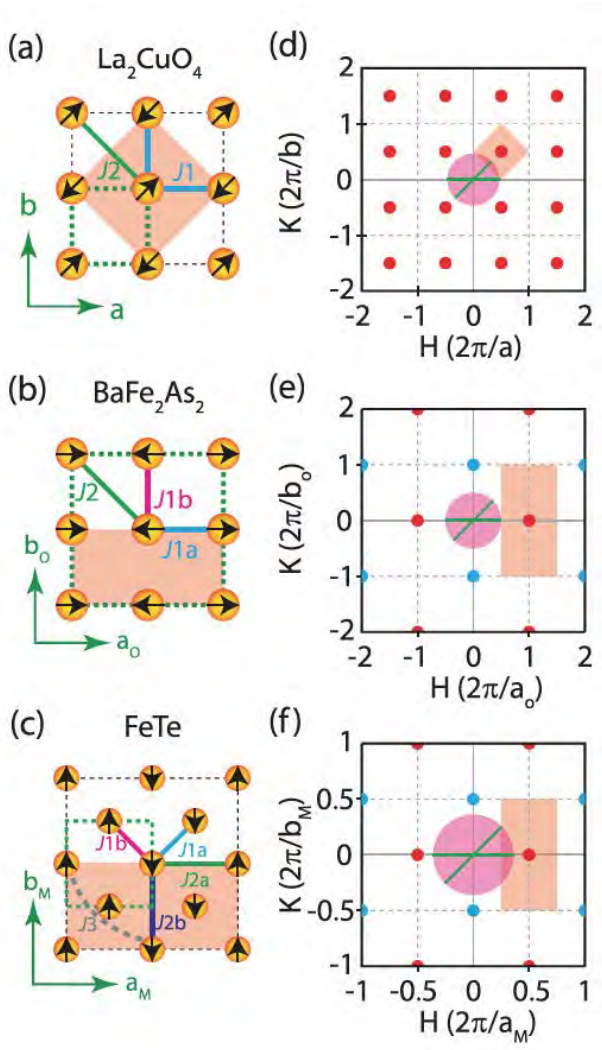


FIGURE 1e.1. Real and momentum space lattices of several compounds. The circles surrounding zero momentum show the region of momentum space accessible to resonant inelastic X-ray scattering, while the squares mark complete Brillouin-zones studied by neutron scattering.

Source: "Antiferromagnetic Order and Spin Dynamics in Iron-Based Superconductors," Pengcheng Dai, Reviews of Modern Physics, *87*, 855 (2015).)

X-ray studies, is essential. Because the neutrons interact only with nuclei and not with electrons, useful scattering signals can normally be achieved without causing radiation damage. Element specificity can sometimes be achieved in neutron scattering by isotope substitution, and this is particularly valuable in biological matter studies where deuterium can be substituted for hydrogen.

X-rays see magnetic properties in a less direct way than neutrons, and typically with poorer energy resolution and weaker signals that are more difficult to interpret quantitatively. In X-ray scattering, the dominant magnetic signal typically comes from the response of the electronic system to the X-ray's electric field, which

is normally characterized by its conductivity at X-ray frequencies. In magnetic systems the conductivity at X-ray frequencies has an antisymmetric Hall contribution, analogous to the Kerr or Faraday response at optical frequencies. Although this response can be viewed as a magnetic order parameter, its relationship to the moment distribution in the material is not as direct as the corresponding relationship for neutrons. Typically the magnetic signal in inelastic X-ray scattering must be enhanced by taking advantage of a core-to-valence resonance. The energy of this resonance sets the X-ray wavelength, and hence the maximum excitation momentum that can be probed in a resonant inelastic scattering experiment. As illustrated by the examples in Figure 1e.1, for some materials this can leave the momenta of greatest interest outside the range that can be explored.

In addition to this fundamental limitation, the energy resolution that can be achieved with resonant inelastic X-ray scattering is not yet competitive with what can be achieved with neutron scattering. Furthermore, because X-rays are absorbed by most materials, it is technically difficult to surround samples within environments such as magnetic field coils, hydrostatic pressure cells, and dilution refrigerators. On the other hand, these are easily accommodated in neutron scattering setups.

Finally, due to the large absorption coefficient of air at soft X-ray energies, X-ray scattering samples must be placed in a vacuum, imposing severe limitations on sample environments, scattering geometries, and sample changes. ■

BOX: Oxide Heterojunction Magnetism

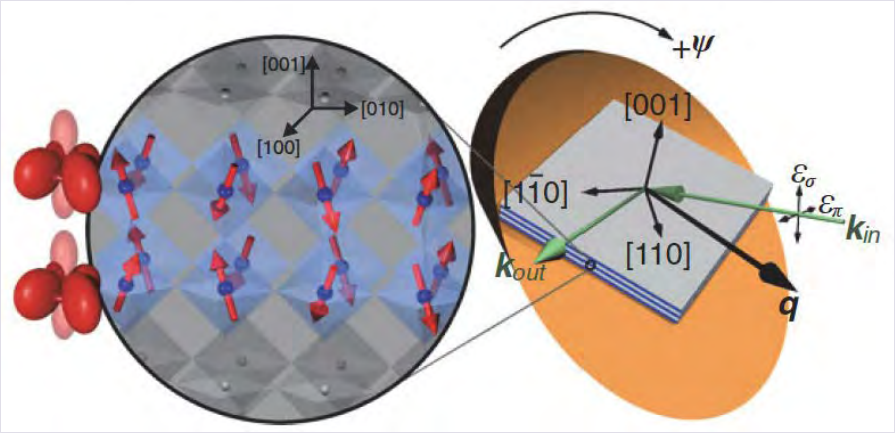


FIGURE A. Schematic illustration of resonant X-ray diffraction from a thin film of $LaNiO_3$ that is only two layers thick. Frano et al. were able to demonstrate that these films order magnetically, whereas films of larger thickness do not.

Source: Illustration from Alex Frano, "Spin Spirals and Charge Textures in Transition Metal Oxide Heterojunctions," Springer Theses [2014]. ISBN 978-3-319-07069-8

Resonant X-ray scattering can sometimes reveal magnetic order that would not be detectable using neutrons. In an important experiment, Frano et al.* were able to measure magnetic diffraction from the magnetic order in a very thin films containing only two layers of $LaNiO_3$ by scattering resonantly at a nickel p-core to d-valence transition. LaNiO3 is a member of a family of rare earth nickelates, many of which have an interesting type of non-collinear magnetic order. However, bulk $LaNiO_3$ is a non-magnetic but highly correlated metal. Frano et al. demonstrated that $LaNiO_3$ films are magnetic when two layers thick, but that the magnetism is lost already at three layer film thicknesses. This experiment demonstrates the potential of oxide heterojunctions for tunable strong-correlation physics, and for tunable magnetism that may be valuable in spintronics.

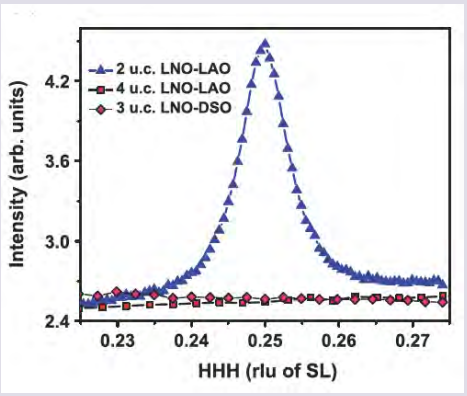


FIGURE B. Resonant X-ray magnetic diffraction peak which demonstrates magnetic order in two-unit cell thick films of $LaNiO_3$ on $LaAlO_3$. Magnetism does not appear when the $LaNiO_3$ film thickness is larger than two layers.

* Orbital Control of Non-Collinear Magnetic Order in nickel oxide heterojunctions," Phys. Rev. Lett. 111, 106804 (2011).

2. Industrial Applications of Neutron Scattering

This section offers a perspective on industry use of neutrons from reactors and spallation sources for research and development. These sources are available only at dedicated facilities. In the U.S., such facilities are found at a few national laboratories (Los Alamos, Oak Ridge, and Idaho National Laboratories, as well as the National Institute of Standards and Technology). They are also found at more than 20 universities with research reactors. Industrial research often involves staff both at the company and at the neutron center. Industry staff are typically generalists tasked with solving problems relevant to the company, whereas those at a neutron center are of course experts in their particular type of neutron research.

Research reactors and spallation sources have different characteristics. While some work can be done more or less equally well at either, some studies are better or uniquely performed with only one source type. Industrial uses that are uniquely suited to research reactors include isotope production and materials testing, both of which are covered elsewhere in this report. Many of the uses described in this chapter can be performed at either type of source. In many cases, research reactors—by virtue of the number of scattering stations they can support—offer more prompt user access or faster data collection than spallation sources, which is often important to schedule-driven users from industry.

2a. Industrial Applications

Neutron scattering and imaging provides unique contributions to the discovery, development, and processing of new and improved materials for industrial applications owing to the way in which they interact with matter. Neutrons interact only with the atomic nuclei in a material. As a consequence, dense materials are easily penetrated, so that complex systems (e.g., an operating internal combustion engine,[1] batteries,[2] or water flow in a fuel cell[3] can be observed *in operando*. Frequently, neutron studies are components of a suite of measurement techniques that are needed to untangle a multi-disciplinary issue.

The large cross section for neutron scattering from hydrogen, and especially deuterium, make neutrons especially well-suited for exploring organic, polymer, and biological materials and structures. Industrial researchers, often in collaboration with others, have tackled such challenges as:

- in situ studies of molecular alignment in semi-crystalline polyethylene during processing[4]
- the effect of branching and molecular weight on catalytic properties of polymers[5]
- the shear-dependent interactions on dispersion and viscosity in paint and coating formulations[6]
- the stability, structure, and flow properties of biodegradable surfactant vesicle dispersions used in products such as fabric softener,[7] and
- the atomic and molecular-level details of the interaction between different adhesives and their substrate.[8]

The biopharmaceutical industry applies neutron scattering to topics such as: understanding the effect of drug preparation on stability and shelf life;[9] elucidating the structures and processing effects on drug viscosity, with implications for delivery;[10,11] and optimizing drug processing and formulation.[12]

The oil and gas industries employ neutron scattering as one of a suite of techniques to understand the composition and molecular structures of non-traditional petroleum sources including heavier non-volatile components, leading to enhanced oil recovery.[13] It is also useful for determining the architecture and connectivity in gas-bearing shale.[14] Alternative energy technologies have also benefitted from neutron studies. For example, fuel cell development has been aided by neutron radiography studies that enabled visualization of water flow in a PEM fuel cell as a function of water channel geometry, material, and surface.[15]

In the transportation industry, neutron diffraction and imaging have provided useful insights into the residual strain in single crystal high-performance turbine blades.[16] Neutrons are also useful for detecting corrosion, for example in aluminum aircraft components,[17] although the major interest in that case is in a portable system rather than a reactor or accelerator-based system. Interest in neutron studies extends

BOX: Exxon and Neutron Scattering

Exxon was an early adopter of neutron scattering, investigating systems of interest to the corporation since the early 1980s. This has resulted in science that impacts technology and also has impacted the broader scientific community through opening up areas of investigation now pursued by academic groups. The origin of soft-matter physics is traced to the researchers at Exxon from this period, and neutron scattering investigations significantly contributed to this area of study. Neutron investigations in this period and into the 90s were focused on several main themes: fluids for enhanced oil recovery, polymer blends, fluids in porous media, and fuel cells. Building on the impacts of these earlier studies, the corporation began to further explore areas in which neutron research could have an impact on technology. Starting in the early 2000s, the neutron work was extended to new areas: gas hydrate inhibitor polymers, polymers for cold flow of diesel, thermodynamics of petroleum, polymer composites, and residual strain in metal welds. The study of polymers for cold flow of diesel resulted in a commercial additive in use today, with extensive neutron scattering studies defining an optimized structure. In recent years, neutron investigations have helped with understanding the new class of hydrocarbon resource that has revolutionized the oil and gas industry via the rock structure of gas shale. There has also been a revolution in new understanding of polymer architecture, structure property, and deformation thanks to extensive new neutron scattering investigations.

ExxonMobil's leadership in industrial uses of neutron-based R&D extended to the development and deployment of new capabilities at user facilities. The ExxonMobil Participating Research Team built the 30 m Exxon/NIST SANS beamline at NCNR that was completed in 1991. It immediately superseded other SANS capabilities in the U.S. Its impact was felt immediately across the research community, particularly for soft matter research. A team of Exxon researchers led an active, highly productive research effort, becoming one of the best neutron programs in industrial research ever carried out, as documented in some of the examples cited in the previous paragraph. The Center for Interfacial Engineering at the University of Minnesota also joined the Exxon/NIST partnership and continues as a major user of NIST SANS instruments. The partnership continues to this day.

to the automotive industry, where investigations have used neutron diffraction to measure residual stress in weldments, an essential characteristic for predicting fatigue life.[18]

General Atomics has demonstrated that it considers neutrons to be important for sustaining the infrastructure for nuclear research and work on radioactive materials. Their EM2 advanced reactor provides an example of a major development effort that has run experiments at both HFIR and SNS. These investigations provide critical information on swelling and thermal conductivity during neutron irradiation, which is essential data needed for qualifying new fuels for nuclear reactors. ■

2b. Industry-Related Consortia for Use of Neutrons

Neutron scattering and imaging are complex and continuously evolving techniques whose sophistication precludes casual use. Reasonable familiarity with the field and the information that different neutron techniques can provide is necessary to have a sense of the types of R&D questions that are well-, or even optimally-suited to exploration with neutrons. This has led major neutron facilities to establish pre-competitive consortia and other means of supporting first-time industrial users that enable them to work with neutron science experts to learn the capabilities of neutron science, and optimize and apply neutron techniques to address their challenges.

nSoft is a NIST-based industrial consortium[1] with more than a dozen members across a range of industries. The consortium is designed to deliver technology and expertise in neutron-based measurement science to U.S.-based industrial researchers as they perform precompetitive research. The collaboration model is built around "expertise transfer" rather than traditional technology transfer, in recognition of the very significant knowledge and financial barriers to entry into neutron-based research. Researchers from member companies participate in non-proprietary research led by NIST staff at the NIST Center for Neutron Research (NCNR). Consortium members drive the research

topics, taking advantage of NIST expertise to develop new measurement methods, data models, and performance metrics in collaboration with member researchers. Member companies often station staff at NIST for extended periods. Staff at member companies gain expertise in the use of equipment and software appropriate for their business sector. The interaction also helps companies understand how neutron-based techniques might be applicable to other R&D challenges.

In the U.S., the Shull Wollan Center[2] provides a gateway for U.S. industry to use the High Flux Isotope Reactor (HFIR)/Spallation Neutron Source (SNS). Following the DOE Office of Science model for access to user facilities, industrial access for pre-competitive (i.e. non-proprietary) research is determined through the same proposal process that is used for all proposals for open research. Successful proposals are provided access at no cost to the researchers or their institution. Proprietary research is also possible on a full cost recovery basis.

The LANSCE accelerator at Los Alamos provides a test-bed for semiconductor irradiation damage used by many aerospace and computing companies.[3]

2c. Neutron Techniques with Potential Industrial Applications

In addition to the cases where industry is already making use of neutron techniques to develop and improve products, there are many instances where researchers in other sectors are developing and deploying new methods that are providing fundamental understanding that should have impact on the industrial sector.

One example is provided by VULCAN, located at the SNS at Oak Ridge National Laboratory.[1] The goal of VULCAN is to provide understanding of engineering and functional materials behavior under complex environments. The instrument is designed for deformation, phase transformation, residual stress, texture, and microstructure studies. In situ and time-resolved measurements are possible under many conditions, thanks to load frames, furnaces, battery chargers, and other auxiliary equipment that have been incorporated into the instrument. Capable of accommodating large specimens, spatial and time resolutions relevant to industrial problems are accessible. This unique instrument has been used for research of relevance to industry, frequently with industry collaborators, in areas including additive manufacturing, alloy development, and observation of manufactures parts under operating conditions.[2]

2d. Barriers to Broad Industry Use of Neutrons

Many challenges remain that affect industry perception of neutrons. Quick and easy access to the correct facilities is challenging for a potential industry user who lacks direct experience because they are expected to be problem-solving generalists. Even for common applications such as residual stress measurement, it is a challenge for the industry user to gauge how well validated the technique may be, regardless of the source. Industry users need access to consultation services when things are unclear to the engineer who is unlikely to be an expert in the method to be used. Making it easy for people in industry to find an appropriate beamline without preexisting knowledge would facilitate expanded application of neutrons (and advanced characterization in general). It is notable that the neutron community in Europe has taken some actions in this direction (for example, the SINE initiative), although this has now ended. Proprietary research at a neutron user facility in the U.S. requires that the company pay the full costs associated with its studies. While this may be reasonable for a business that has sufficient in-house expertise to know what neutron studies can (and cannot) provide, it is a significant barrier to entry for new users. Pre-competitive consortia or exploratory non-proprietary access is likely a reasonable first step for this population, since the financial barriers are low. Both experiences and new industry users need assurances and procedures that ensure that a number of conditions are fulfilled, including:

- IP will be protected (via, e.g., NDAs)
- Proper handling and control of data
- Export control is correctly followed
- Facilitation of remote operation so that multiple (industry) individuals can participate without having to travel

- Users have access to data during an experiment and after they return to their company
- Results processed to the point where they are comprehensible to non-expert users, as opposed to raw data that has to be processed by a specialist at the facility

The nSoft consortium at NIST addresses these issues for non-proprietary work. DOE may find it useful to consider an analogous model to provide non-proprietary access to its user facilities. In Europe, the Sine2020 Initiative (https://www.sine2020.eu) aimed to maximize industrial use of those neutron facilities but is no longer active. One target of opportunity was revenue generated from industrial use of their facilities to mitigate some of their funding issues. Another was to demonstrate their importance to sponsoring governments, along with encouraging internal investment in equipment and software appropriate to industry use such as handling heavy samples and remote operation. ■

2e. Summary

This brief examination of industrial use of neutrons demonstrates its significance as well as the breadth and depth of the applications. Advances in neutron sources and instrumentation have dramatically increased the universe of industrial problems that are amenable to study using neutron-based techniques. Despite the various challenges, there is no doubt that industry will continue to exploit the available facilities. Actions that could increase industrial demand in the future include:

- Continued and increased communication about the capabilities of neutron user facilities, with particular attention to industrial problems which are especially amenable to neutron studies
- Extensive support for first-time industrial users to ensure that they have a positive experience and come to appreciate the value of neutron studies in addressing their problems
- Continued development of advances in instrumentation and timely processing of data to provide information that can address important industry problems
- Clear communication about neutron source availability to give industrial users confidence that a facility will be available when they need it, or to give them sufficient time to identify alternative approaches to address their problems in the event of a long shutdown.

Acknowledgments

Dr. Michael Glavicic (Rolls-Royce) and Hubert King (ExxonMobil Research and Engineering Co.) are acknowledged for their input on industrial needs for, and uses of, neutrons. ■

3. Fundamental Physics at Reactors and Spallation Sources

Neutrinos and Neutrons from Reactors and Spallation Sources

Since the first observation of the free antineutrino by Reines and Cowan at the Savannah River reactor, fundamental physics at reactors in the United States has been at the forefront of discovery science. For decades, U.S. scientists have led experiments investigating the properties of neutrinos and neutrons from nuclear reactors and, more recently, spallation neutron sources.

Neutrons and neutrinos play a key role in fundamental and applied science and enable scientists to study the constituents of nuclei, search for new forms of matter, and understand the symmetries that govern fundamental laws of physics and the evolution of the Universe. Neutrons are also powerful probe of materials, and neutrinos carry the signatures of nuclear decays in fission processes making them a probe of nuclear reactions and a monitor of nuclear fuel.

Reactors and spallation sources are unique sources of neutrons and neutrinos. In reactors the fission products of heavy elements beta-decay and generate a large isotropic flux of electron antineutrinos along with the neutrons produced during the fission process. While the neutrons are guided out of the reactor core in beamlines to experimental stations, the antineutrinos are emitted isotropically. The antineutrino flux falls off with the inverse square law 1/R^2, making distances as close as possible to the reactor core a desired location for high-statistics experiments. The energy spectrum of emitted antineutrinos is determined by the nuclear beta decay energies. It peaks at ~4 MeV and ranges up to a maximum 10 MeV. Reactors are a pure source of electron antineutrinos making them ideally suited for neutrino oscillation studies and other experiments without backgrounds from other neutrino flavors. With its highly-enriched fuel, compact but powerful core, regular cycle of operations, and user facility, the High Flux Isotope Reactor (HFIR) at ORNL is a unique facility for research and scientific users from the U.S. and overseas. It has enabled a broad program of studies with neutrons as well as select neutrino experiments.

Neutrons can be created by nuclear reactions in reactors and accelerators. Spallation sources are the most intense accelerator-based neutron sources. They use a high-powered proton accelerator to generate a beam of protons on a heavy metal target. During the collision, free neutrons are generated from the heavy metals creating a directed beam of neutrons and neutrinos. The accelerator facility allows spallation sources to be generally pulsed, unlike most reactors that generate neutrons and neutrinos constantly while operating. With GeV proton energies in the primary accelerator, spallation sources create neutrinos with energies of tens of MeV, a distinct time structure and variety of neutrino flavors.

While research reactors and spallation sources are typically designed for the optimum production of neutrons, antineutrinos are a byproduct of these facilities. The abundance, energy spectrum, and flavor purity of antineutrinos from reactors and the pulsed time structure and direct beams of high-energy neutrinos from spallation sources make reactors and spallation facilities unique sources of neutrinos with complementary characteristics. They provide well-controlled laboratory environments that enable a suite of precision experiments for fundamental and applied science (See Figure 3.1 and Box 3.1).

Fundamental Science with Discovery Reach

Neutrons and neutrinos are key to our understanding of the constituents and forces of matter, the properties of elementary particles, and the symmetries of nature. Precision experiments using neutrons and neutrinos measure the neutron lifetime, probe the electric dipole moment, search for sterile neutrinos as a new form of matter, and constrain our understanding of nuclear reactions inside a nuclear reactor through precise measurements of the reactor neutrino spectrum. The neutron structure and the decay of neutrons are critical for describing matter and the visible world as we know it. The neutron lifetime is key to the synthesis of elements, and the charge distribution of neutrons may hold the clue to understanding the violation of CP symmetry and the resulting baryon asymmetry in the Universe.

Neutrinos, on the other hand, are point-like elementary particle with no charge and little mass. They

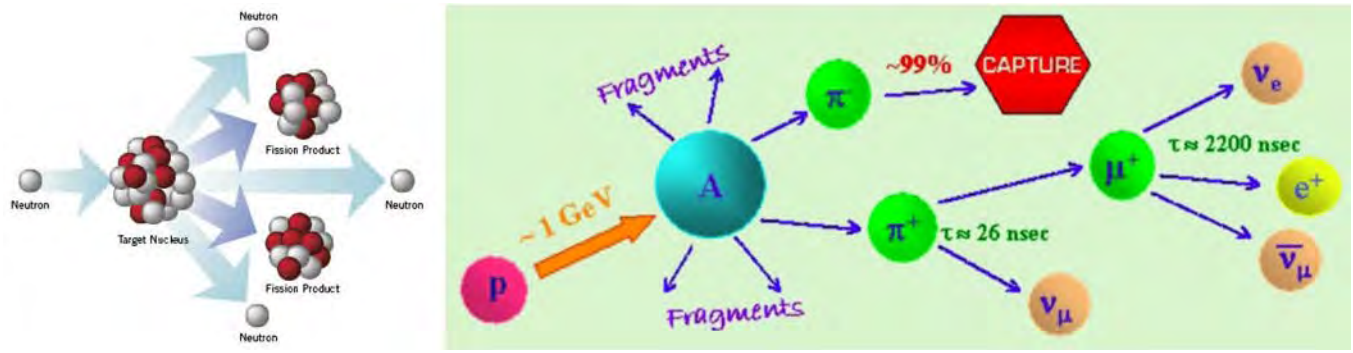


FIGURE 3.1. Left: Fission process in a nuclear reactor. The fission products beta-decay to produce a flux of pure MeV electron antineutrinos emitted isotropically from the reactor. Right: Neutrino and neutrino production in a spallation neutron source. Several neutrino and antineutrinos are produced from the pulsed beam of pions generated in the spallation process.

Sources: Nuclearconnect

BOX 3.1. High Flux Isotope Reactor – A Compact Source for Neutrino Science

HFIR is one of the most compact but powerful reactors available for neutrino science in the world. With a size of < 0.5m in height, a radius of 0.2m, and a power of 85MW it is an abundant "point" source of electron antineutrinos making it ideal for distant-depend neutrino oscillation studies and precision measurements using antineutrinos. With its highly-enriched fuel, > 99% of electron antineutrinos come from the fission of ^{235}U making it a spectroscopically clean antineutrino source. The regular operations cycle of HFIR allow for controlled signal and background studies.

Image: Model of the HFIR core fuel assembly

Source: PROSPECT collaboration

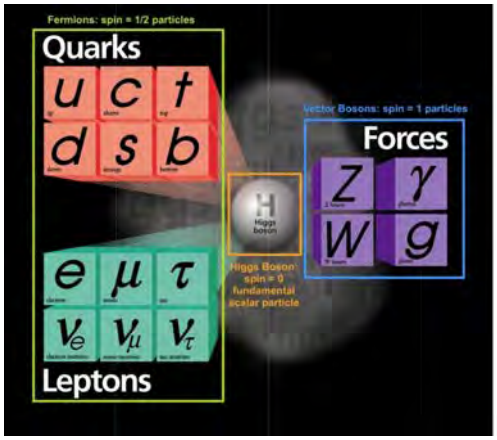
only interact through the weak interaction making them a clean probe of the principles and physics that govern the Standard Model of Particle Physics. Their weak interaction and little mass allow neutrinos to freely stream effectively through the Universe close to the speed of light making them effective carriers of energy through the cosmos. Neutrinos have played a key role in the evolution of the Universe and the formation of large-scale structures since the beginning of time.

Their tiny mass compared to other particles is a mystery, and a direct measurement of the neutrino mass is still outstanding. Since neutrinos have no charge, they may even be their own antiparticles. Understanding the Majorana nature of neutrinos through the search for neutrinoless double beta decay is one of the top priorities in neutrino science.

Since their postulate by Wolfgang Pauli in 1930, three Nobel Prizes (1995, 2002, and 2015) have been awarded for the observation and studies of neutrinos, the highest number of Nobel Prizes for any single particle. The 2015 Nobel Prize in Physics was awarded for the experimental observation of neutrino oscillation, a quantum mechanical transition of one neutrino flavor into another.

Understanding the properties of neutrons and neutrinos holds the key to some of the biggest and fundamental questions in physics.

- Why does the Universe have matter?
- How were the elements made in the Big Bang?
- What is the nature of physics beyond the Standard Model? (See Figure 3.2)



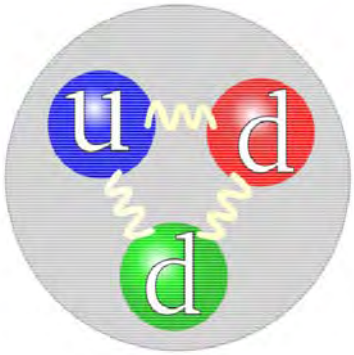


FIGURE 3.2. Left: Neutrinos are elementary particles with no charge in the Standard Model of Particle Physics. Right: The neutron is a composite particle consisting of 3 quarks held together by gluons, the carrier of the strong fore.

An Experimental Quest

Studies of neutrons and neutrinos require highly sensitive detectors to discern the interaction and faint signatures of these neutral particles. Advanced instrumentation and novel detector concepts are critical to the recent discoveries in the field. The fundamental physics studies with neutrinos and neutrons at reactors and spallation sources have led to a broad experimental program with a range in size, cost, and timeline.

From the COHERENT project's smallest neutrino detector (not larger than a milk carton) to the EDM mid-scale experimental facility for the study of the neutron, scientists have developed a variety of custom approaches to study the unique properties of these particles. Fundamental physics experiments with neutrinos and neutrons are typically custom-designed instruments following years of R&D advancing the frontiers of technology, materials and instrumentation. The development of neutron and neutrino experiments for fundamental science also enables a synergistic program in applied science ranging from the development of sensitive neutron detectors for portal monitoring to reactor monitoring and nuclear non-proliferation studies through neutrino detection.

For years, U.S. scientists and experiments at U.S. facilities have led the field in understanding the neutron lifetime and electric dipole moment and in probing the nature of neutrinos and properties of neutrino oscillation. The HFIR and the SNS facilities at Oak Ridge National Laboratory have provided a unique environment for studying fundamental physics with neutrinos and neutrons.

The first unambiguous experimental observation of coherent elastic neutrino-nucleus scattering with the COHERENT experiment at the SNS confirms the prediction of a fundamental physics process predicted in 1974. The unique time structure of the accelerated beam and the synergistic use of neutrinos from the SNS made this discovery possible. (See Box 3.2.)

The Spallation Neutron Source is host to a suite of experiments in neutron science. Among them is the U.S. neutron EDM experiment, one of the most technically challenging and ambitious fundamental physics experiments in nuclear and particle physics. By pushing the technological capabilities of every single part of its experiment, the nEDM project aims to improve sensitivity in the study of the neutron electric dipole moment by a factor of 100, thereby resolving whether the neutron electric dipole moment can explain the observed matter/antimatter asymmetry in the Universe. (See Box 3.3.)

The High Flux Isotope Reactor is a unique source of reactor antineutrinos in the U.S. with user access. Over the years, it has enabled the study of reactor antineutrinos and nuclear processes with a variety of small R&D efforts. PROSPECT was the first particle physics project at HFIR designed and built in collaboration with ORNL leveraging the unique features of the HFIR facility. PROSPECT was designed to measure the flux and energy spectrum of reactor antineutrinos from HFIR in search of short-baseline oscillation as a signature of sterile neutrinos. PROSPECT reported its first results in 2018, leading the worldwide effort in the search for sterile neutrinos at research reactors and probing our understanding of the nuclear reactor data and models (See Box 3.4.)

The range of the experimental neutrino program at both HFIR and SNS is currently constrained by the size of the available experimental space near the reactor core and the beamline. The shielding requirements for surface-based neutrino detectors make the placement of detectors particularly challenging, and it is difficult

BOX 3.2. Precision Studies of Reactor Antineutrinos with PROSPECT

PROSPECT, the Precision Reactor Oscillation and Spectrum Experiment, is located at HFIR at a distance of < 10m from the reactor core. PROSPECT measures the relative flux and energy spectrum of antineutrinos emitted from the reactor as a function of distance from the core with a surface-based detector using a novel, segmented ^{6}Li-doped liquid scintillator detector. PROSPECT demonstrated the successful measurement of reactor neutrinos with a surface-based detector with high signal-to-background, and made the first modern measurement of the reactor antineutrino spectrum from ^{235}U in a highly-enriched reactor. The results form PROSPECT yield some of the world's most stringent limits on the existence of eV-scale sterile neutrinos as a new form of matter and inform the nuclear modeling of the reactor neutrino spectrum. PROSPECT was designed, built, and operated with a collaboration of 10 universities, three national laboratories, and the National Institute of Technology. It draws on the multidisciplinary expertise of the collaborating institutions in particle physics, nuclear science, as well as instrumentation development and applied science. PROSPECT uses synergistically the "free" flux of antineutrinos emitted by HFIR. Its scientific results are critical for understanding the properties of neutrinos as well as informing nuclear data for reactor modeling and R&D for safeguard and reactor monitoring purposes.

HFIR was chosen as the preferred site for the PROSPECT experiment following a detailed characterization of backgrounds at several high-powered research reactors in the U.S. and an extensive evaluation of site characteristics including ease of access, infrastructure, and user support.

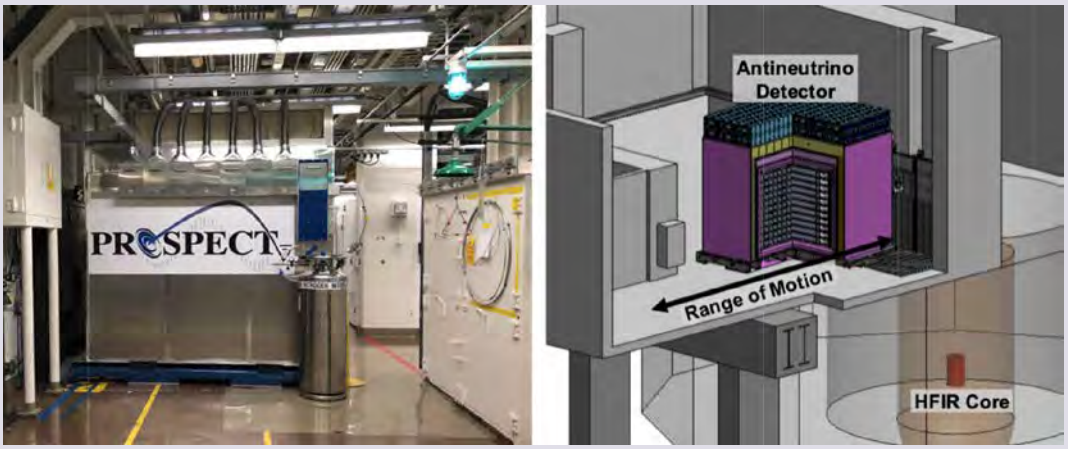


FIGURE A. Left: The PROSPECT detector inside its containment and shielding package inside HFIR next to the reactor wall. Right: Conceptual drawing of the PROSPECT detector with regards to the location of the HFIR reactor core.

Sources: PROSPECT collaboration

FIGURE B. Assembly of the segmented PROSPECT detector at the Yale Wright Laboratory prior to its shipment to ORNL/HFIR

Source: Yale/PROSPECT collaboration

BOX 3.3. Probing the Neutron Electric Dipole Moment and CP Symmetry

The neutron electric dipole moment (EDM) is a measure of its charge distribution. A permanent, non-zero electric dipole moment would violate both parity (P) and time reversal symmetry (T), and indicate that the neutron charge distribution is not perfectly round. A non-zero neutron EDM might explain the matter antimatter imbalance in the Universe. Violation of the CP symmetry has been observed in weak interactions and is part of the Standard Model of Particle Physics via a CP-violating phase, but its amount is too small to explain the baryon asymmetry.

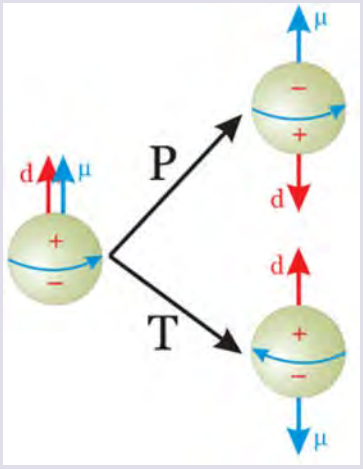


FIGURE A. Parity (P) and time-reversal (T) violation due to an electric dipole moment.
Source: Wikipedia

ORNL has had a long-standing history in this field. The first measurement of the neutron EDM in 1950 by Smith, Purcell, and Ramsey using neutrons from the Oak Ridge Reactor showed the roundness of the charge distribution to better than one part in a million. Since then, precision has improved by more than 6 orders of magnitude. The nEDM experiment under preparation at the Fundamental Neutron Physics Beamline at the Spallation Neutron Source will improve on this result by another factor of 100. The proposed measurement will utilize a large density of ultracold neutrons (UCNs) that will be produced through a superthermal process involving scattering off of excitations in superfluid Helium. The UCNs will be stored in a material bottle in strong electrical fields for times longer than their decay lifetime.

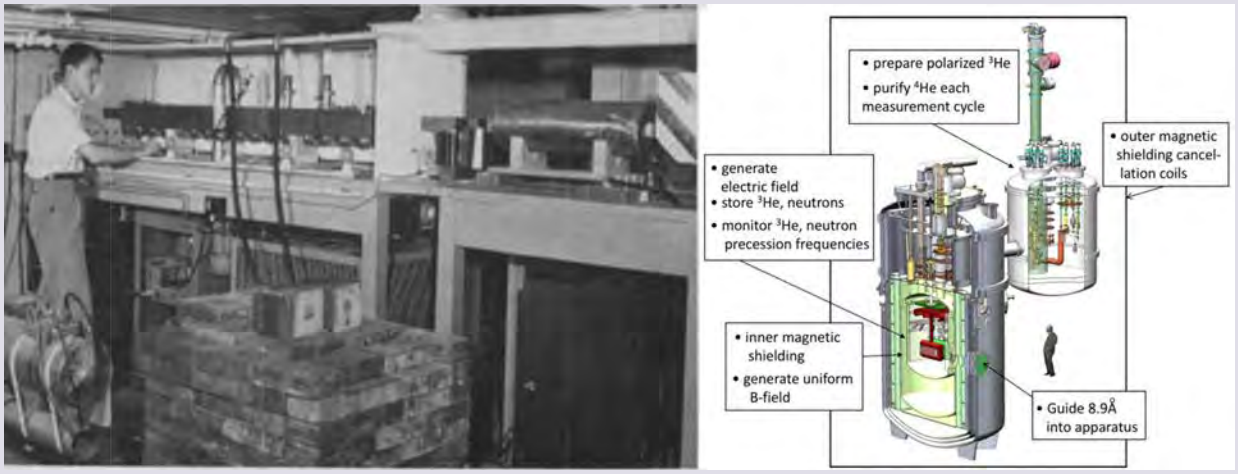


FIGURE B. Left: First measurement of the neutron electric dipole moment at the Oak Ridge Reactor in 1950. Right: Conceptual drawing of the planned nEDM experiment.
Source: Oak Ridge National Laboratory – The News

BOX 3.4. First Observation of Coherent Elastic Neutrino-Nucleus Scattering of Neutrinos

Coherent Elastic Neutrino-Nuclear Scattering is a process predicted by the Standard Model of Particle Physics. It was first predicted in 1974 by Freedman, and was finally observed in 2017 by the COHERENT collaboration. The process depends on the nuclei used as a target, and is a sensitive probe of the underlying physics of coherent scattering of neutrinos off nuclei. The experimental detection requires a source of low-energy neutrinos and detectors that contain nuclei of optimal mass. The SNS provides an intense flux of neutrinos in the few tens-of-MeV range, with a sharply-pulsed timing structure that is beneficial for background rejection. In 2017, Akimov et al. observed this process with 6.7sigma confidence by using a comparatively tiny, 14-6 kg sodium-doped CsI scintillator exposed to neutrinos from the spallation neutron facility. This measurement makes use of the distinct time structure of the neutrino beam from the SNS which enhances the background rejection in the signal. The discovery places tight bounds on exotic interactions beyond the Standard Model of Particle Physics.

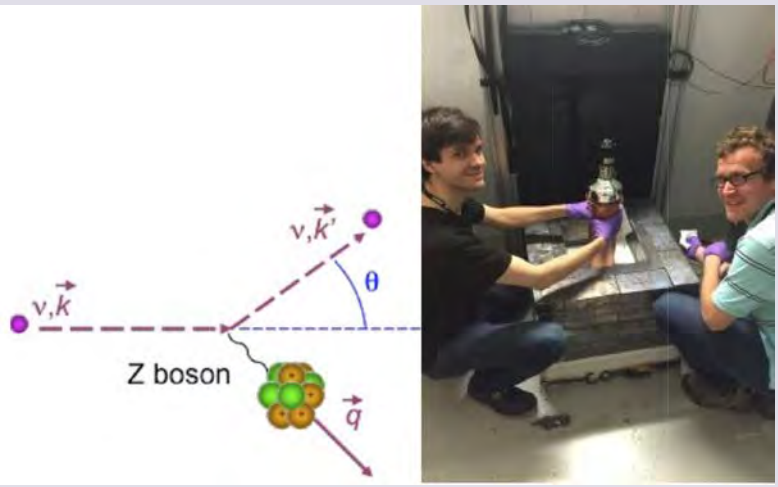


FIGURE A. Left: Coherent scattering process of neutrinos off nuclei. Right: Assembly of the CsI[Na] detector at the SNS. The CsI[Na] detector is the world's smallest working neutrino detector at 14.6 kg and has been operational at the SNS since July 2015. The CsI[Na] crystal is shielded with low background materials and instrumented with a super-bialkali photo-multiplier tube

Source: COHERENT Collaboration

to retrofit current available space. While the direct beam of neutrinos at the SNS and their time structure allows detectors to be farther away and provides experiments with an additional background rejection, the isotropic emission of antineutrinos from reactors demands experiments to be located as close as possible to the core.

The PROSPECT experiment was designed into the available space inside the HFIR building next to the core containment wall, but its sensitivity and scientific reach were limited by the available space and floor loading capacity. A dedicated shielded room for neutrino detectors and detector R&D at HFIR would provide the U.S. community with a unique and world-leading capability to advance the field. It would provide the neutrino program at ORNL and HFIR with a range of opportunities spanning fundamental particle physics, nuclear physics, and applied detector development.

Over the years, neutrino experiments at ORNL have made opportunistic use of the neutron (and neutrino) sources at HFIR and the SNS, leading to a series of impactful results and first measurements in neutrino science. The ease of access to HFIR and SNS, the ORNL user community, and to existing infrastructure were critical for the success of these experiments. The neutron program continues at dedicated beamlines, but would also benefit from increased space and user access.

Future Opportunities, Synergies, and Outlook

Neutrons and neutrinos are a unique way to study the fundamental forces of nature. HFIR and SNS at ORNL are operated as user facilities for neutron and materials science and isotope production. Until now the scientific community has made creative and opportunistic use of these facilities for a fundamental physics program. And yet the neutron and neutrino programs in the U.S., at ORNL in particular, have obtained world-leading results with highly visible impacts. The recent results in neutrino physics from COHERENT and PROSPECT,

as well as the planned nEDM project define the state of the art in their respective fields. Their proximity and co-location on the ORNL campus have created a new and growing user community for neutrino science.

The fundamental physics program with neutrons and neutrinos is carried out by multi-institutional collaboration including other national laboratories, universities and research institutes, and has created a fertile environment for multi-disciplinary R&D and discovery science. The neutron and neutrino programs at ORNL are examples of truly synergistic programs that leverage BES facilities across the portfolio of activities in the Office of Science from experiments in High Energy Physics (HEP) and Nuclear Physics (NP) to instrumentation R&D for nuclear non-proliferation.

With a potential upgrade to HFIR or a new research reactor facility, there is an opportunity to establish an experimental laboratory with a well-planned research program. We can move from being opportunistic to a more strategic plan for fundamental physics that includes discovery science, development of novel instrumentation and detectors, and workforce development and training.

Dedicated laboratory space for neutrino experiments, detector R&D, and fundamental physics at a reactor or spallation source are at a critical shortage and represent the most urgent needs to advance the field. A dedicated fundamental physics laboratory at an upgraded HFIR or a new reactor could have a transformative impact on the field of fundamental physics and the synergistic and collaborative effort of scientists within the Office of Science. ■

4. Isotope Production

4a. Isotope Production at HFIR

Since the advent of the nuclear era, the use of radioactive isotopes has brought tremendous benefits to society in a multitude of ways, from expanding our knowledge of the world around us to improving the lives of millions of people through medical diagnoses and treatment. No fewer than 16 Nobel prizes have been awarded in the fields of nuclear chemistry and applied radiochemistry. The use of radioactive isotopes has allowed researchers to answer a myriad of questions about wide-ranging subjects from plant metabolism and ocean currents to the behaviors of ancient peoples and indigenous trade routes. Radioactivity has brought immeasurable benefits to industry as well, allowing the analysis of material densities, the inspection of critical systems, and product sterilization, while radioactive tracers have been integral in oil and gas exploration and monitoring fluid flows and detecting leaks in remote and inaccessible networks.

In healthcare, radioactivity and radioisotopes have been instrumental in diagnosing and treating disease, improving the lives of millions of people. Ever since ^{131}I became the first radioisotope approved by the U.S. FDA in 1951 for treatment of thyroid cancer, researchers and clinicians have employed numerous additional radioisotopes for both diagnostic and therapeutic applications. Technetium-99m is used in over 16 million people per year in the U.S. as an imaging agent for numerous applications, with the most frequent use being heart perfusion studies and bone cancer diagnoses. Recently approved by the FDA, ^{177}Lu is showing tremendous success in markedly improving progression-free survival in patients with metastatic gastroenteropancreatic neuroendocrine tumors, and is showing great promise in clinical trials in the treatment of patients with prostate cancer.

The vast majority of radioactive isotopes used in medicine, industry, and research are produced by irradiating materials (targets) with neutrons in nuclear reactors. While numerous strategies are employed, the radioactive isotopes of interest are all created by atoms in the target capturing one or more neutrons. Our ability to generate radioactive materials in this way is primarily determined by two factors: the number of neutrons per second that impinge upon the target (the neutron flux density or n/cm^2·s), and the kinetic energy of the neutrons that interact with the target. Hence, while power reactors generate an order of magnitude or more neutrons per second than isotope production reactors, their neutron flux density is several orders of magnitude below facilities designed to produce isotopes. Moreover, because the probability of capturing a neutron increases dramatically as the kinetic energy of the neutron decreases, isotope production reactors are designed to have a high neutron flux density of thermal neutrons or neutrons with a most probable kinetic energy of 0.025 eV. ***Because the High Flux Isotope Reactor provides the highest thermal neutron flux density (2.5 x 10^{15} n/cm^2·s)*** of any reactor operating today in the western world***, it plays a unique role in producing critical radioactive isotopes for industry, medicine, and research.***

Californium-252 is used by industry as a small, robust, self-powered, economical source of neutrons for a wide range of applications including energy, homeland security, and agriculture. It has a half-life of 2.6 years, and 1 milligram of this isotope emits over 1 billion neutrons per second. The isotope is used by the nuclear energy industry to confirm the fissionable content of nuclear fuel rods and for determining the fissile content of nuclear waste. In addition, ^{252}Cf provides the source of neutrons needed to start up nuclear reactors, including those on nuclear powered submarines. The isotope is used by the mining and minerals industry to measure the amount of sulfur in coal, the ash and stone content of cement, and for oil well logging. It is also used as a calibration source to test the sensitivity of radiation detection equipment at ports of entry. The annual global demand for ^{252}Cf for these and other applications ranges from 20 to 40 milligrams per year and the HFIR is the only reactor outside of Russia capable of producing this isotope. The importance of the high thermal neutron flux at HFIR for producing an isotope like ^{252}Cf that requires multiple neutron captures is illustrated in Figure 4a.1. Aside from HFIR and the SM-3 reactor in Russia, the other research/isotope production reactors in the world have a peak thermal flux around 1 x 10^{14} n/cm^2·s. As shown in Figure 4a.1, ^{252}Cf cannot be produced at these lower thermal fluxes. Without HFIR, the western world would not have an independent, reliable supply of this critical isotope.

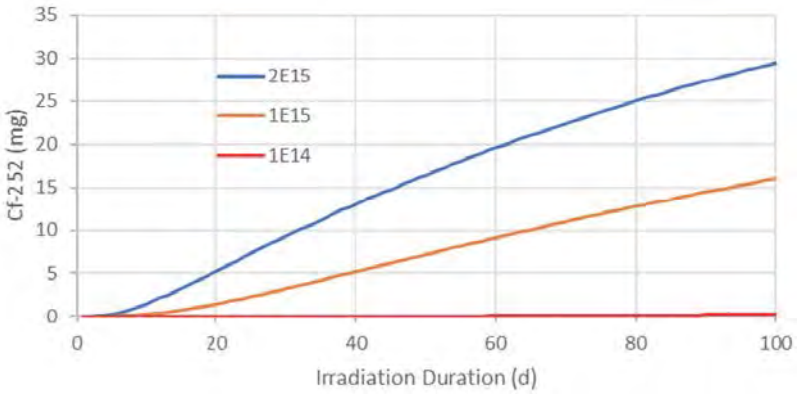


FIGURE 4a.1. Cf-252 production from a 7 gram mixed curium target at different thermal neutron fluxes

Source: Dr. Marc Garland, DOE Isotope Program

Nickel-63 is a low-energy beta emitter with a long half-life (100 y) that is available in a convenient physical form that enables repeatable, low-waste manufacturing of the radioactive source. Gas chromatography systems that utilize ^{63}Ni electron capture detectors are up to 1,000 times more sensitive than gas chromatography systems that use either flame ionization or thermal conductivity detectors. The applications of these systems include food and pesticide analysis, forensic toxicology, controlled substances identification, and environmental monitoring for greenhouse gasses. In addition, ^{63}Ni sources are used as the electron source in field deployable ion mobility spectrometry systems. These systems are extensively deployed by the Department of Homeland Security and the U.S. military for detecting trace amounts of explosives, narcotics, chemical warfare agents, and industrial chemicals in the field. As with ^{252}Cf, this critical isotope requires a high thermal neutron flux for its production and is only available from HFIR and the SM-3 reactor in Russia.

Barium-133 has a half-life of 10.5 y and emits a large number of gamma rays (ranging in energy from 30 to 400 keV) in its beta decay to stable ^{133}Cs. This multi-line gamma ray source is used to simultaneously monitor the oil, gas, and water flow rates in a system without any phase separation. Multi-phase flow meters based on this radioactive source provide detailed, real-time flow data to the oil and gas industry. Like ^{63}Ni and ^{252}Cf, ^{133}Ba is only produced at the high-flux reactors HFIR and SM-3. Industry reported to the committee that demand for both ^{63}Ni and ^{133}Ba exceeds the current production capacity of these two high-flux reactors.

Targeted radiotherapies based on alpha emitters are a promising new cancer therapy. Because of their short range in tissue, targeted α-radiotherapy (TAT) agents have great potential for application to small, disseminated tumors and micro metastases and treatment of hematological malignancies consisting of individual, circulating neoplastic cells. Because the energy deposited by the α particle in a cell is approximately four orders of magnitude greater than the energy deposited by a β^- particle, the relative biological effectiveness of α particles is much greater than that of β^- particles. In addition, the biological effectiveness of α particles does not depend upon hypoxia or cell cycle phase. As a result, far lower amounts of radioactivity are required to achieve the desired therapeutic outcome, which can be critical in those cases when the number of receptor sites is limited. The first TAT agent approved for clinical use by the U.S. FDA (May, 2013) is the *in vivo* α-generator radionuclide ^{223}Ra, which has a half-life of 11.4 d. In contrast to many single alpha-emitting isotopes, ^{223}Ra dramatically increases the therapeutic efficacy of endoradiotherapy as it emits four α particles in its decay chain, and the half-life of ^{223}Ra is long enough for the isotope to accumulate at the target site. ^{223}Ra-dichloride[1] is a targeted therapy for symptomatic bone metastases in prostate cancer, a common cause of morbidity and mortality in patients with metastatic disease. In metastatic castrate resistant prostate cancer patients, ^{223}Ra therapy improves the overall survival with a 30% reduction in mortality. While still under active investigation, the utility of ^{223}Ra therapy in bone metastatic disease in breast cancer and renal cell carcinoma appears very promising. The sole source of the parent radioisotope (^{227}Ac) used by Bayer to provide ^{223}Ra is from irradiation of ^{226}Ra targets at the HFIR followed by processing of this highly radioactive target material at a radioisotope processing facility at Oak Ridge National Laboratory. Both the high thermal neutron flux of HFIR and the close proximity of specialized radiochemical processing facilities are required to meet

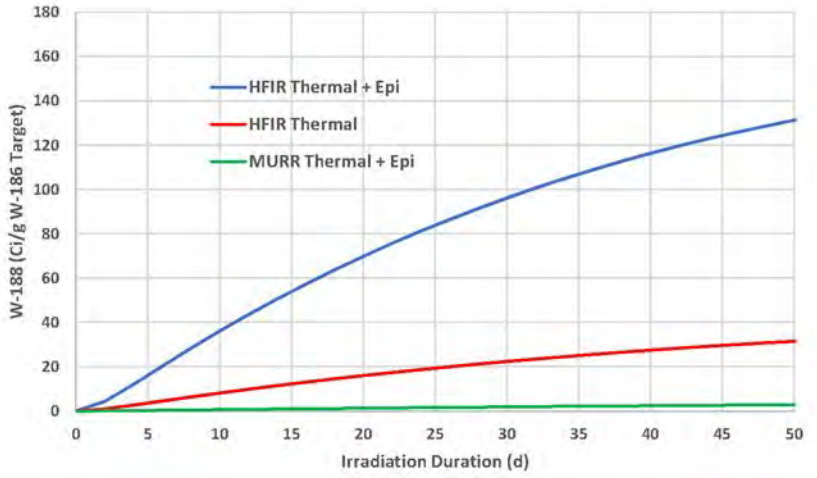


FIGURE 4a.2. A comparison of W-188 production at HFIR to what can be achieved at other research/isotope production reactors

Source: Dr. Dave Robertson, University of Missouri Research Reactor

the current and emerging demand for this important medical isotope.

In addition to the aforementioned isotopes, a high-flux reactor will be required to produce new, emerging life-saving radioactive isotopes. For example, industry is currently evaluating the use of ^{227}Th for the TAT treatment of multiple cancers including breast, prostate, mesothelin, and lymphoma. The advantage of using ^{227}Th is that it can be chemically conjugated to established targeting vectors like HER2, PSMA, MSLN and CD22. Again, only HFIR can provide the amount of this isotope that will be required when one or more of these TAT agents is employed in the clinic.

Another example is the use of ^{188}Re as the therapeutic agent in theranostics based upon ^{99m}Tc and radioactive rhenium. A driving force behind the clinical application of radiopharmaceuticals in precision medicine is the ability to selectively direct—or target—radiolabeled molecules to active sites of human disease. In order to effectively accomplish this goal, both a diagnostic (^{99m}Tc) and therapeutic (^{188}Re) radionuclide must be strategically attached to a biological targeting vector for delivery to a disease biomarker (e.g., a cancer-specific cellular receptor). Theranostic radiopharmaceuticals offer the unique opportunity to use information derived from patient specific diagnostic imaging studies to determine the therapy approach with respect to drug pharmacokinetics, biomarker density, and patient dosimetry. Because rhenium's chemistry is nearly identical to that of technetium, the availability of this therapeutic isotope would build on the more than thirty approved ^{99m}Tc imaging agents already approved by the U.S. FDA. As can be seen in Figure 4a.2, the high thermal flux of HFIR is required to produce any significant quantity of the parent isotope ^{188}W from which ^{188}Re can be generated in the clinic. ■

4b. Heavy Element Chemistry

The heaviest elements on the periodic table are the ones that we know the least about. The BES program on Heavy Element Chemistry (HEC) supports basic research on the fundamental chemistry of these elements, which are called actinide and transactinide elements. The goal of this research program is to understand the underlying chemical and physical principles that determine their behavior. The actinide series of elements are characterized as those elements with electrons in the 5*f* orbitals, which begins with thorium (atomic number of 90), and ends with lawrencium (atomic number 103) and a full inner 5f electron shell. Within this series of elements, thorium and uranium can be found in nature, but the remaining twelve actinides are not naturally occurring. The term "transactinides" is used to refer to all elements beyond the actinides—that is, those elements with atomic numbers larger than 103. According to atomic relativistic calculations, the filling of the 6d electron shell takes place in the first nine of the transactinide elements (those with atomic numbers 104 through 112). Consequently, they are currently placed as a 6d transition series under the 5d transition series. None of the transactinide elements are naturally occurring.

Understanding the role of 5*f* electrons is an important frontier for chemists, as this knowledge is essential

to fully grasp the fundamental properties of all matter, as exemplified by the periodic table. This includes fundamental insights into bonding, which drives physical properties and reactivity of the heavy elements, across multiple length scales. For example, the 5*f* orbitals participate in the band structure of metallic and ceramic materials that contain the actinides, and the nature of this participation down the actinide series is an area of active research. Theory and experiment show that 5*f* orbitals participate significantly in molecular actinide compounds (e.g., compounds required for advanced nuclear energy systems). Resolving the role of the *f*-electrons is one of the three grand challenges identified in the report *Basic Research Needs for Advanced Nuclear Energy Systems* (2006) and echoed in the report from the Basic Energy Sciences Advisory Committee, *Science for Energy Technology: Strengthening the Link between Basic Research and Industry* (2010).

The unique molecular bonding of the heavy elements is explored using theory and experiment to elucidate electronic and molecular structure, along with reaction thermodynamics. Emphasis is placed on:

1. The chemical and physical properties of these elements to determine their bonding and reactivity in solution, at the interface, and in the solid-state
2. The fundamental transactinide chemical properties; and
3. The overarching goal of resolving the *f*-electron challenge. (The *f*-electron challenge refers to the inadequacy of current electronic structure methods to accurately describe the behavior of *f*-electrons, in particular: strong correlation, spin-orbit coupling, multiplet complexity, and associated relativistic effects.)

Because much of this research is experimental, it requires manipulation of pico- to milligram quantities of plutonium and trans-plutonium isotopes, which are generated for researchers by irradiation of targets of actinide elements in HFIR. Initial production at the start of the HFIR program involved irradiating ^{239}Pu fuel to generate important activation products such as ^{244}Cm. Separations of elemental fractions of these isotopes were then completed. These separated fractions of trans-plutonium elements were then fabricated into new targets for subsequent irradiations to produce trans-curium activation products, as shown in Figure 4b.1.

This process of activating ^{239}Pu, separating the heavier elements that are created, and re-irradiating them to produce even heavier isotopes is the framework by which trans-plutonium elements are generated. These elements are essential to the researchers in the BES heavy element chemistry program.

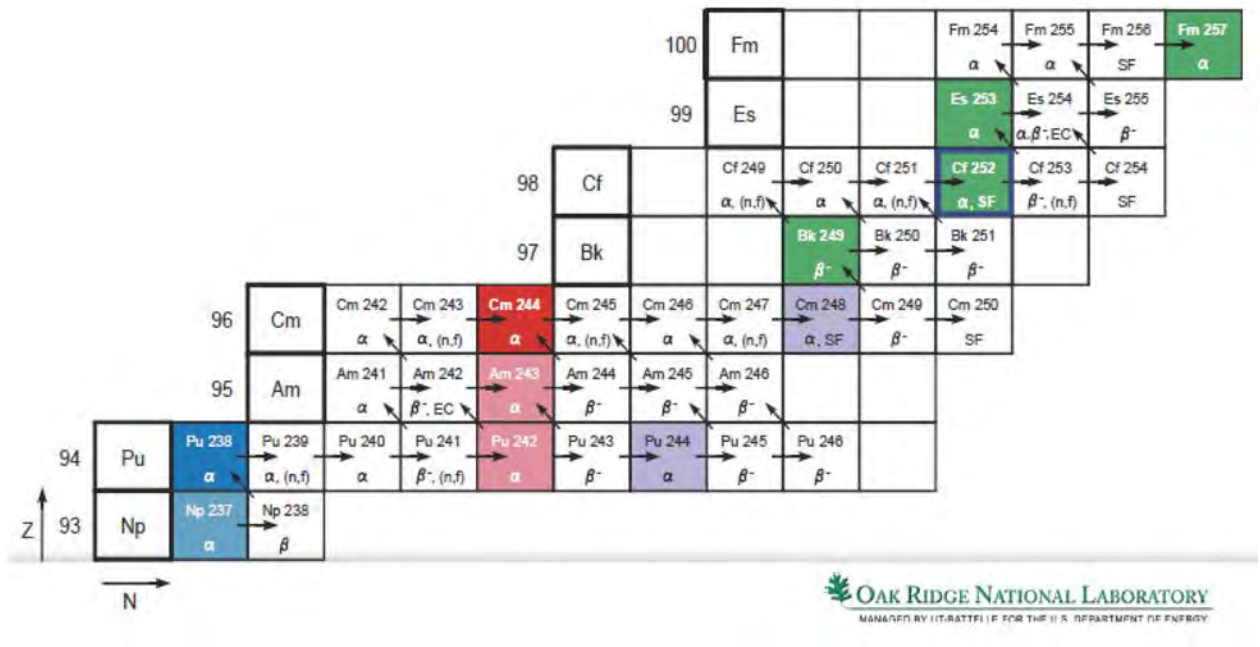


FIGURE 4b.1. Producing Trans-curium Heavy Isotopes
Source: Oak Ridge National Laboratory

Driving the activation of plutonium and curium isotopes to produce milligram quantities of the heavy elements requires larger neutron flux densities than that obtained by the fleet of U.S. commercial reactors. As illustrated in Figure 4b.2, the unique thermal neutron flux of (2.5×10^{15}) of HFIR is required to produce measurable quantities of very rare trans-plutonium and trans-curium elements. The isotopes of these elements have relatively short half-lives, and therefore must be continuously produced for the research community. Because multiple neutron captures are required to produce these heavy elements, they cannot be created at the lower neutron fluxes available at other research/isotope reactors.

Today, HFIR produces these isotopes in measurable quantities, as shown by Figure 4b.3. Over the last several years, heavy elements produced at HFIR were used in international collaborations to discover elements 114, 115, 117, and 118, and HFIR is currently providing targets of ^{244}Pu for the search for element 119.

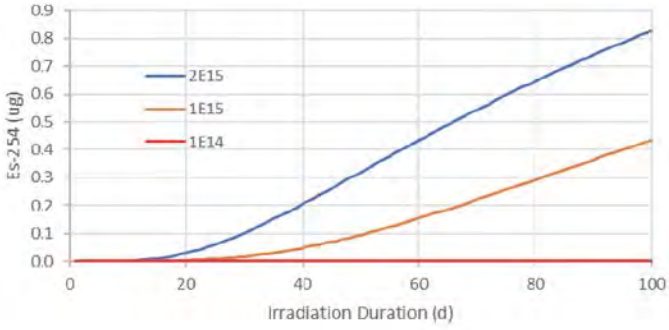


FIGURE 4b.2. Production of Es-254 at HFIR compared to the production that can be achieved with typical research and test reactors

Source: Dr. Marc Garland, DOE Isotope Program

Radiochemical Engineering Research Center (REDC)

In addition to irradiation in HFIR, production of these isotopes requires the ability to chemically separate the irradiated materials. These separations are done in the REDC. The REDC is a Category II multipurpose radiochemical processing facility based around the use of heavily shielded hot cells and is located immediately adjacent to HFIR. The historical mission of the REDC has been to provide Cf, Bk, Es, and Fm for research purposes and industrial uses. Post-irradiation separations of elements and the preparation of targets for irradiation are completed in hot cells in the REDC, with the heaviest isotope typically produced being ^{257}Fm. After separations and purification, actinide products are packaged and shipped to the research community as well as other users.

Heavy element processing campaigns are conducted approximately every 24 months, and BES staff canvass investigators in advance to identify needs for specific elements and isotopes for upcoming processing campaigns. The co-location of REDC with the world's highest thermal neutron flux reactor is critical for supplying researchers with the heaviest elements.

The BES program on HEC is the only source of funding for the discovery science associated with the actinide and trans-actinide elements. New knowledge generated by the HEC is fundamental to our understanding of matter and the periodic table, and the role of the 5*f* electrons in physical properties and reactivity across multiple length scales. This program requires the use of small quantities of these elements, which must be produced through neutron activation using the neutron flux density of HFIR and separated for use in the REDC. ■

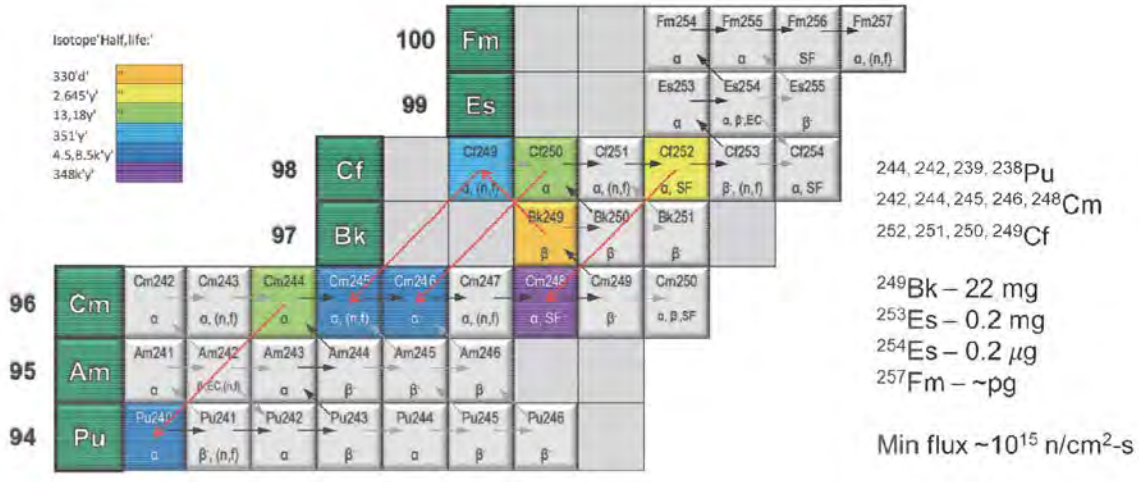


FIGURE 4b.3. Isotope Production Quantities

Source: Felker, ORNL, 2014

5. Materials Irradiation

5a. Materials Irradiation — General

Isotope production and materials irradiation testing in HFIR are very similar activities and use many of the same or similar experimental positions. The primary irradiation position with the highest neutron flux is the HFIR central flux trap. There are 31 target positions in the flux trap utilized for radioisotope production. Six positions in the outer area of the target basket are designated as Peripheral Target Positions (PTP) and shown in Figure 5a.1. The PTP has the highest fast-neutron flux available in the reactor (~1.2 x 10^{15}). A high fast neutron (> 1 Mev) flux is important for reactor materials irradiation testing because it accelerates the damage (as compared to lower power density reactors such as nuclear power plants) caused by the high energy neutrons.

HFIR produces the highest displacements per atom (dpa) of any operating thermal reactor today. This accelerated damage mechanism enables researchers to see results much faster, or to partially mimic the neutron spectrum of a fast reactor (e.g. liquid sodium or gas cooled reactors) or the radiation environment of a fusion reactor. It should be noted that the planned fast neutron Versatile Test Reactor (VTR) will have a higher dpa but will not be designed to replace HFIR or any thermal reactor that produces radioisotopes or performs nuclear materials testing for light water reactors (LWR). In addition, high powered pulsed or spallation neutron sources are unable to simulate the energy distribution and radiation fields found within operating reactors.

Flux Trap capsules (PTP and central facilities) can be full-length or a series of shorter capsules. These full-length or short capsules are static and only removed when HFIR is shutdown. The short capsules are stacked inside of a holder tube for easy handling, and HFIR coolant flow through this holder tube is critical to heat removal from the capsule experiments. Each experiment is designed to have neutron absorption characteristics equivalent to 200 g of aluminum and 35 g of stainless steel. These limits are established to minimize perturbation of the existing neutron flux in the target and a reduction in the fuel cycle length.

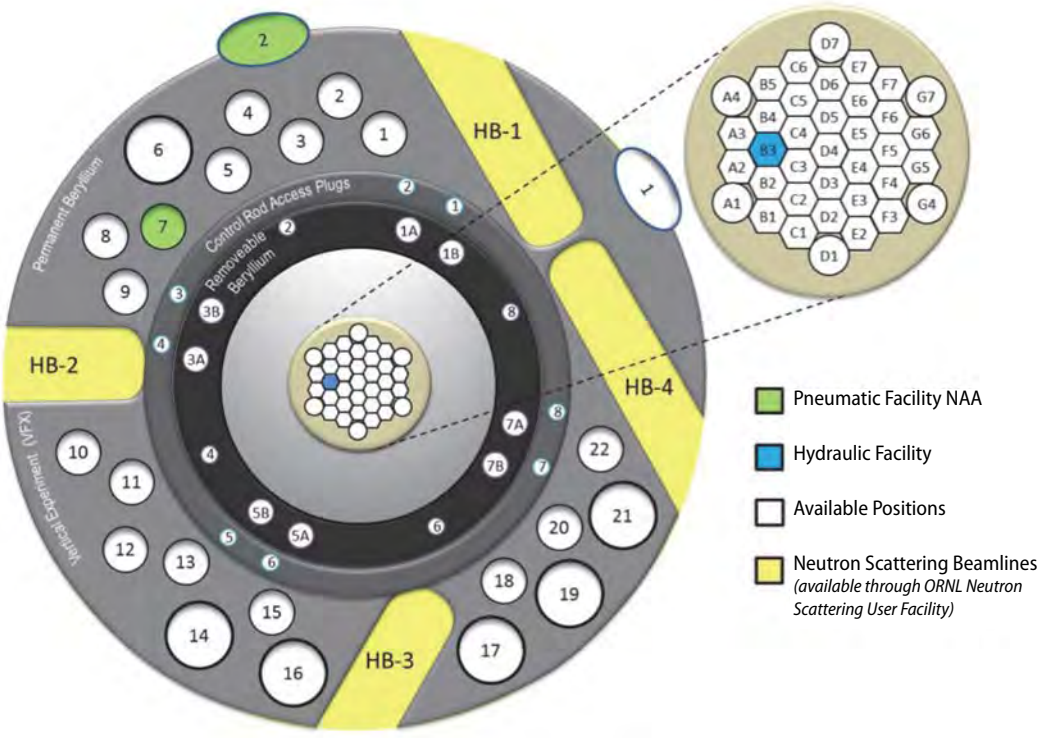


FIGURE 5a.1.
Es-254 Production from 7g Mixed Cm Target
Source: Oak Ridge National Laboratory

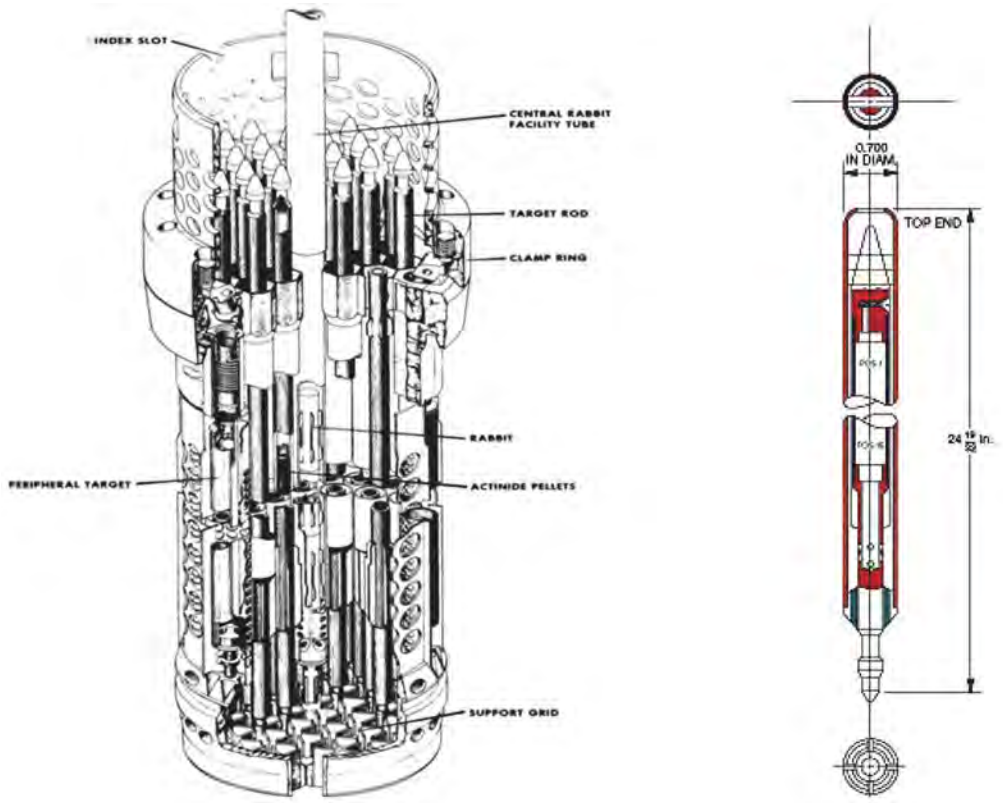


FIGURE 5a.2.
Target Basket and Example PTP Target

Source: Oak Ridge National Laboratory

As shown in Figure 5a.2, PTP capsules are typically 2.625 inches in length and are stacked in a secondary encapsulation for handling. The capsules have relatively limited internal volume to accommodate materials and fuels irradiation samples. There are currently six options for short capsule designs that are available with internal diameters less than 0.4 inch. All of these capsules are fabricated from aluminum with one capsule design perforated with 82 small holes to allow primary coolant flow to cool the internal sample.

To accommodate larger volumes for experiments, there are eight large and four small diameter positions in the removable beryllium (RB) reflector area. The large locations may have instrumented or non-instrumented experiments. Instrumented experiments may utilize thermocouples to monitor temperatures, and flow cooling or sweep gases as well as resistance heaters through the experiment to control temperature. Experiments in these locations may use neutron shields to tailor the spectrum for materials testing, but the quantity of neutron absorbing material is limited due to the proximity to the reactor fuel region and the potential impact to fuel cycle length and fuel element power distribution. Additionally, unshielded experiments in these positions are ideal for studying combination effects of fast neutron damage coupled with thermal neutron generation of helium (through transmutation) in certain reactor materials.

The HFIR thermal neutron flux levels in the flux trap at 85 MW are too high for most nuclear fuel designs. However, nuclear fuels and materials are routinely tested in the various beryllium reflector locations. The large Vertical Experiment Facility (VXF) positions are the furthest from the reactor fuel with thermal flux levels lower by a factor of five. The addition of thermal neutron absorbers can further reduce those levels as needed. The Large Removable Beryllium Facilities (RB*) directly adjacent to the reactor core may have the thermal neutron flux reduced by the use of Eu_2O_3 shields for nuclear fuels testing, but this is generally not required for non-fuel materials testing. Various fast and thermal neutron flux levels in HFIR experimental positions are given in Table 5a.1.

HFIR is currently supporting the DOE Advanced Fuels Campaign with a primary focus on accident tolerant fuels and clad materials. Irradiation of Fe-Cr-Al alloys, materials that could potentially replace traditional zirconium-based cladding materials, has been performed recently in the HFIR flux trap to evaluate the radiation tolerance of the material. To support more experiment sample throughput and reduce the time and cost of irradiation experimental programs, ORNL has

TABLE 5a.1
Irradiation Test Parameters in HFIR Experiment Positions

PARAMETER	FLUX TRAP	RB*	RB* SHIELDED	SMALL VXF	LARGE VXF
Fast Flux, E > 0.1 MeV (10^{14} n/cm^2 sec)	11	5.3	4.9	0.5	0.13
Thermal Flux (10^{14} n/cm^2 sec)	25	11	0.19	7.5	4.3
Peak displacements per atom (dpa) per cycle	1.8	0.67	0.58		

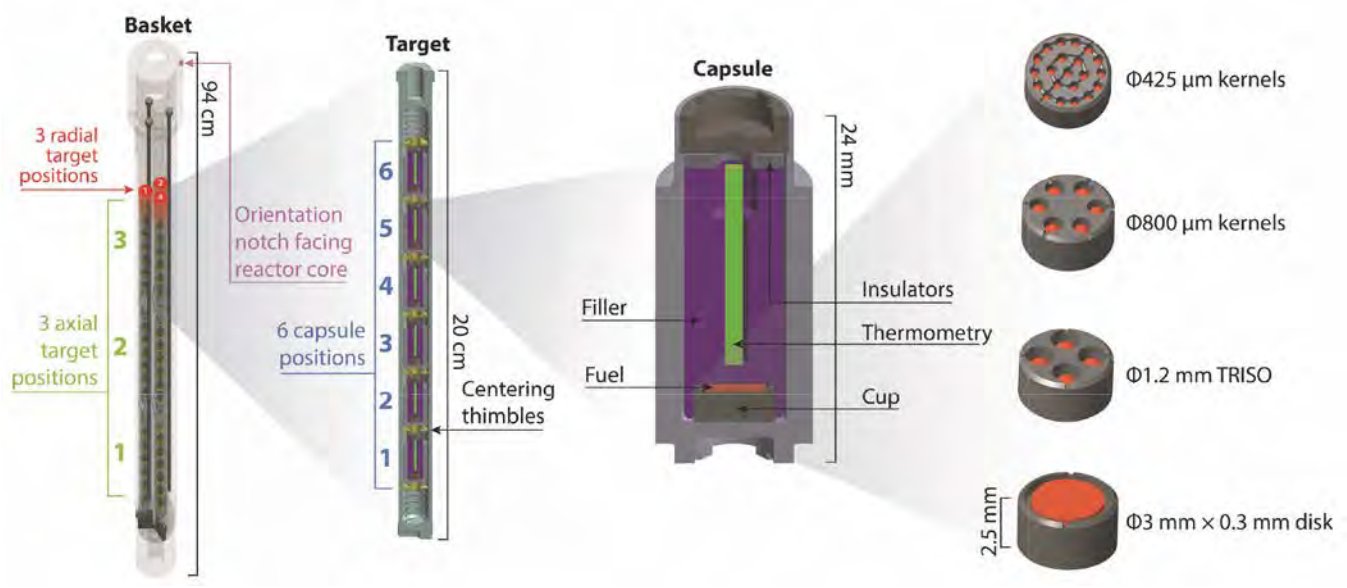


FIGURE 5a.3. HFIR MiniFuel Experiment System
Source: Petrie, Christian M., et al. "Separate effects irradiation testing of miniature fuel specimens." *Journal of Nuclear Materials* 526 (2019): 151783.

begun a new program to test nuclear materials. Rather than traditional nuclear fuel testing utilizing full-size pellets, the new approach uses much smaller samples (i.e. miniature) with more samples simultaneously irradiated to explore many more variations in fuel and materials design in one experimental campaign.

Various advanced fuel forms are currently being tested or planned for irradiation in the MiniFuel test facility. These materials include uranium nitride (UN) kernels, tristructural-isotropic (TRISO) UN particles, and fully ceramic microencapsulated (FCM) pellets. The facility allows concurrent and accelerated separate-effects irradiation testing of small fuel samples. These facilities may reduce the cost and time to perform nuclear fuel and material testing, but also compensate for the lack of irradiation test reactor capacity in the world today by increasing experimental throughput in the limited HFIR test positions. ■

5b. Fusion Materials Irradiation

The performance degradation of structural steels in nuclear environments may limit the extended operation of current generation light-water nuclear reactors and restrict the design of advanced fission and fusion reactors.[1,2,3,4,5,6,7,8] This neutron induced degradation to the physical and mechanical properties was first recognized by Eugene Wigner during the design of the Hanford production reactors during the Manhattan project.[9] The underlying physics controlling neutron radiation damage, and its consequence to physical and material property degradation, is inherently hierarchical and multiscale. Pertinent length and time scales controlling radiation effects range from neutron collision-reactions on the scale of the nucleus to the size and service lifetimes of structural components, spanning factors in excess of 10^{14} (length) and 10^{22} (time).[10,11]

Correspondingly, a valuable, albeit often underappreciated, component of the scientific contribution of reactor based neutron sources is the irradiation of materials to support the fundamental investigation of radiation degradation mechanisms and to spur the development of advanced fuels and structural materials technology for future fission and fusion reactors. As pointed out in the November 2019 presentation of Dr. Kurtz, "a high-performance, steady-state mixed spectrum nuclear reactor is an indispensable tool for fusion materials science research.[12] In particular, the HFIR provides a high dose capability associated with a high fast flux that enables material irradiations to produce more than 10 displacements per atom (dpa) per year in steels. This flux and damage production rate is currently the highest in the Western world, and enables scientific investigation into a number of challenging radiation damage phenomena, including questions related to:

- deciphering the irradiation and material variables controlling the nucleation onset of void swelling;
- developing predictive capability of phase transformations in complex alloys during irradiation; and
- determining the extent to which property degradation saturates under high dose neutron irradiation[13]

The study of radiation damage in fusion materials shares many commonalities with the degradation of fission structural materials in the neutron irradiation environment. As pointed out in the November 2019 presentation of Dr. Back,[14] this leads to a complementarity amongst the available research and test reactors within the U.S. (see Figure 5b.1) Smaller University based research reactors, like the MIT research reactor (MITR), provide lower neutron fluxes that can be appropriate for fundamental radiation damage studies and initial feasibility testing of novel materials.

Likewise, the Missouri University Research Reactor (MURR) has a high thermal neutron flux that can be used for the neutron transmutation required to create special use materials, in addition to radioactive isotopes for medical and industrial applications. Along the upturn of the reactor power arrow in Figure 5b.1 are the National Institute of Standards (NIST) Center for Neutron Research (CNR, although this reactor is labeled NBSR, National Bureau of Standards Reactor) that provides state of the art facilities for neutron scattering and non-destructive characterization. HFIR has a reactor power level and multi-program mission that enables it:

- the performance of basic research into neutron-induced materials degradation;
- the critically important integration of basic science with engineering that is required to develop materials and technology for advanced fission and fusion energy sources.[15,16]

While common degradation mechanisms exist for fission and fusion materials, a confounding factor for fusion structural materials arises from the very high energy of the neutron spectrum, which peaks at 14.1 MeV. High neutron fluxes at high energy (above 2-3 MeV) can produce significant neutron induced transmutation reactions, most notably (n,p) and (n,α) reactions with neutron energy thresholds above 1 MeV. The H and He products, in addition to the transmuted elements, can alter microstructural evolution from the simultaneous radiation damage. In the absence of a high flux, volumetric source of 14 MeV neutrons to provide a representative fusion materials testing environment, the combination of the high thermal and fast neutron flux at HFIR provides a unique and indispensible role in both the U.S. and International fusion materials research programs. HFIR has been used for fusion materials irradiations in a long-standing U.S.-Japan International collaboration, and more recently as part of a U.S.-EU collaboration. These collaborations have assisted with the qualification of the stainless steel vacuum vessel for ITER, and provide critically important neutron irradiations for developing materials that are capable of withstanding the harsh fusion neutron environment anticipated in a fusion demonstration reactor or pilot plant.

In fact, HFIR is the only mixed spectrum reactor in the world that has completed materials irradiations to doses exceeding 100 dpa.[17] The high thermal neutron flux in HFIR has enabled fusion materials research to mimic certain aspects of H and He transmutation effects through the use of isotopic tailoring experiments (e.g., Ni-58, B-10, or Fe-54) using isotopes that undergo such transmutations either with thermal neutrons or a lower threshold energy, or through in-pile helium injection that takes advantage of a two step nuclear reaction in Ni from thermal neutrons.

Thus, HFIR currently represents a unique and central facility for conducting fusion material research.

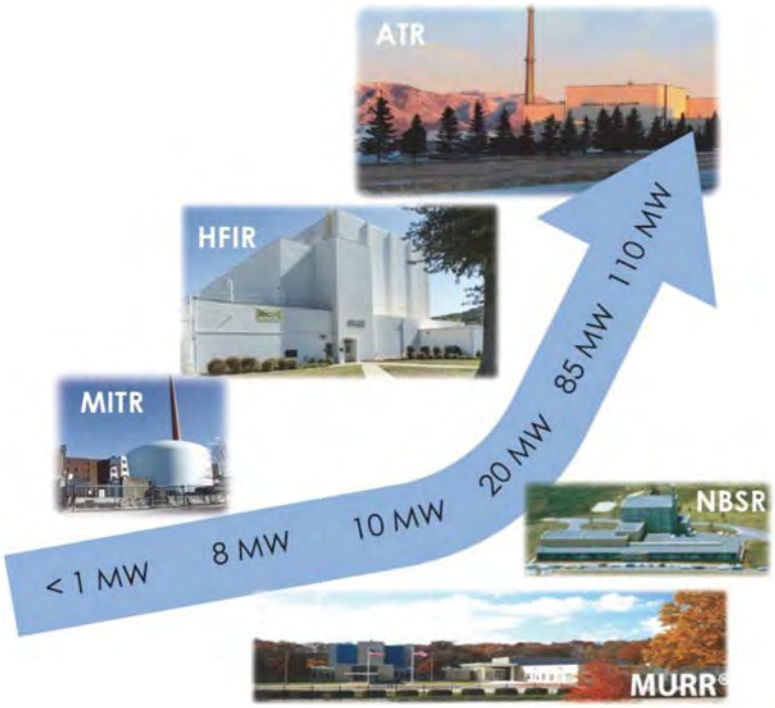


FIGURE 5b.1. Complementarity of research reactors based on the power output. The MITR, HFIR, and ATR reactors shown above the arrow are used for neutron irradiations to study materials degradation, while the MURR reactor provides irradiation to create special materials. The larger reactors also provide non-destructive characterization.

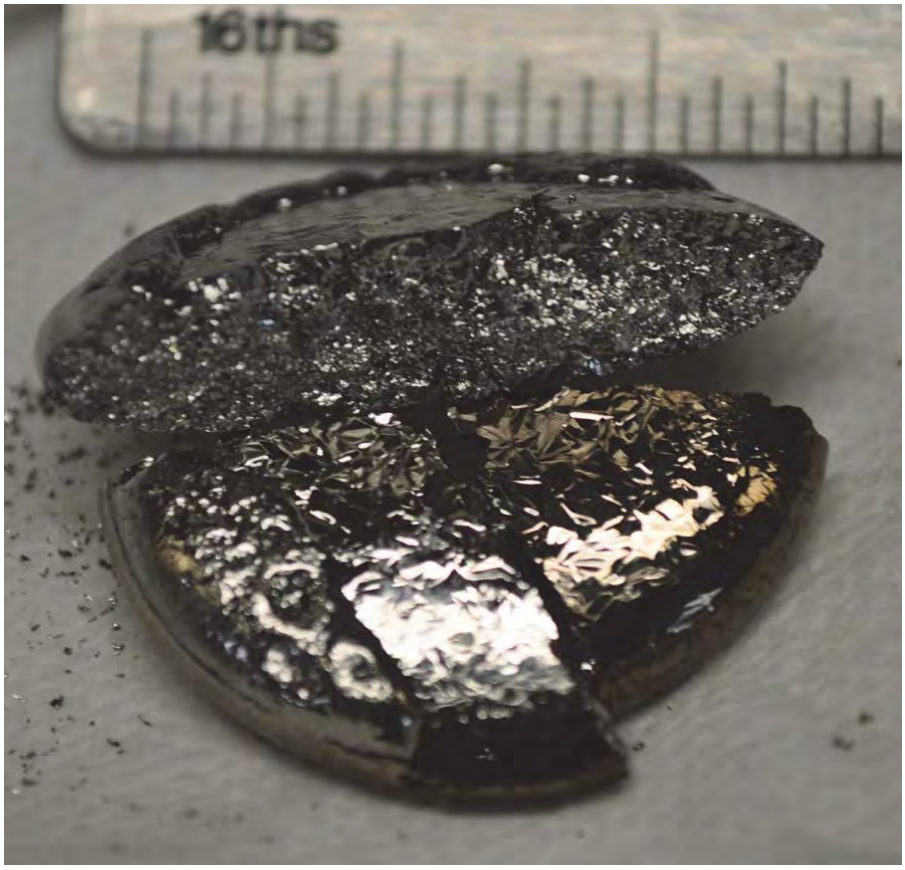
Source: C.A. Back, "Materials Irradiation,", presented to BESAC Subcommittee on HFIR Long Term Strategy, Nov. 15, 2019.

Existing and future fast spectrum reactors (e.g., BOR-60 in Russia, or the VTR in planning and design in the U.S.) can provide high atomic displacement damage irradiations of fusion structural materials, but lack the ability to simultaneously study the nuclear transmutation effects since high thermal neutron fluxes are required to take advantage of isotopic tailoring.

The research production of the fusion materials community with HFIR has been extensive, and indeed, historically, the number of peer-reviewed journal papers emanating from the HFIR in-core neutron materials damage studies has rivaled that of the neutron scattering community. As noted by the Kurtz presentation at the November meeting, HFIR has been a versatile and workhorse materials irradiation facility heavily used for fusion materials research, and contributes to U.S. leadership in the worldwide fusion materials research community.[18]

Finally, it is worth noting that a subset of the committee visited the Jules Horowitz Reactor (JHR), currently under construction at CEA-Cadarache. When completed and operational in 2025, the JHR will provide an alternative mixed spectrum reactor specifically designed to provide a high thermal and fast neutron flux that can provide in excess of 10 dpa per year, with the ability to utilize isotopic tailoring or in pile helium injection similar to HFIR. The JHR reactor costs in excess of 2.4 billion euros, and will also likely take a decade or more to demonstrate the diverse and extensive materials irradiation capabilities similar to what HFIR currently offers. ■

HEU-LEU CONVERSION



A button of uranium silicide (U_3Si_2) alloy prior to grinding to powder for use in Low Enriched Uranium (LEU) fuel. Uranium silicide is the fuel form being qualified for conversion of HFIR to LEU fuel.

Image credit: PNNL. Provided by C.A. Lavender, personal communication, July 23. 2020

Preservation of Reactor Capability with Low Enriched Uranium Fuel

Since 1978, the U.S. government has worked with civilian research reactors and medical isotope production facilities domestically and internationally to minimize, and, when possible, eliminate weapons-usable nuclear material around the world.

As indicated in Figure HL.1, there has been a great deal of success converting reactors around the world, including 24 reactors with experimental peak thermal fluxes above E14 n/cm²/s. A total of 71 reactors converted from Highly Enriched Uranium (HEU) fuel to Low Enriched Uranium (LEU) fuel in the period 1978-2019, and an additional 31 reactors that used HEU fuel have been confirmed permanently shutdown.

Though the global community has converted 24 reactors with high flux, unique challenges remain for a group of highly optimized HEU reactors in the U.S. and Europe. The U.S. High Performance Research Reactors (USHPRR) and European High Flux Reactors (EUHFR) are each quite distinct, and have less fuel assembly design and/or grid-plate flexibility than prior conversions; high power density in the fuel in order to provide intense experimental fluxes; and high burnup in those reactors that reload fuel in order to minimize fuel costs. Appendix A2 describes many of the details of the efforts to convert the USHPRR and EUHFR reactors. This section summarizes aspects of that effort that are most relevant to the capabilities of HFIR, whether as a HFIR LEU conversion or a refurbished HFIR with LEU fuel.

It must be emphasized that to preserve capability, the Conversion Program addresses actual performance metrics rather than simple flux values. Such metrics are quite reactor-specific, but might include: isotope production rates; cold-source brightness; experiment temperature (gamma heating); silicon doping homogeneity; etc. Upon conversion, some specific performance metrics may decrease more than others, but the overall capability is preserved to the maximum degree. In a number of cases such as the Rhode Island Nuclear Science Center reactor or the VVR-K reactor in Almaty, Kazakhstan, the more compact cores possible with an LEU fuel that has U-235 density higher than the prior HEU fuel has allowed significant increases in flux intensity and associated mission capabilities.

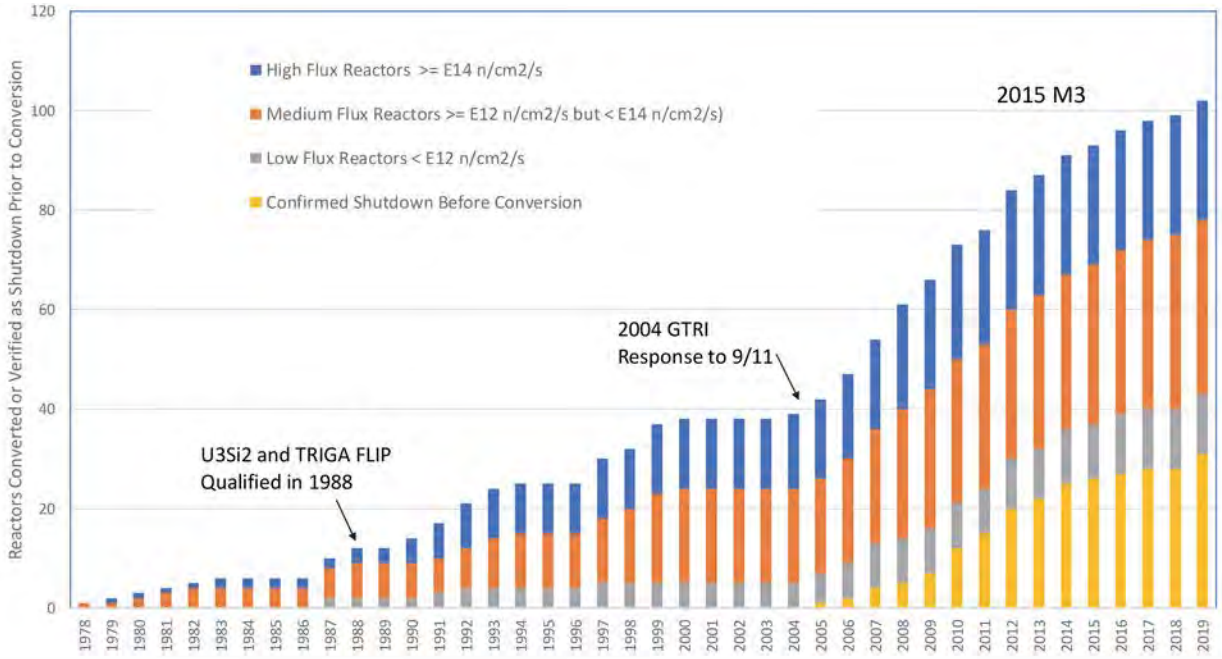


FIGURE HL.1. Timeline of the Global Reactor Conversions, 1978–2019

U_3Si_2 and TRIGA FLIP fuels were key higher-density fuels to allow conversion from HEU to LEU
GTRI: Global Threat Reduction Initiative organization within NNSA
M3: Material Management and Minimization organization within NNSA
NNSA: National Nuclear Security Administration

Source: John Stevens, Argonne National Laboratory

In other cases, such as the RPI reactor in Portugal, the flux in a specific energy range for a specific beam port was increased as part of conversion, with less emphasis on less utilized in-core irradiation sites.

The reactor conversions have been possible due to the development, qualification, and creative application of LEU fuels with uranium density higher than the HEU fuels already in use. The change in enrichment from 93% HEU to 19.75% High Assay LEU (HALEU) implies the need to increase uranium density in the same core volume by a factor of 4.7. However, the additional U-238 in LEU absorbs some neutrons parasitically, so a density increase greater than the factor of 4.7 will be required to preserve reactivity worth of the core volume if nothing else about the system is changed. Fortunately, fuel reactivity is only one factor of effective operation. Since the reactivity worth of fuel and experimental performance are both highly dependent on neutron spectrum, changes to fuel geometry, reflectors, and/or multi-cycle fuel utilization strategy can mitigate the effect of the U-238 absorption in order to preserve mission capability. Changes to fuel layout on the grid plate and/or operating power of the reactor can also be used to preserve mission capability after conversion. Modernized safety bases that employ high-fidelity modeling for neutronics and heat removal analyses with a rigorous grounding in phenomenological safety basis rather than antiquated "conservatisms" can enable core operation at higher local power densities to facilitate compact cores and higher neutron fluxes.

In 2005, the U.S. organized the effort to convert the five USHPRR including HFIR into a coordinated subprogram. In 2008, the U.S. and the EUHFR formed a similar coordinated effort. The primary focus of the high-performance reactor groups was development and qualification of an LEU fuel that could be fabricated for use in the distinct systems. Uranium-molybdenum alloy fuel (UMo) was selected for the combination of high density and effective retention of fission gas upon irradiation. However, significant research and development was necessary to address an unstable interaction between UMo alloy and aluminum and to develop a sustainable fabrication capability for the UMo fuel.

The USHPRR team pursued a *revolutionary* monolithic fuel, in which a diffusion barrier is applied to a U-10Mo (where 10 indicates 10% Mo in the alloy) foil and then clad in aluminum using Hot Isostatic Pressing (HIP) rather than typical roll bonding. The EUHFR team pursued an *evolutionary* dispersion fuel with U-7Mo powder dispersed in an aluminum matrix and then clad by aluminum using typical rolling methods of plate-type fuel.

In response to the challenges encountered for both monolithic and dispersion UMo fuel systems, in 2012-2013 the NNSA Reactor Conversion fuel development and qualification efforts were significantly restructured for both the USHPRR and EUHFR. The European collaborators also restructured their approach. Both teams rebaselined the plans for the reactor conversions.

The USHPRR and EUHFR teams learned from each other regarding the UMo fuel systems. The EUHFR team adopted the diffusion barrier and heat treatment approaches that had proven vital for excellent irradiation performance of the U-10Mo monolithic fuel. The USHPRR team adopted inclusion of a commercial fuel fabricator and pilot-line-production that had proven predictable and effective for EUHFR experiment fabrication. Both teams slowed the pace of irradiation experiments to assure that maximum data value would be generated by each experiment, in terms of both fabrication data and irradiation performance data. In addition, both teams have had independent expert reviews to assure appropriate creativity, transparency, and rigor.

Selection of U_3Si_2 for HFIR Application, and the Path to Conversion

The independent expert review of the EUHFR plan in 2015 suggested that the EUHFR pursue U_3Si_2 dispersion fuel as a backup to their work on U-7Mo dispersion.

SCK CEN reconsidered their BR2 fuel element plate thickness and radius constraints, and determined that a modified geometry would allow preservation of mission capabilities with an LEU 5.3 g/cm^3 U_3Si_2 dispersion fuel incorporating gadolinium as an integral burnable absorber.

Since the promising results for LEU U_3Si_2 application to a redesigned BR2 fuel element, the conversion design teams for HFIR and the RHF reactor at ILL in France have both reconsidered geometric constraints and have developed design candidates for variants of U_3Si_2 details that would preserve mission capability.

In the case of HFIR, U_3Si_2 is not the backup solution, but was established as the baseline solution in 2019. The unique fuel shape of HFIR will require fabrication capabilities quite distinct from the baseline U-10Mo monolithic plan for the other USHPRR. The U_3Si_2 dispersion fuel system will allow the HFIR-

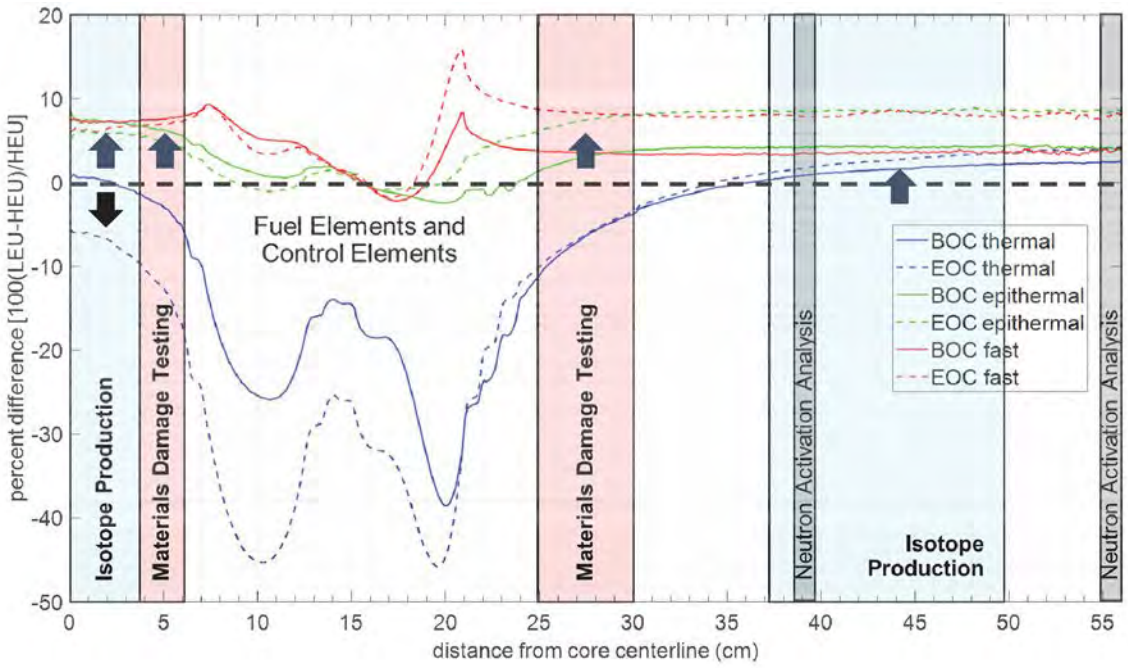


FIGURE HL.2. Three Group Neutron Flux Radial Profiles on Core Midplane

Typical positions for Isotope production and materials damage testing irradiations illustrated BOC and EOC: Beginning and End OF Cycle. HEU operation at 85 MW is compared to LEU U3Si2 operation at 95 MW. Safety margins have been preserved for the LEU at higher power..

Source: David Chandler, presentation to BESAC subcommittee, January 2000

specific characteristics of the current HFIR design to be leveraged for the LEU design (i.e., fuel zone shaped rather than uniform inside the cladding and burnable poison distributed adjacent to the fuel). The U-10Mo fuel system will be a backup for HFIR conversion.

The HFIR design calculations for LEU conversion have included detailed simulation of a wide variety of metrics that represent the experimental capabilities of HFIR over the course of each operating cycle, including cold-source flux detail (intensity and cold-to-total flux ratio), ^{252}Cf production rate, flux trap fast flux in material irradiation locations, flux trap fast-to-total flux ratio, reflector fast flux in material irradiation locations, and reflector fast-to-total flux ratio.[1,2] In their presentation to this BESAC Subcommittee, the HFIR Conversion Team reported preservation of all missions, as summarized on Figure HL.2.

It is important to remember that no successful experimental results have been published for U_3Si_2 at the challenging irradiation conditions required by BR2, RHF, and HFIR. The JHR confidence in EVITA results that have not been published is encouraging, but not a basis for qualification at any other reactor. Furthermore, the EVITA tests did not include integral burnable absorber in the fuel meat.

Thus, both the HERACLES Consortium and the HFIR team within USHPRR have initiated experiment campaigns to qualify U_3Si_2 with the appropriate fuel meat characteristics (density, specific integral burnable absorber if present) for the required operating conditions. The HFIR U_3Si_2 dispersion fuel qualification plan will move through a series of tests at BR2 and ATR to address the distinct fuel configuration and irradiation conditions of the inner and outer cores of HFIR fuel. The HFIR qualification may be adapted depending on the path forward selected by BR2 and RHF, to the degree that U_3Si_2 experimental synergies might accelerate the three conversions.

Progress on High Flux Reactor Conversion since 2016 NAS and 2018 APS Studies

The 2016 NAS "Reducing the Use of Highly Enriched Uranium in Civilian Research Reactors"[3] and 2018 APS "Neutrons for the Nation"[4] studies each raised concerns about the credibility of conversion program schedules due to repeated delays prior to the rebaselines, followed by significant delays announced as part of the 2012 and

2013 rebaselines of the USHPRR and EUHFR efforts relative to the schedules that had been reported prior to rebaselines.

The need to restore schedule credibility with stakeholders was understood by reactor conversion leadership during the rebaseline processes, and the USHPRR and EUHFR teams have worked to maintain schedule despite the complexities of the programs. In July of 2015 the NNSA reported to the NAS review committee that the projected conversion dates of the 5 USHPRR, the ATRC, and 3 EUHFR reactors would occur during the span from MURR in 2026 to FRM-II in 2033 (i.e., first licensed LEU fuel on the grid plates for operation). In January 2020, the NNSA reported to the BESAC Neutron Subcommittee that those 9 conversions will occur during the span from MITR in 2028 to HFIR in 2034.

Appendix A.2 lists a number of key deliverables toward high-performance research reactor conversions that have been accomplished in the US and Europe since the 2016 NAS report was published. Significant progress has been achieved in the areas of detailed LEU reactor design and safety analysis; fuel qualification of the UMo and U_3Si_2 fuel systems; and fabrication of the UMo and U_3Si_2 fuel systems, including cost projection and associated process optimizations.

The ORNL neutron science team (HFIR, SNS, and senior laboratory management) and the M3 Reactor Conversion team (NNSA, the collaborating national laboratories, and BWXT) agree that they are on a sound coordinated path to a U_3Si_2 conversion that will maintain the mission capabilities of HFIR, as reported in publications and the presentations by ORNL to this BESAC Subcommittee.

MAJOR U.S. NEUTRON FACILITIES: Status and Future Plans

360-degree panoramic of the HFIR Reactor at Oak Ridge National Laboratory in Tennessee
Credit: Jason Richards

High Flux Isotope Reactor (HFIR)

The need for a high neutron flux reactor to support transuranium isotope research and development was identified in 1958, and construction of the High Flux Isotope Reactor (HFIR) began in 1961. HFIR achieved first criticality in 1965 and reached full design power of 100 MW in August 1966. The reactor was designed around the concept of a neutron flux trap, which generally consists of an annular region of fuel surrounding a thermalization area to create a thermal neutron flux peak. The HFIR achieves the highest neutron flux density of any reactor operating today in the western world (2.5×10^{15} n/cm^2/s at 85 MW) by utilizing a beryllium reflected, light-water cooled and moderated highly-enriched uranium fueled reactor core surrounding the center flux trap in the center (see Figure US.1).

HFIR Core

The HFIR core is a cylindrical assembly approximately 2 feet tall and 17 inches in diameter consisting of inner and outer fuel elements. The center of the HFIR core contains a five-inch diameter flux trap. The inner fuel element contains 171 fuel plates, and the outer element contains 369 fuel plates. The fuel plates are curved in the shape of an involute to provide a constant coolant flow channel width between plates. To minimize power peaking, the uranium in the aluminum-clad fuel is non-uniformly distributed along the arc of the fuel plate. Boron-10 is added within the inner fuel plates to flatten the radial peak neutron flux and extend the operating cycle for the core.

The fuel region is surrounded by a cylindrical beryllium reflector approximately one foot thick and consisting of three regions or sections. These sections include the inner removable reflector, the semi-permanent reflector, and the outer permanent reflector. All sections of the beryllium reflector must eventually be replaced due to damage, growth, and cracking caused by irradiation from the reactor. The next beryllium reflector replacement is scheduled for 2024 and will require a nine-month outage. The reactor core and beryllium reflector are cooled and surrounded by light-water reactor primary coolant which is contained in the eight-foot diameter reactor pressure vessel.

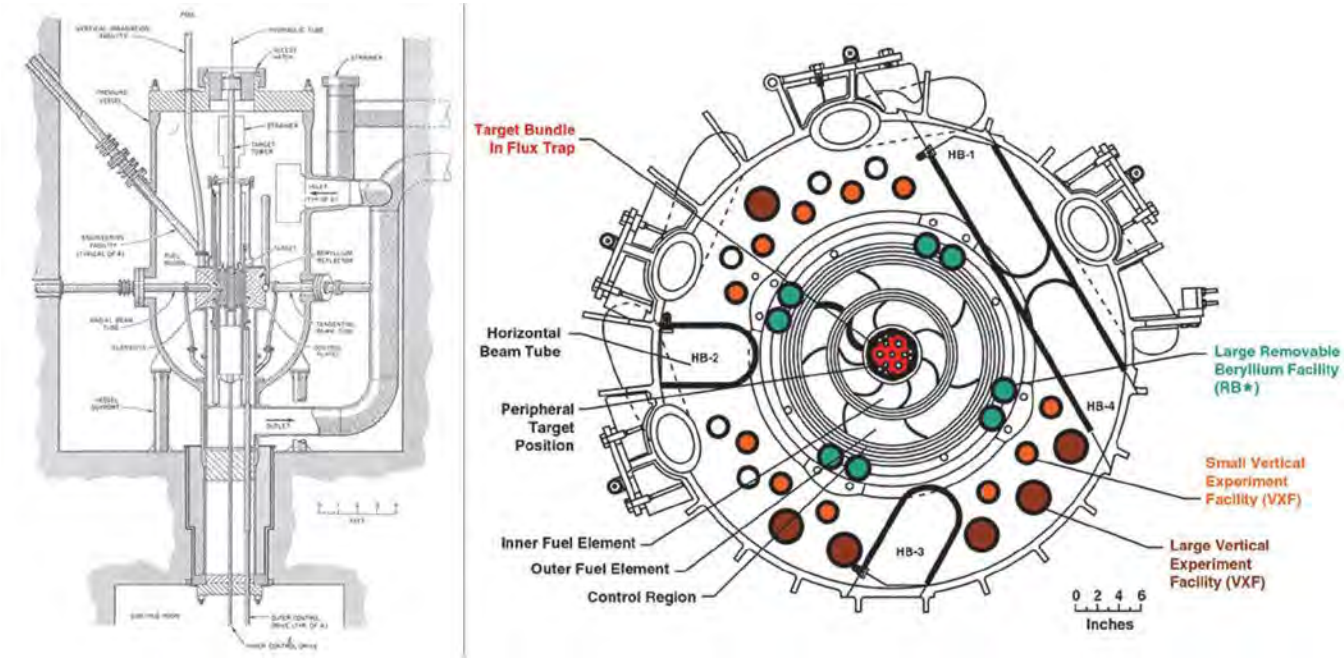


FIGURE US.1. HFIR Axial and Radial Cross-Sections
Source: Oak Ridge National Laboratory

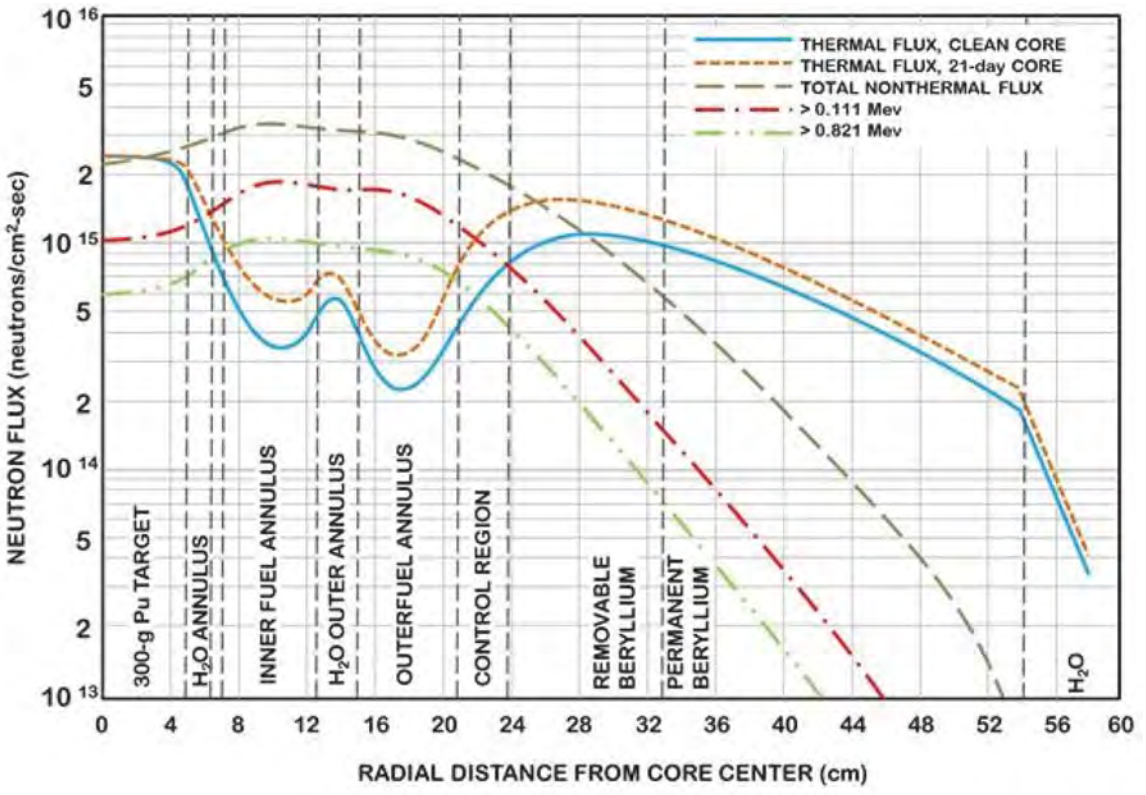


FIGURE US.2. Neutron Flux and Energy Across the HFIR
Source: Oak Ridge National Laboratory

In-Vessel Isotope Production and Materials Irradiation

HFIR was originally designed specifically to enable the production of transuranium isotopes for research, industrial, and medical applications utilizing the high thermal neutron flux in the center flux trap. The neutron flux energy spectrum across the HFIR reactor and the reflector is shown in Figure US.2. Today, HFIR is the only reactor outside of Russia capable of producing significant quantities of californium-252. Californium-252 is a very strong neutron source (with a half-life of only 2.645 years) used for well-logging, neutron radiography, reactor startup sources, and other industrial and medical uses. Other isotope productions for which HFIR is unique or particularly effective are discussed in The Scientific Case section of this study.

The HFIR flux trap has 30 target positions in the flux trap basket that are used for isotope production and materials irradiation testing or other experiments. Two of these locations will accommodate instrumented experiments which would allow, for example, temperature monitoring.

One location in the HFIR target basket is reserved for a hydraulic facility which permits insertion and removal from the reactor during operation. The hydraulic tube (HT) transfers aluminum capsules from a loading station into the flux trap and back using the differential pressure across the HFIR core. HT samples and their effect on the reactor are carefully evaluated prior to approval to ensure that the insertion or withdrawal of the experiment does not cause a power transient that results in a reactor trip.

By design, the peak thermal flux occurs near the center of the flux trap. There are six peripheral target positions (designated as PTP) in areas on the outside edge of the target basket. These positions receive the highest fast and epithermal neutron fluxes in the HFIR, making these locations useful for materials irradiation testing. Strong neutron absorbers are limited in the flux trap and some other positions as they could reduce the length of the HFIR experimental cycle.

HFIR has additional irradiation capacity located in the removable beryllium (RB) and permanent beryllium surrounding the HFIR core. Because the RB locations are closer to the reactor fuel, they are often used

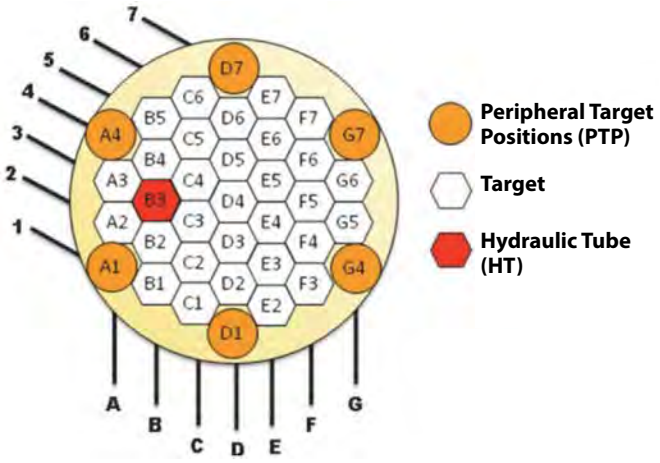


FIGURE US.3. HFIR Target Basket Locations
Source: Oak Ridge National Laboratory

for instrumented and non-instrumented experiments. Within limits, the neutron spectrum in this area may be filtered to reduce the thermal neutron component of the spectrum. The vertical experiment facilities (VXF) in the permanent reflector normally will only contain non-instrumented experiments or target materials for isotope production.

HFIR has two pneumatic tube facilities supporting the neutron activation analysis program. These tubes allow the rapid insertion and removal of irradiation samples while the reactor is operating. One of the pneumatic tubes uses one of two engineering facilities that enter the edge of the beryllium reflector at an angle.

Neutron Scattering

HFIR has four horizontal neutron beams (HB-1 to -4) with the thimbles located in the beryllium permanent reflector. HB-1 and HB-3 are configured as thermal neutron beams that are tangential to the reactor core to reduce the gamma and fast neutron radiation in the beams. HB-2 is a radial beam tube which utilizes beryllium inserts and fast-neutron filters to increase the signal-to-noise ratio at the neutron scattering instruments. HB-4 is a tangential tube and contains the cold neutron source (commissioned in 2007) which is one of the brightest sources in the world today. The cold neutron source uses supercritical hydrogen operating near 17K to increase the available flux of neutrons at wavelengths 4 to 12 Angstroms for the cold neutron instruments.

Together, the HFIR thermal and cold neutron beams support 12 neutron scattering instruments. A cold neutron guide hall was constructed in 2007 to provide greater space for small-angle scattering (SANS) instruments and other instruments optimized for the longer wavelength cold neutrons. As a continuous neutron source, HFIR's fluency rate is 50 times greater than a Long or Short pulse source. The range of HFIR scattering experiments is discussed in The Scientific Case section of this report, together with the HFIR capability complementarity to the Spallation Neutron Source and other scattering facilities.

HFIR Status

The HFIR pressure vessel shown in Figure US.1 has a design lifetime of 50 effective full-power years (EFPY) for 100 MW operations. Tests performed on irradiation surveillance specimens in November 1986 indicated that the HFIR reactor vessel was being embrittled by radiation exposure at a higher than predicted rate. Following detailed evaluations and extensive reviews, HFIR was permitted to restart on April 18, 1989, but did not return to normal operations at a new maximum power level of 85 MW until May 18, 1990. The lower power level significantly reduces the rate of pressure vessel embrittlement and extends the operating life of HFIR, based on the vessel, to approximately 2050 assuming six 23-day operating cycles per year.

HFIR has an extensive age management program that evaluates equipment and systems condition to determine a priority for refurbishment or replacement. Virtually all major components have been replaced, with many of those remaining scheduled to be replaced during the next reflector replacement in 2024. Since 1995, this life extension strategy has improved HFIR reliability and assured a predictable (98.5% in FY19) operational schedule to support the ORNL neutron scattering science program. Predictability and reliability are essential for HFIR to support the strong neutron science user facility program.

Although the HFIR reactor pressure vessel has approximately 30 to 40 years of life remaining, it is considered the life-limiting component of HFIR. Similar to the 1995 replacement of the High-Flux Reactor pressure vessel at the Institut Laue-Langevin in France, ORNL has developed a tentative plan to replace the HFIR reactor vessel and extend the operating life of the facility beyond 2040. In a process already used for nuclear power plant decommissioning, vessel sectioning could be performed remotely using an underwater plasma torch and the segments could then be packaged

for disposal. A replacement vessel could be fabricated using improved materials that are less susceptible to radiation embrittlement, such as stainless-steel, and allow HFIR to return to 100 MW operations. A project to fully design and procure a replacement reactor vessel, which would require three to five years for fabrication, could be aligned with DOE planning to coincide with LEU conversion in the 2030 to 2035 timeframe and could include an early beryllium reflector replacement. HFIR and ORNL staff have drafted a preliminary project plan to replace the HFIR pressure vessel, upgrade some reactor systems, and improve the cold neutron source to improve brightness by 50%. A potential LEU replacement fuel, expected to begin testing soon, could be incorporated into an upgraded or enhanced HFIR reactor core design, possibly allowing a higher reactor power level to compensate for the LEU fuel neutron flux distribution. All of these activities could also support the installation of an HB-2 guide hall with a new suite of thermal and cold instruments to capitalize on the enhanced HFIR, which would in turn enable high quality neutron science research well into the 21st century. ■

NIST Center for Neutron Research (NCNR)

The NIST Center for Neutron Research (a major operating unit within the National Institute of Standards and Technology in the U.S. Department of Commerce) is a national user facility that operates world-class facilities for neutron-based research. The mission of NIST, "to promote U.S. innovation and industrial competitiveness by advancing measurement science, standards and technology…," drives a robust engagement with industry in the application of neutron measurements to problems of technological interest and in the development of standard reference materials. Access to NIST neutron facilities is provided to scientists from industry, government, and academia through several different channels:

- a general user program based on anonymous peer-reviewed proposals
- partnerships with government, private sector, or academic organizations
- collaborations on NIST-mission activities, and
- proprietary research performed with full cost recovery

In 2019 alone, more than 300 articles were published that were fully or partly based upon research performed at the NCNR, and the facility served scientists from 50 U.S. corporations.

NCNR research facilities are centered around the NBSR, a 20 MW steady-state research reactor first commissioned in 1969, that has a heavy water moderator and reflector. The NBSR is licensed by the Nuclear Regulatory Commission; the current license was issued in 2009 and runs through 2029. No short-term issues that might limit operations beyond that time have been identified. The NBSR uses Highly Enriched Uranium (HEU) fuel, but a conversion to Low Enriched Uranium (LEU) will occur when such fuel is qualified. The liquid deuterium cold source now being constructed is partially funded by the NNSA Material Management and Minimization Program to compensate for the 10% reduction in neutron flux that will result from LEU conversion.

The neutron beam instrument layout shown in Figure US.4 is the result of the cold sources developed and the research needs of the neutron community. Note that MACS views its own small cold source, meaning that more than ¾ of the neutron beam instruments at the NCNR use cold neutrons.

Neutrons interact with both the nucleus and spin of atoms, which makes it possible to obtain information on atomic and magnetic structures, respectively. These interactions are weak, which result in some simplification in analysis but also weak signals. Thus, neutron scattering is an intensity-limited probe, and good instrument design is critical to successful studies.

The development of innovative instrumentation is a priority at the NCNR with a very high payoff. This is exemplified by the recent construction of CANDOR, a state-of-the-art instrument that multiplexes many HOPG monochromators in a row, each set to diffract a different wavelength. This allows much more rapid measurements of neutron reflectometry, as illustrated in Figure US.5 in the first scan taken with the new instrument compared to a single reflectometer.

In addition to the neutron scattering instruments, there are several thermal-neutron irradiation facilities

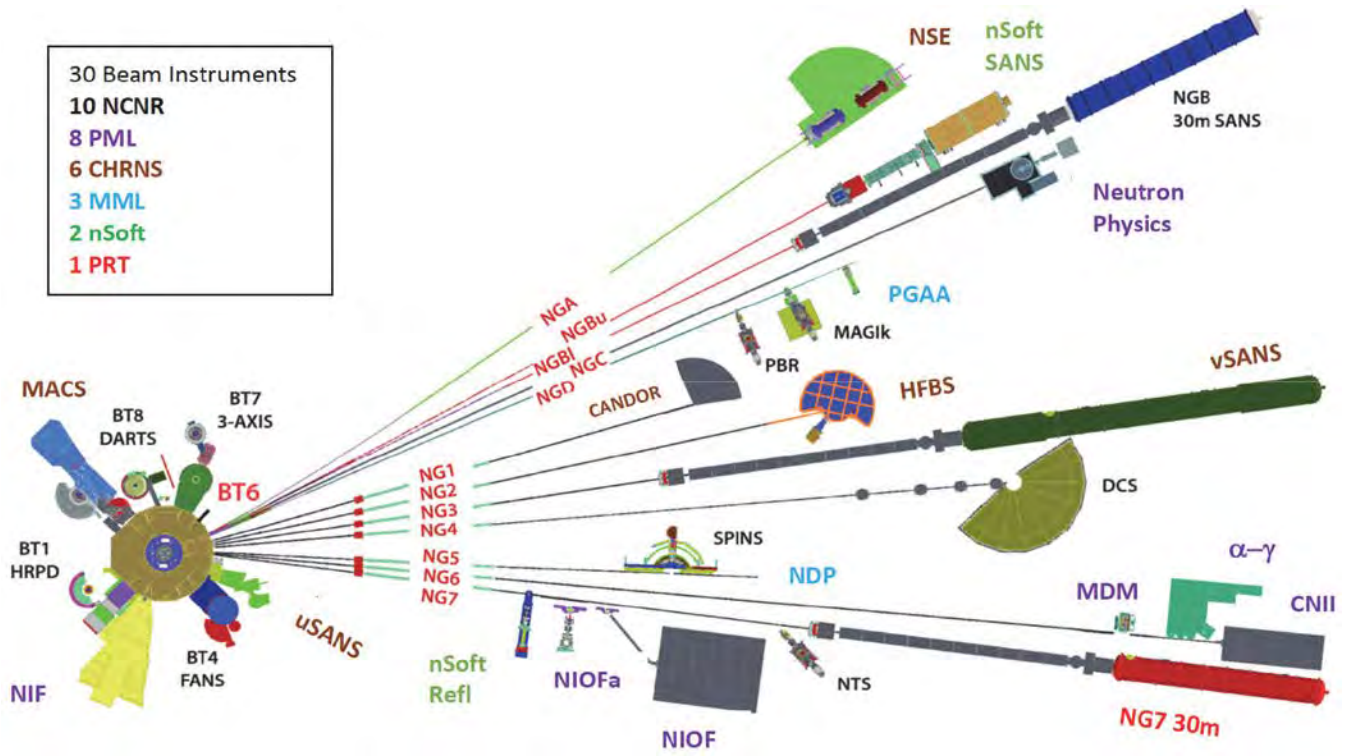


FIGURE US.4. NCNR Reactor Layout
Source: Dan Neumann NCNR

including pneumatic rabbit tubes, fixed vertical facilities, a thermal column, through tubes, and other facilities inside the reactor confinement building. Although these facilities may be used by outside users in a collaborative or service mode, they primarily serve the mission needs of NIST, including calibrations, activation analysis, and sample irradiations.

The Chemical Sciences Division of the NIST Material Measurement Laboratory uses these facilities for elemental analysis by neutron activation to support NIST's role as the nation's reference laboratory for measurements and standards of chemical composition. Neutron activation analysis (NAA) complements more common analytical methods and often serves as one of the two independent measurements required for the certification of Standard Reference Materials (SRMs). NAA is particularly advantageous for analyzing materials that are hard to dissolve, such as glasses, ceramics, geological specimens, metals, *etc*. Furthermore, NAA can quantify hydrogen in materials, a difficult measurement by other means. Since 2000, NAA has contributed to the certification of more than 120 SRMs with 55,000 units sold, covering a wide variety of materials ranging from industrial commodities to food.

Beyond SRMs, the research, development, and application of new non-destructive *in-situ* measurement capabilities are a major emphasis of this program. For example, an effort is underway to develop and demonstrate the measurement of chlorine distribution in concrete by prompt-γ activation analysis, a potentially field-deployable capability to assess the corrosion of concrete structures. A second example is the application of neutron depth profiling (NDP) to help elucidate battery failure mechanisms by measuring the complete lithium ion distribution during charge/discharge cycles.

The Neutron Physics Group of the NIST Physical Measurements Laboratory provides measurement services, standards, and fundamental research in support of NIST's mission serving national interests, including industrial research and development, national defense, homeland security, and electric power production. This group provides measurement capabilities and services ranging from neutron imaging, instrument development and calibration, neutron source calibration and standards, detection of concealed nuclear materials, and radiation protection. Basic physics experiments probe the symmetries and parameters of the weak nuclear interaction, including measurements of the

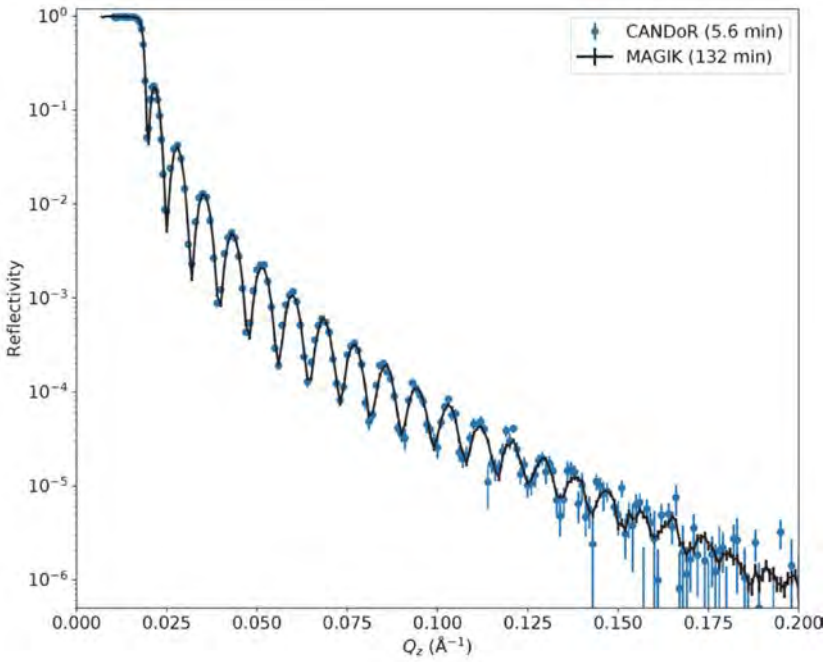


FIGURE US.5. Neutron Beam Resources at NCNR

Source: NCNR/National Bureau of Standards and Technology

lifetime of the free neutron, improved cold-neutron counting techniques, setting a limit on the time-reversal asymmetry coefficient, and the radiative decay of the neutron.

Neutron-imaging studies of water transport in fuel cells and hydrogen distribution in hydrogen storage devices have been performed using an imaging system (NeXT) that combines the power of neutron and X-ray 3-D tomography into a single-pass probe for materials structure and composition analysis. This provides an entirely new approach to resolving longstanding problems in materials science, including concrete degradation, and advances the state of the art of energy technologies, including lithium batteries, and unconventional gas reservoir geologies.

The NCNR has established long-term partnerships with the National Science Foundation (Center for High-Resolution Neutron Scattering), the University of Delaware (Center for Neutron Science), and the University of Maryland to develop new instruments and science, and to expand the use of neutrons beyond traditional fields. Another collaboration that seeks to expand the use of neutrons by industry is the *n*Soft consortium, which is a group of industrial partners that currently comprises 3M, Amgen, Aramco Services Company, Braschem North America, Colgate Palmolive, Dow Chemical, Genentech, Procter & Gamble, Regeneron, Solvay USA, and Toyota Research in North America. The members have access to small-angle neutron scattering to conduct research on problems of industrial interest with results that are freely available to the general public. Membership fees support the development of new methods and instrumentation and the investigation of novel applications of neutrons by industrial partners. The operations are governed by a CRADA that establishes the terms of use.

In the short term, NIST is committed to continuing upgrades of the NBSR reactor and neutron scattering facilities. There are no known lifetime-limiting conditions for the NBSR, which is now over 50 years old. An aging management plan has been established to continually inspect and maintain the reactor for the foreseeable future. One major ongoing improvement is the design, construction, and installation of a new liquid deuterium cold neutron source in conjunction with the conversion of the reactor to Low Enriched Uranium (LEU). This will maintain and improve the NCNR facilities with increased flux for all cold neutron facilities, more than compensating for the losses expected as a result of higher absorption in the LEU. During the shutdown required for conversion activities, NIST will perform several maintenance activities, modifications, and replacements of aging components. At the same time upgrades to the existing scattering facilities (guides, instruments, and other capabilities) will provide the opportunity to increase performance even further.

For the longer term, a replacement of the NBSR will be required, and a project to explore and determine possibilities of an optimum design for cold neutron performance in an LEU reactor has been initiated. NIST expects to construct and commission such a reactor while the NBSR is still operational, so that there will be no interruption of the NCNR. NIST has begun the process of obtaining funding for this project.

In summary, NIST operates a full-capability, world-class neutron facility at the NCNR to serve U.S. researchers from industry, government, and universities. ■

SNS Present and Future

The First Target Station (FTS) at the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory is a third-generation neutron source capable of delivering the world's brightest beams of pulsed neutrons that provide research capabilities across a broad range of disciplines including physics, chemistry, materials science, and biology. The FTS, operating at a power of 1.4 MW, provides beams of neutrons in short pulses at a repetition rate of 60 Hz with the highest peak brightness in the world. Figure US.6 shows the layout of the instrumental hall at FTS of SNS. There are currently a total of 19 user instruments plus an additional 5 instruments under consideration.

The user instruments at FTS cover a wide range energy and momentum space; they have opened new avenues for examining materials over greatly increased length, energy, and time scales. The materials that can be investigated by FTS include magnetic materials,

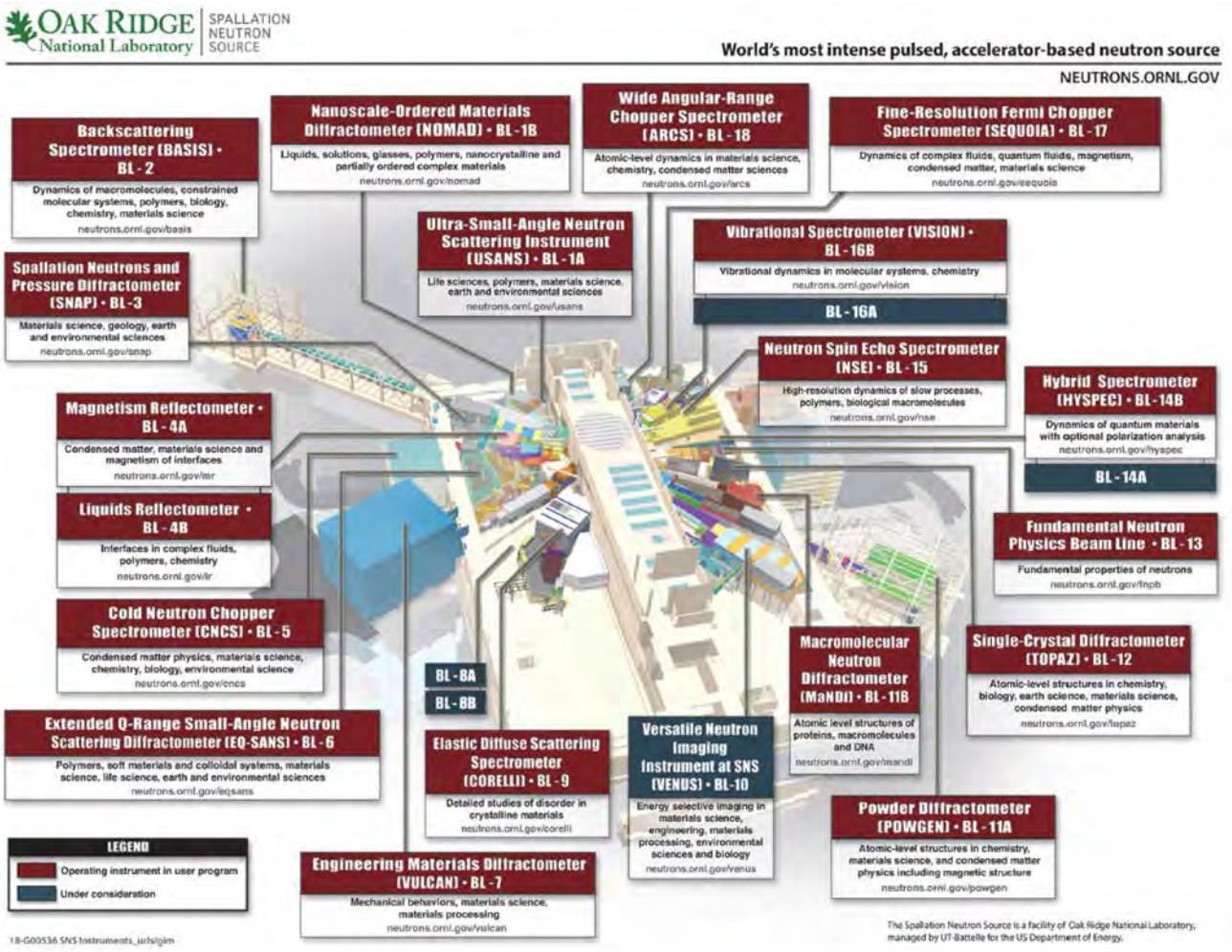


FIGURE US.6. The Instrumentation Layout at FTS, SNS
Source: ORNL

polymers, engineering materials, as well as nanoparticles. In combination with sample environments, advances in neutron optics and detectors, and new computational methods, SNS has transformed the landscape of neutron science in the US. In the early part of the 2000s, the number of neutron scattering scientists and their concomitant activities in Europe have significantly exceeded those in the US. The situation has changed considerably after the completion of the FTS of SNS in 2006. Since that time, the numbers of users, operation hours, and publications from SNS have continued to increase with each passing year. For example, there were 644 unique users in FY 2018, and 780 unique users in FY2019. Between SNS and HFIR, approximately 650 scientific publications were produced in the calendar year 2019, 467 of which are instrument-based publications. SNS is currently undergoing a proton power upgrade (PPU), which will be completed in 2024, to double its power capability to 2.8 MW. This upgrade will deliver 2 MW of proton beam to the FTS, resulting in a significant increase in thermal neutron brightness to enable faster experiments and potentially time-resolved neutron spectroscopy experiments for materials research in the thermal energy (shorter wavelength) range. With this upgrade, FTS at SNS will be competitive with spallation neutron sources in Japan (J-PARC) and the future European Spallation Source (ESS), which is currently 68% complete and expected to have a user program starting in 2023.

In addition to continued improvement of the FTS at SNS, which is mostly focused on thermal energy neutron users, there is tremendous interests in cold neutron spectroscopy. In fact, the 9 cold neutron spectrometers at the FTS are some of the most oversubscribed spectrometers (by a factor of 4). Currently, the Second Target Station (STS) at SNS is in the detailed design stage and will be under construction soon. Compared with the FTS, the STS will be pulsed at 15 Hz (using one out of every four pulses from the target, the rest being used by FTS) and deliver cold neutrons with the highest peak brightness in the world (Fig. US.7). The construction of STS in the coming years will be expected to alleviate considerably the oversubscriptions of the cold neutron spectrometers at the FTS. In addition, STS will enable kinetic process and time-resolved measurements of quantum and biological materials. The ability to produce high flux cold neutrons will also make possible investigations of smaller samples and samples with large length scales of interest. In short, the continued improvement of the FTS and the near future construction of the STS at SNS, complemented by an upgraded and improved high-flux Isotope Reactor, will ensure the US leadership position in neutron sources. ■

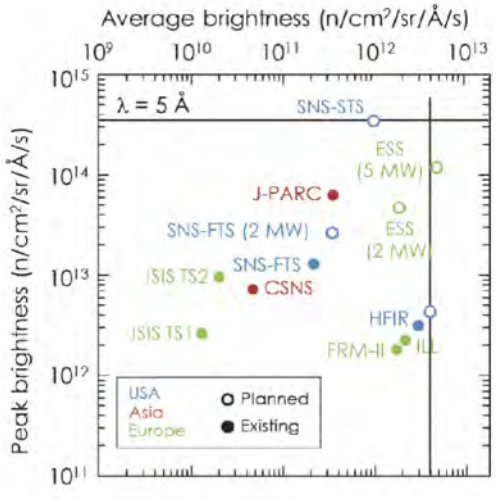


FIGURE US.7. Peak and time-averaged brightness of current (closed circles) and planned (open circles) neutron sources, illustrated at 5 Å. CSNS: China Spallation Neutron Source, China; ESS: European Spallation Source, Sweden; FRM-II: Forschungsreaktor München II, Germany; ILL: Institut Laue-Langevin, France; ISIS: ISIS Neutron and Muon Source, UK (TS: Target Station); J-PARC: Japan Proton Accelerator Research Complex, Japan.

Source: ORNL

INTERNATIONAL NEUTRON FACILITIES

The Institut Laue-Langevin in Grenoble, France, and its reactor (in the dome) that provides an intense source of neutrons for research
Source: Wurzeller - English Wikipedia, Public Domain, https://commons.wikimedia.org/w/index.php?curid=6405870

Institut Laue-Langevin (ILL)

Background

The ILL is located in Grenoble, France, in close proximity to the European Synchrotron Radiation Facility (ESRF), an outstation of the European Molecular Biology Laboratory (EMBL), the University Grenoble Alpes, and several institutes operated by French national research agencies CEA and CNRS. Funding for the ILL comes from a consortium of European countries including the "ILL Associates" (Germany, France, and the United Kingdom), which cover two thirds of its annual budget of about €100M. 10 other countries have signed shorter-term scientific membership agreements that give them privileged access to beam time in exchange for a more modest budget contribution. The ILL currently has a staff of about 520, including roughly 75 instrument scientists.

With a thermal power of 58.3 MW, the ILL Reactor delivers a flux of 1.5×10^{15} neutrons per second per cm^2 to a suite of currently about 40 instruments, which are housed in the confinement building and two cold-neutron guide halls. It currently operates in four 50-day cycles per year. Reactor operations began in 1972, and the reactor vessel was replaced in the years 1993–1995. Since then, the reactor and instrument suite have undergone several upgrade programs. The two-phase "Millennium Program" (2000–2018) supplied funding of €85M for the replacement of the neutron guide system, 7 new instruments, and 25 instrument upgrades. The "Refit Program" (2002–2007) improved security and seismic reinforcement. In 2016, the ILL launched the two-phase "Endurance Program." Phase 1 (2016–2019) was funded at a level of €22M and enabled 14

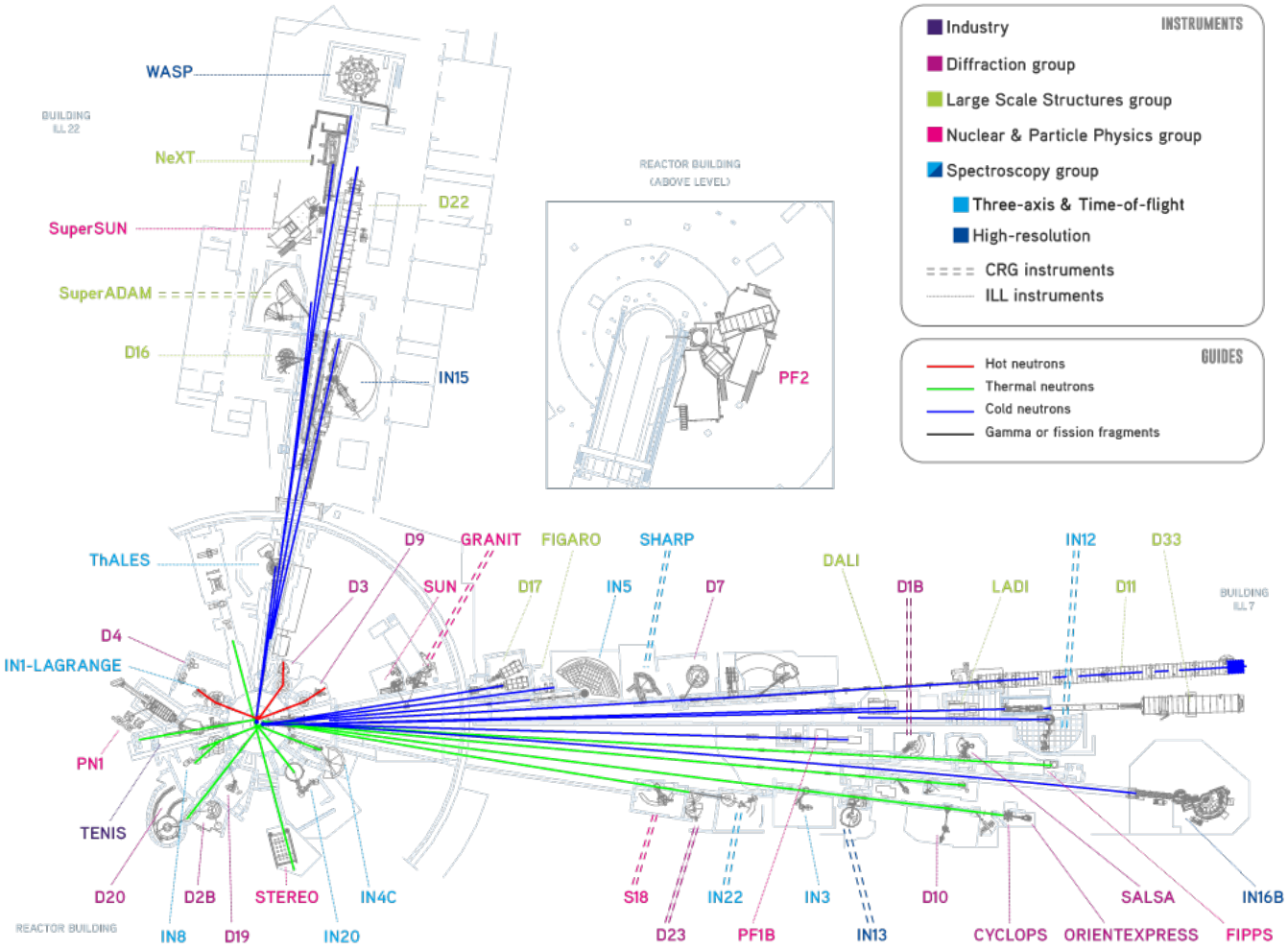


FIGURE I.1. Floor Plan of the ILL
Source: https://www.ill.eu/users/instruments/

instrument upgrade projects as well as upgrades of the sample environment and data collection software. Phase 2 (2019–2023) will fund 10 additional upgrade projects at a level of €40M. In addition to the neutron instruments, the ILL also operates a deuteration laboratory and chemical laboratories for sample preparation. In 2002, the ILL, together with surrounding institutions, founded the "Partnership for Structural Biology" which promotes complementary use of scientific facilities.

Most of the scientific instruments at the ILL are operated by staff scientists who are organized in four scientific groups: Diffraction, Large Scale Structures, Spectroscopy, and Nuclear and Particle Physics. The beam time is allocated via an external user program. In addition, eight instruments are operated by Collaborative Research Groups (CRGs), which either lease an instrument owned by the ILL and receive privileged access to 50% of the beam time (CRG-A), or build and operate their own instrument with privileged access to 70% of the beam time (CRG-B). In the following, the CRG instruments are described alongside those operated by ILL staff.

Diffraction

Powder diffraction accounts for a substantial fraction of the ILL's publication output. The instrument suite includes three general-purpose diffractometers and three more specialized instruments. In the former category, D1B (a CRG instrument) and D20 are optimized for high intensity and are therefore in high demand for parametric studies and real-time experiments, in addition to standard crystal and magnetic structure determination. The flagship instrument D20 also allows stroboscopic experiments with duty cycles up to 33 kHz, with a minimum counting time of 1 μs. D2B is optimized for high momentum-space resolution and thus allows efficient determination of medium-scale structures such as zeolites and quasicrystals. Among the specialized powder diffractometers, D4 uses short-wavelength neutrons from a hot source to measure diffraction patterns of liquids and structurally disordered systems over a large Q-range. D7 focuses on diffuse scattering from magnetically disordered systems, using a spin-polarized beam and uniaxial as well as XYZ polarization analysis. SALSA is designed for strain imaging of engineering materials with dimensions ranging from a few millimeters to more than one meter.

Single-crystal diffractometers include the hot-neutron instruments D3 and D9 for accurate crystal and magnetic structure determination. D3 was upgraded in Phase 1 of the Endurance program, and includes a spherical neutron polarimetry (CRYOPAD) facility for determination of non-collinear magnetic structures as well as a dedicated setup for experiments on liquids. In addition, two thermal instruments, D10 and D19, are optimized for high flux and high Q-space resolution respectively. The Diffraction Group also operates two Laue diffractometers, CYCLOPS and Orient-Express, which allow users to rapidly characterize their samples on-site.

Large-scale Structures

Three *small-angle neutron scattering* (SANS) instruments (D11, D22, and D33) are dedicated to structure determination in soft and hard condensed matter as well as life sciences on length scales ranging from 1 nm to 1μm. With about 50–60 user experiments per year on each instrument, they are the workhorses of the ILL. All instruments have been extensively upgraded in both the Millennium and Endurance Programs. The flagship, D22, is currently the world's highest-flux SANS machine. Its high flux and optimized detection capabilities enable applications in life sciences and microfluidics as well as time-resolved studies with μsec resolution (TISANE). Further special capabilities include a USANS option for extremely low momentum transfer on D11, and time-of-flight (TOF) and spin-polarization-analysis options on D33.

The three *reflectometers* at the ILL (FIGARO, SuperADAM, and D17) were either newly built or extensively upgraded in the Millennium Program. FIGARO, a high-flux TOF machine with a horizontal sample geometry, is mostly used to study liquid interfaces in biophysics, soft matter, and environmental science. D17 is a versatile machine that can be used both in TOF and monochromatic modes. With its vertical sample geometry, it is complementary to FIGARO. The CRG instrument SuperADAM, a monochromatic machine with a vertical sample geometry and polarization analysis option, is mostly used for solid thin films and multilayers.

The Large Scale Structures Group also operates two Laue diffractometers dedicated to protein crystallography (LADI-III and LADI-B), as well as a diffractometer optimized for the investigation of partially ordered structures in soft matter and biology (D16).

Spectroscopy

The ILL houses a suite of six *three-axis spectrometers,* including two dedicated cold-neutron machines (IN12 and ThALES, both CRG instruments), three thermal machines (IN8, IN20, and IN22) and a hot-neutron instrument (IN1). Over the past few years, the beam optics of most of these instruments were upgraded, and new setups were installed to enhance the detection efficiency (e.g., the multi-analyzer "FlatCone" option on IN8, IN20, and ThALES), polarization-analysis capabilities (i.e., a spherical neutron analyzer on IN22), and energy resolution (e.g., a spin-echo option on IN20).

The ILL's suite of *time-of-flight spectrometers* is being extensively refurbished in the Framework of the Endurance Program. Two ageing TOF spectrometers (IN6 and IN14) are being replaced by new instruments—the cold-neutron instrument SHARP and the thermal instrument PANTHER. In addition, the guide system and focusing optics of the general-purpose spectrometer IN5 has just been upgraded.

The Spectroscopy Group also operates several instruments for spectroscopy with high energy resolution, including two *spin-echo spectrometers* (IN11 and IN15) and two *backscattering spectrometers* (IN16B and IN13) for cold and thermal neutrons, respectively. With a sensitivity to relaxation times from 0.001 to 1000 ns, the spin-echo spectrometer IN15 is reported to be the world's highest-resolution spectrometer of its kind. The newly commissioned WASP spin-echo spectrometer will complement the suite. WASP will cover a wider range of scattering angles than IN15 and thus bridge the gap to backscattering spectroscopy.

Nuclear and Particle Physics

The ILL also operates an extensive suite of spectrometers for nuclear physics (FIPPS, PN1, PN3-GAMS), cold (PF1B) and ultracold (PF2) neutron sources for high-precision measurements of fundamental properties of the neutron, and interferometers (S18, GRANIT) for experiments on fundamental physics, including gravitational bound states of the neutron. ■

Forschungsreaktor München II (FRM-II)

Background

The FRM-II is located on the campus of the Technical University of Munich (TUM) in Garching, a suburb of Munich, Germany, and is operated by the TUM. Funding for operation of the reactor and about half of the instruments is provided by the science ministry of the state of Bavaria at a level of €55M per year. Additional funding for operation of about a dozen instruments at the FRM-II comes from the German federal ministry of science (BMBF) via the Jülich and Geesthacht Research Centers, both members of the Helmholtz Association of Research Centers. The BMBF also funds instrumentation design or upgrade projects by nine German university groups currently, often in cooperation with the TUM. The Max Planck Society (MPG) operates two instruments. The Maier-Leibnitz-Zentrum (MLZ), a partnership of all instrument groups, coordinates research at the FRM-II and hosts regular workshops and conferences. The FRM-II currently has a staff of about 400, including roughly 130 scientists.

With its thermal power of 20M, the FRM delivers a flux of $8x10^{14}$ neutrons per second per cm^2 to a suite of currently about 28 instruments, which are housed in the confinement building and a cold-neutron guide hall (Guide Hall West in Figure I.2). Access to 70% of the FRM-II beam time is managed through an external-user system. Instrument operators receive privileged access to the remaining 30%. A second guide hall with five instruments (Guide Hall East in Figure #.2) has been completed, but is awaiting safety approval by state authorities. Following the closure of the BER-II Reactor in Berlin at the end of 2019, 2–3 additional scattering instruments will be transferred to the FRM-II. With the transfer of the BER-II instruments and the opening of the second neutron guide hall, all available beam ports of the FRM-II will be occupied. Plans for a third guide hall have been discussed, but funding for conceptual design has not yet been secured.

Diffraction

The FRM-II was initially equipped with only a single general-purpose *powder diffractometer* (SPODI), a monochromatic instrument that is optimized for high resolution rather than flux. A complementary high-flux monochromatic instrument (FIREPOD) will be transferred from the BER-II in the course of the next two years. Construction of two additional powder diffractometers (POWTEX and SAPHIR) has been largely completed,

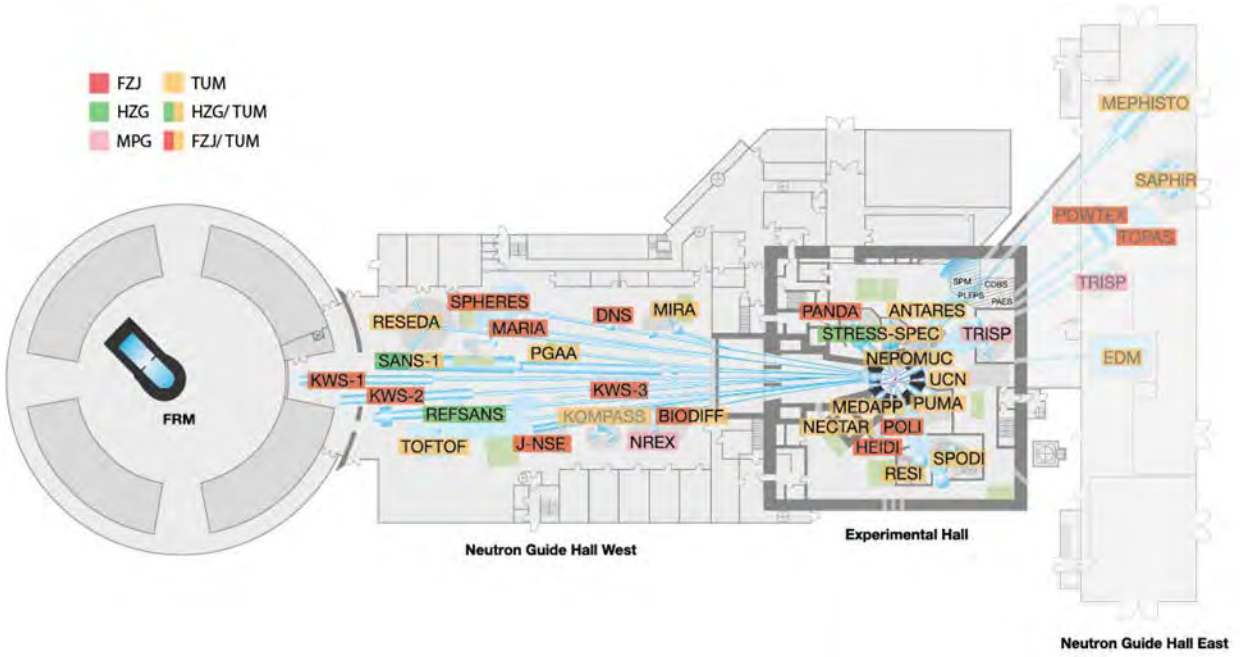


FIGURE I.2. Floor Plan of the FRM-II

TUM = Technische Universität München, FZJ = Forschungszentrum Jülich, HZG = Helmholtz-Zentrum Geesthacht, MPG = Max-Planck-Gesellschaft, FRM = Forschungsreaktor München (the FRM-II's predecessor which is no longer operational)

Source: https://www.mlz-garching.de/instrumente-und-labore.html]

and the instruments are ready for use once the second guide hall can be made operational. POWTEX is a TOF diffractometer with a texture analysis facility and associated sample environment targeted for use in solid-state chemistry and materials science. SAPHIR is also a TOF machine, specialized for diffraction and radiography of samples under extreme conditions of pressure (initially up to 15 GPa, with further upgrades anticipated) and temperature (up to 2000°C). Finally, STRESS-SPEC is a two-axis spectrometer optimized for residual-stress and texture analysis in engineering materials.

Single-crystal diffractometers include BIODIFF, which is situated on a cold-neutron guide and whose high momentum resolution is optimized for macromolecular crystals, as well as HEIDI and POLI, which are located on a hot source in the confinement building. Whereas HEIDI is mostly used for crystal structure determination, POLI is equipped with polarization analysis facilities for magnetic structure determination. An additional diffractometer, LaDIFF, will be transferred from the BER-II Reactor and will be used mostly for Larmor diffraction, a variant of spin-echo spectroscopy that provides extremely high momentum resolution ($\Delta Q/Q \sim 10^{-5}$) independent of sample mosaicity.

Large-scale Structures

The FRM-II instrument suite includes four *SANS machines* with complementary (partially overlapping) capabilities. KWS-1, KWS-2, and SANS-1 are classical pin-hole instruments. KWS-1 is optimized for high Q-resolution and includes spin-polarization analyzers as well as a grazing-incidence (GISANS) setup. KWS-2 is optimized for high intensity and wavelength coverage, and allows kinetic measurements with high time resolution. KWS-3 is a diffractometer designed for extremely small scattering angles and thus extends the coverage of real-space structures up to about 10 µm.

The *reflectometers* NREX and MARIA are monochromatic machines located on cold-neutron guides. Both instruments offer polarization analysis capabilities. Whereas MARIA has a vertical sample geometry, both horizontal and vertical geometries are possible at NREX. An x-ray diffractometer installed at NREX enables simultaneous x-ray and neutron scattering experiments, which is advantageous especially for degradable samples where consecutive measurements are impractical. The horizontal TOF reflectometer RESEDA is optimized for studies of liquid surfaces and interfaces, and also includes a GISANS option.

Spectroscopy

Four *triple-axis spectrometers* are operational at the FRM-II. PANDA and PUMA are high-flux cold-neutron and thermal-neutron instruments, respectively, without polarization-analysis located in the confinement building. KOMPASS, a cold-neutron machine with extensive polarization analysis capabilities, has just been commissioned in the first guide hall. TRISP is a thermal triple-axis instrument with a zero-field spin-echo setup that allows measurements of the lifetimes of dispersive excitations with 1 μeV energy resolution.

The flagship multi-chopper *time-of-flight spectrometer* TOFTOF, which sits at the end of a focusing neutron guide, combines high neutron flux and high energy resolution for a wide range of experiments in hard and soft condensed matter research. DNS is a TOF spectrometer with polarization analysis capabilities specializing in diffuse scattering measurements. An additional TOF spectrometer (TOPAS) with polarization-analysis will become operational as soon as the second guide hall is opened for experiments. Currently the FRM-II is considering the possible transfer of the high-flux TOF spectrometer NEAT from the decommissioned BER-II Reactor. Since a suitable beam port is no longer available, it would have to replace an instrument that is currently in operation.

The FRM-II also operates classical *spin-echo* (J-NSE) and *backscattering* (SPHERES) *spectrometers* for spectroscopy with high energy resolution. An additional spin-echo instrument (RESEDA) has just been extensively upgraded and now includes a longitudinal spin-echo setup that allows high-resolution spectroscopic measurements on ferromagnetic samples as well as experiments under high magnetic fields, which are not possible with standard spin-echo machines. A similar setup has also been installed at the cold-neutron triple-axis diffractometer MIRA.

Imaging

The cold-neutron imaging instrument ANTARES is targeted for radiography and tomography of a wide array of industrial machinery in operation. A second imaging station is located in the confinement building and serves two irradiation rooms (MEDAPP and NECTAR). The front end of this station is equipped with a converter plate for the production of fission neutrons. MEDAPP has been designed for radiation therapy of cancer patients, taking advantage of the high biological activity of fission neutrons compared to standard hospital-based therapies. NECTAR uses the high penetrating power of fission neutrons for radiography and tomography of bulky industrial objects.

Elemental Analysis and Positron Spectroscopy

A prompt-gamma activation instrument for elemental analysis (PGAA) is operational in the cold-neutron guide hall. The FRM-II also operates a high-flux positron source (NEPOMUC) that delivers positrons to three dedicated setups for positron annihilation spectroscopy of bulk solids (CDBS), Auger-electron spectroscopy of surfaces (PAES), and positron microscopy (SPM). A low-energy positron source intended for experiments on thin-film structures is under development.

Nuclear and Particle Physics

Plans for instrumentation for nuclear and particle physics at the FRM-II include a spectrometer for spectroscopy of neutron-induced fission reactions (MEPHISTO), a setup for precision measurement of the neutron lifetime (PENELOPE), an experiment for the determination of the neutron electric dipole moment (EDM), and a source of ultracold neutrons (UCN) for neutron interferometric measurements. All of these experiments have experienced major delays, in part because of difficulties in the safety certification of the second guide hall. ■

Jules Horowitz Research Reactor (JHR)

The JHR is a 100 MW materials test reactor currently under construction at the French Alternative Energies and Atomic Energy Commission (CEA) site in Cadarache, France. It is scheduled to be commissioned by the end of this decade. When it comes on-line, JHR will alleviate much of the material test reactor capacity shortage created by the closures of the HALDEN and OSIRIS facilities. JHR is designed to provide a fast neutron flux of 5.5 x 10^{14} n/cm^2·s in the core. In contrast to HFIR which yields up to 10 dpa/y, the fast flux in JHR

will generate up to 16 dpa/y. The core of JHR is being designed to accommodate up to 20 simultaneous experiments, many of which can be highly instrumented. The facility will also have the capability to perform in-core, on-line fission gas analysis from a pressurized fuel rod.

The maximum thermal flux in the reflector region of JHR will be 5.5 x 10^{14} n/cm^2·s. While useful for production of many industrial and medical isotopes, this value is well below the peak thermal flux HFIR. Six displacement systems are being incorporated into the reflector region to accommodate nuclear fuel experiments and isotope production. These include test devices for nuclear fuel behavior dedicated to characterization and qualification under nominal, off-normal, and accident conditions as well as a system for irradiating low-enriched uranium targets for the weekly production of up to 4,800 6-day Ci of ^{99}Mo. Numerous fixed irradiation positions in the beryllium reflector will allow JHR to produce a range of medical and industrial isotopes. The reactor cannot, however, be used to produce those isotopes which can only be created at HFIR and SM-3.

The JHR project is backed by an international consortium led by the CEA which is the project owner, nuclear operator, and contracting authority of the facility. The consortium includes AREVA and EDF for France, CIEMAT for Spain, NRI for the Czech Republic, SCK.CEN for Belgium, VTT for Finland, DAE for India, IAEC for Israel, NNL for Great Britain, STUDSVIK for Sweden, JAEA for Japan, and the European Commission. In exchange for their financial participation, JHR consortium members have guaranteed access to experimental capacities of the facility to conduct their own material test research. ■

Belgian Reactor 2 (BR2)

The BR2 light water cooled, beryllium moderated materials test reactor is located near Mol, Belgium and was first operated in January 1963. It has a very unique design with a central vertical channel and all other fuel and experimental channels inclined to form a hyperboloidal arrangement around the central channel. This compact geometry leads to a high fission power density with easy access at the top and bottom covers allowing for complex irradiation devices to be inserted and withdrawn. The reactor load is optimized for each cycle allowing for unique flexibility in the position of fuel, control rods, and experiments. When BR2 operates at its maximum power (100 MW), it provides thermal neutron fluxes up to 1 x 10^{15} n/cm^2·s. The reactor has an active refurbishment plan for continued operation through 2026 and plans to run through 2036. Operations beyond this date will be determined by the lifetime of the current pressure vessel.

BR2 is used to simulate other reactor environments to perform tests of fuels and materials under representative conditions for light water reactors, gas-cooled or sodium-cooled fast reactors, and fusion reactors. The test reactor is also used to study accelerated ageing of materials under high neutron flux and behavior of materials under accidental conditions such as fuel transients and power excursions. While the facility has taken over a number of fuel experiments with the closure of HALDEN, it was reported during the committee's visit that they are "struggling with capacity" to accommodate all of the requests from industry.

As an isotope producer, BR2 currently has the world's largest installed irradiation capacity for the world's most used nuclear medicine isotope; 7,500 6-day Ci per week for ^{99}Mo. The facility also produces a wide array of other medical and industrial radioisotopes. While BR2 plays a critical role in meeting the world's demand for these isotopes, it cannot provide several of the key isotopes produced at HFIR. For example, BR2 is used to make ^{188}W as a generator for the production of ^{188}Re (the therapeutic analogue of the most used nuclear medicine imaging agent ^{99m}Tc). The maximum specific activity of ^{188}W from BR2 is on the order of 1 Ci/g whereas the ^{188}W from HFIR is on the order of 100 Ci/g. As noted earlier in the report, higher activities will be required to take this promising isotope from research to clinical application. ■

CONCLUSIONS

This comprehensive study was carried out in response to a request by J. Stephen Binkley, the Deputy Director for Science Programs, Office of Science, Department of Energy, to Marc A. Kastner, Chair of the Basic Energy Sciences Advisory Committee (BESAC). Dr. Binkley asked BESAC to form a subcommittee to assess the scientific justification for a U.S. domestic high-performance reactor-based research facility, taking into account current international plans and existing domestic facility infrastructure. Dr. Binkley then proposed six specific questions as the framework for our study. We will address these questions below. This study has provided, in great detail, the scientific justification which Dr. Binkley has requested.

An important part of the impetus for Dr. Binkley's request was two previous studies. The first was a congressionally mandated study carried out by the National Academy of Sciences entitled "Reducing the Use of Highly Enriched Uranium in Civilian Research Reactors," completed in 2016. The second was a Report commissioned by the American Physical Society's Panel on Public Affairs (APS POPA) entitled "Neutrons for the Nation: Discovery and Applications while Minimizing the Risk of Nuclear Proliferation," published in 2018. These studies focused on the need for conversion of current research reactors from Highly Enriched Uranium (HEU >90% U-235) to Low Enriched Uranium (LEU <20% U-235) fuel to preclude any possible concomitant losses in U.S. scientific and technological capabilities.

An additional issue for the Department of Energy is the known finite lifetime of its flagship research reactor facility, the High Flux Isotope Reactor (HFIR), at Oak Ridge National Laboratory. The steady exposure of HFIR's steel pressure vessel to neutron bombardment has caused embrittlement of the steel. This, in turn, means that the vessel will have to be replaced within two to three decades, if not sooner (for example if the theoretical estimates for the rate of embrittlement are too optimistic or if failure occurs for some other reason).

As stated eloquently in the POPA study and as documented in detail in this report, neutrons are essential, precious, and powerful. Their unique properties as probes of the structure and dynamics of materials have led to numerous advances in basic materials science. Indeed, whenever a new class of materials is discovered or new properties are observed in an old class of materials, immediately the basic structural and magnetic properties of these materials are characterized using neutron scattering techniques. This has happened repeatedly over the past several decades.

Neutrons have also become invaluable tools in industrial product development and manufacturing. The range of applications varies from studying the microstructure of high-performance batteries to optimizing drug preparation and delivery to determining the properties of gas-bearing shale rock. The penetrating power of neutrons has made possible direct observation of operating internal combustion engines, the optimization of high-performance turbine blades, and the measurement of stress in welds for the auto industry.

Nuclear reactors also play an essential role in providing both neutrons and neutrinos for studies in fundamental physics; they are key to our understanding of the constituents and forces of matter, the properties of elementary particles, and the symmetries of nature. For example, precision experiments using neutrons and neutrinos measure the neutron lifetime, probe the neutron electric dipole moment, and search for sterile neutrinos as a new form of matter. Understanding the properties of neutrons and neutrinos holds the key to some of the most important fundamental questions in physics, including the nature of physics beyond the standard model.

Nuclear research reactors also play an indispensable role in isotope production and materials irradiation. Indeed, initially HFIR's primary mission was radioactive isotope production. The vast majority of radioactive isotopes used in medicine, industry and basic research are produced by irradiating materials with neutrons in nuclear reactors. Specifically, because of HFIR's intense neutron flux, it plays a central role in producing many critical radioactive isotopes. These include the first targeted alpha therapy agent approved for clinical use by the U.S. FDA. Radium-223 is a therapy for symptomatic bone metastases in prostate cancer that improves overall patient survival with a 30% reduction in mortality. Californium-252 and Nickel-63 are both used extensively in industry and by the Departments of Defense and Homeland Security.

Finally, the heaviest element radioactive isotopes are used in fundamental materials research to understand their physical and chemical properties. Materials irradiation studies are critical to developing accident tolerant fuels and clad materials for nuclear reactors and are essential to the fundamental investigation of radiation degradation mechanisms and, importantly, for the development of structural materials technology for future fission and fusion reactors.

We now turn to the questions posed by Dr. Binkley:

1. "What is the merit and significance of the science that could be addressed by a high-performance, steady-state reactor, and what is its importance in the overall context of materials sciences and related disciplines?"

As documented in great detail in this report, neutron scattering carried out at steady-state reactors plays a fundamental role in virtually all areas of the condensed matter sciences including solid state physics, quantum materials, high temperature superconductors, topological magnets, spintronic materials, polymer melts, microemulsions, block copolymers and gels. In addition, neutron scattering is playing a progressively more important role in biology including protein crystallography and studies of membranes, pharmaceuticals, and biotic/abiotic interfaces. Importantly, for both soft condensed matter and biological hydrogenous systems, scattering contrast may be controlled by H/D labelling providing structural information that is not available by any other technique. Progress in all of these fields would be greatly hindered if not stopped entirely if the information provided by neutron scattering was not available.

It is important to point out that the nature of research in the condensed matter sciences has changed dramatically over the past several decades. It is now rare for a single probe to elucidate completely the fundamental science underlying any given material. As an example, Fe-based superconducting systems are characterized by competing antiferromagnetism, electronic nematic order, charge density order, structural order, and superconductivity. Furthermore, each of these orders may be important on different length scales. In order to elucidate the fundamental science in such materials, one needs to carry out a wide variety of studies including crystal synthesis, measurements of the macroscopic electronic, magnetic and structural properties, neutron scattering studies of the static and dynamic structural and magnetic properties, angular resolved photoemission and inelastic x-ray scattering studies of the electronic excitations, electron microscopy for thin film materials, and optical studies using both laser and synchrotron light source. All of this information must then be integrated together to understand the physics underlying the material. Neutron scattering is almost always one of the essential tools in these studies; without world leading neutron facilities, both steady state and pulsed, the U.S. would be relegated to a secondary role in modern materials science and technology.

Separate from the above, steady-state reactors play a dominant and often unique role in both isotope production and materials irradiation studies. Radioactive isotopes contribute to science, technology, and medicine in a myriad of ways as documented in detail in this report. As mentioned earlier, they are used routinely in a wide variety of imaging technologies and to treat cancers. Steady state reactors also produce the heaviest elements on the periodic table. These heavy elements have fascinating electronic and chemical properties, representing one of the important frontiers in basic solid state physics and chemistry.

Clearly, in both the operation of current generation reactors and the design of advanced fission and fusion reactors, the performance of structural metals in nuclear environments must be understood. A critical role of reactor-based neutron sources is the irradiation of materials to support the investigation of radiation degradation mechanisms and to spur the development of advanced fuels and structural materials technology for future fission and fusion reactors. HFIR in particular plays a central and often unique role in such investigations.

Finally, steady state reactors provide both neutron beams and an isotropic stream of antineutrinos. This makes possible experiments which probe some of the deepest questions in physics including the nature of physics beyond the Standard Model. Neutrinos have played a key role in the evolution of the universe and the formation of large-scale structures since the beginning of time and yet much remains to be understood about their fundamental character. HFIR is a unique source of reactor neutrinos in the U.S. with user access and, as such, is a critical component of the U.S. research effort in fundamental physics.

2. "What are the capabilities of other domestic and international facilities, existing and planned, to address the science opportunities afforded by such a domestic research reactor?"

In the main text, we have reviewed three major domestic facilities, namely NCNR at NIST and HFIR and the SNS at ORNL. In addition, we have reviewed the scientific capabilities at four European steady state reactor facilities, ILL at Grenoble, FRM-II in Munich, the BR2 reactor in Belgium, and the Jules Horowitz Research Reactor which is currently under construction in France. The latter two facilities serve European materials testing and isotope production needs. We have not explicitly surveyed neutron facilities in China and Japan. We discuss first neutron scattering capabilities.

As stated succinctly in the POPA report, Europe has dominated neutron scattering in recent decades as measured by capabilities, capacity to support users, and scientific output. There are two European world class facilities namely ILL in France, and the ISIS Neutron and Muon Source in the United Kingdom. In addition, there is a network of both reactor and spallation sources throughout Europe which provide for the health of the European neutron scattering ecosystem. An example of the latter is the FRM-II with its 28 well-instrumented spectrometers, cold source and two Guide Halls. Particularly notable is the investment in instrumentation that has been made at the European reactor facilities. Soon, the 5 MW European Spallation Source in Lund, Sweden will come on line. This facility is projected to be the world's leading facility for research using neutrons; it should be operating with an initial suite of 15 instruments in the mid-20s.

The peak of U.S. capacity based on the number of scattering instruments occurred in 1996 with 55 scattering instruments. Currently the number of instruments is approximately 48; this plus the increasing importance of neutron scattering in frontier research and technology is the reason for the huge oversubscription at U.S. neutron facilities. This shortfall will be partly mitigated by the second target station at SNS, but only partly. If HFIR were to be closed down, some U.S. neutron scattering investigators would move their center of gravity to Europe. However, there are institutional and political constraints on U.S. researchers severely limiting available beam time on spectrometers at the lead European facilities. In brief, from the point of view of neutron scattering, losing a well-functioning steady state high flux reactor source would do irreparable damage to U.S. science and technology.

Loss of HFIR would generate similar concerns for the isotope production and materials testing community. In the main text we review the programs at the Advanced Test Reactor, ATR, the Belgian Reactor, BR2, and the French Jules Horowitz Research Reactor currently under construction. While ATR plays a vital role in materials irradiation and nuclear fuel qualification studies for the United States, it does not have the high neutron flux required to produce many of the radioactive isotopes and transuranic elements made in HFIR. BR2 plays an important role in Europe in terms of both materials testing and isotope production. However, it cannot provide a number of the key isotopes made in HFIR. Similarly, the JHR will be an invaluable facility but it will fall short of HFIR's capabilities in many respects in part because its planned peak thermal flux will be well below that of HFIR's.

3. "What are the benefits to other fields of science and technology and to industry of establishing such a capability in the U.S.? In particular, consider applications such as isotope production, materials irradiation, neutron imaging, dark matter research, and neutron activation for trace element analysis."

This question has been answered in detail in both the main body of this report and in the response to the first question.

4. "What are the strengths and limitations of a steady-state research reactor compared to a pulsed spallation neutron source for science, engineering, and technology? What functions currently performed by research reactors can be assumed by spallation neutron sources?"

As discussed in detail in this report, there are many applications where a steady state source is either essential or preferable to a pulsed spallation source of neutrons. Examples of these include any investigations requiring polarized neutrons and studies of the phases and phase transitions in one- and two-dimensional materials. Currently, reactor sources provide a large fraction of the available neutron time on the key instruments in soft matter and biological research. Many investigators in hard condensed matter physics will characterize a material using both pulsed spallation neutron instruments and those at a steady state reactor,

the former to carry out a broad survey of the excitations in momentum and energy space, and the latter to obtain precise information in a particular region of phase space. We expect such dual investigations to continue for the indefinite future.

The question of which functions currently performed by research reactors can be assumed by spallation neutron sources is difficult if not impossible to answer except for isotope production and most materials irradiation studies which require the steady high-fluxes generated by a research reactor. Over the last decade, we have seen extraordinary developments in instrumentation and data analysis capabilities for neutron scattering at both steady state and pulsed spallation sources. Indeed, such instrumentation development has arguably been more important than increases in neutron flux. Thus, experiments which are currently carried out at only one type of source may, 10 years from now, be carried out at both types of facilities.

The fundamental challenge for the neutron scattering community is not which type of neutron source to use for a particular experiment, but rather obtaining beam time at all for any experiment. As shown by the user data for each of NIST, HFIR and the SNS, almost all of the neutron spectrometers are over-subscribed by as much as a factor of three. Further, the proposal cycle time is typically six months. This means that an important experiment can be delayed by a year or more—an unacceptable delay if the U.S. is to maintain leadership in the development of new materials. This is particularly challenging for both graduate students and postdoctoral fellows. Both are typically counting on carrying out experiments which will either lead to their Ph.D., or for the postdocs, enable them to obtain a coveted faculty position. The country needs a steady flow of outstanding young people entering the field of neutron scattering, and this in turn means that we need adequate state-of-the-art facilities. In addition, oversubscription inevitably means that committees allocating beam time tend to favor proposals which guarantee results. This in turn, means that more speculative experiments which may fail, but if successful would produce spectacular results tend to be disfavored.

Therefore, the most important issue is not steady state versus pulsed, but rather how do we ensure that the United States will recover its world leading position in the field of neutron scattering. This means that we need both well-instrumented high flux reactor and pulsed spallation sources of neutrons.

5. "Are there feasible upgrade paths for HFIR to provide world-leading capabilities in serving the Office of Science missions well into the future? What can we learn from the experience at the Institut Laue-Langevin?"

This question is answered in detail in the HFIR strategy document provided to our committee by Oak Ridge National Laboratory. It is reproduced in full in Appendix 1. The lifetime of HFIR is limited by the progressive embrittlement of the pressure vessel. The vessel will most certainly have to be replaced by the middle of this century and possibly sooner. Fortunately, HFIR was designed for pressure vessel replacement. The complete replacement of a research reactor vessel has been previously accomplished at ILL in 1995 and at the Petten research reactor in 1983–85. There is a detailed plan for a similar vessel replacement for HFIR. Almost certainly, any vessel replacement would occur at the same time as the conversion from HEU to LEU fuel, likely in the 2030 to 2035 time frame.

The pressure vessel replacement would allow a number of upgrades and improvements. The new pressure vessel would support large beam tubes and an improved cold source. This would make possible an increase in the number of neutron scattering instruments from 12 to 20. Importantly, it would also allow the construction of a second guide hall with concomitant lower background for neutron scattering experiments. It is envisaged that there would both a thermal neutron and cold neutron guide hall.

The increased irradiation capacity enabled by the new pressure vessel would provide a corresponding increase in isotope production and damage rates for materials irradiation experiments. The changes to the reactor vessel head would facilitate introduction and removal of capsules, including during reactor operations. This would allow increased isotope production, especially for short-lived isotopes, such as Pt195m, Lu-177, W-188/Re-188, and Th-227 for medical applications, Se-75 for radiography, and Es-253 for heavy element chemistry. The improved access would also enable a significant increase in instrumented materials irradiation experiments to advance radiation effects research including the development of accident-tolerant fuels and fusion reactor materials.

6. "Can Low Enriched Uranium (LEU) and High Assay LEU (HALEU) fuels (defined as <20 % enriched U-235) replace Highly Enriched Uranium fuels in research reactors while preserving the needed characteristics of neutrons produced by steady-state reactors? What R&D would be needed to support LEU and HALEU fuels development?"

The research and development of HEU-LEU conversion is discussed in detail in the "HEU-LEU Conversion" section of the main text and in Appendix 2. Many successful conversions have already been accomplished around the world. There is a variety of fuel compositions and configurations. In 2019, it was decided that a fuel based on U3Si2 in a dispersion geometry would be the baseline solution for HFIR. The U3Si2 dispersion fuel system would allow the HFIR-specific characteristics of the current HFIR HEU design to be leveraged for the LEU design. The HFIR HEU-LEU Conversion Team reported preservation of all missions to our BESAC subcommittee. They believe that they are on a sound coordinated path to a U3Si2 conversion that would maintain the mission capabilities of HFIR and they recommend that the pressure vessel and beryllium reflector replacement occur at the same time as the LEU conversion. The necessary U3Si2 fuel element research and development is ongoing.

Finally, there is always the possibility that, for either technical or political reasons, HFIR will have to be closed down and the vessel replacement and HEU-LEU conversion proposed above will not be possible. Indeed, our country has already suffered a major loss with the permanent closure of the High Flux Beam Reactor at Brookhaven National Laboratory. Because of the long times involved between the initial design and the final commissioning of such a reactor, DOE must have an alternative strategy. Specifically, DOE needs to initiate a scoping study for a green field research reactor optimized to perform neutron studies and isotope production that are uniquely suited to a very high flux reactor such as HFIR. The reactor would be designed to operate on LEU fuel. Reactor and fuel assembly designs should be evaluated to optimize simultaneously reactor performance and fuel assembly manufacturability. Further, the design should, to the extent possible, be optimized for neutron needs as currently understood and for flexibility of configuration to enable future, currently unanticipated, applications. Beginning this process now will allow time to evaluate options and proceed with planning and approvals in time to ensure continuing availability of a multiply capable high flux research reactor in the U.S.

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The Scientific Case

1. Neutron Scattering

1a. Solid State Physics Including Quantum Materials

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APPENDICES

APPENDIX 1. Oak Ridge Proposed Strategy for HFIR

The High Flux Isotope Reactor

Opportunities for Sustained Leadership In High-Flux Research Reactors and Related Neutron Science and Technology

Introduction

HFIR is a national scientific user facility funded by the Department of Energy (DOE) Office of Basic Energy Sciences (BES) within the DOE Office of Science. HFIR and the SM-3 Reactor in Dmitrovgrad, Russia, produce the highest steady-state neutron fluxes in the world, with a peak thermal neutron flux of 2.5×10^{15} neutrons/cm^2·s. HFIR is unique and flexible, providing the highest neutron fluxes for missions in neutron scattering, isotope production, materials irradiation, neutron activation analysis, and nuclear physics. SM-3 matches HFIR's peak flux but does not have neutron scattering capability. The Institut Laue Langevin (ILL) reactor in France, with a peak thermal flux of 1.5×10^{15} neutrons/cm^2·s, is optimized for neutron scattering and has limited capability in other mission areas. The HFIR peak flux exceeds that of all remaining research reactors by a factor of 2.5 or more. Table A1.1 provides a summary of higher-flux research reactors currently in service.

Facility Description

HFIR is a pressurized, light water-cooled and -moderated, flux-trap-type reactor with a beryllium reflector. The reactor core, illustrated in Figure A1.1, consists of

TABLE A1.1.

High-flux Research Reactors Currently In Use

REACTOR	LOCATION	INITIAL OPERATION	POWER (MW)	FUEL	REFLECTOR	PEAK THERMAL FLUX1 (1015 N/ CM2·S)	PRIMARY MISSIONS
HFIR	US (ORNL)	1965	85	HEU	Be	2.5 (1.0 fast)	Scattering (12 instruments) Isotopes (including heavy actinides) Materials testing
SM-3	Russia	1961	100	HEU	Be	2.5 (1.0 fast)	Materials testing Isotopes (including heavy actinides)
ILL	France	1972	58	HEU	D_2O	1.5	Scattering (33 instruments)
BR2	Belgium	1962	100	HEU	Be	1.0 (0.7 fast)	Materials testing Isotopes
ATR	Idaho	1967	250	HEU	Be	1.0	Materials testing Isotopes
FRM-II	Germany	2005	20	HEU	D_2O	0.8 (0.5 fast)	Scattering (23 instruments) Isotopes
CARR	China	2010	60	LEU	D_2O	0.8 (0.6 fast)	Scattering (6 instruments) Isotopes Materials testing
NBSR	US (NIST)	1967	20	HEU	D_2O	0.4	Scattering (19 instruments)
OPAL	Australia	2007	20	LEU	D_2O	0.4	Scattering (13 instruments) Isotopes

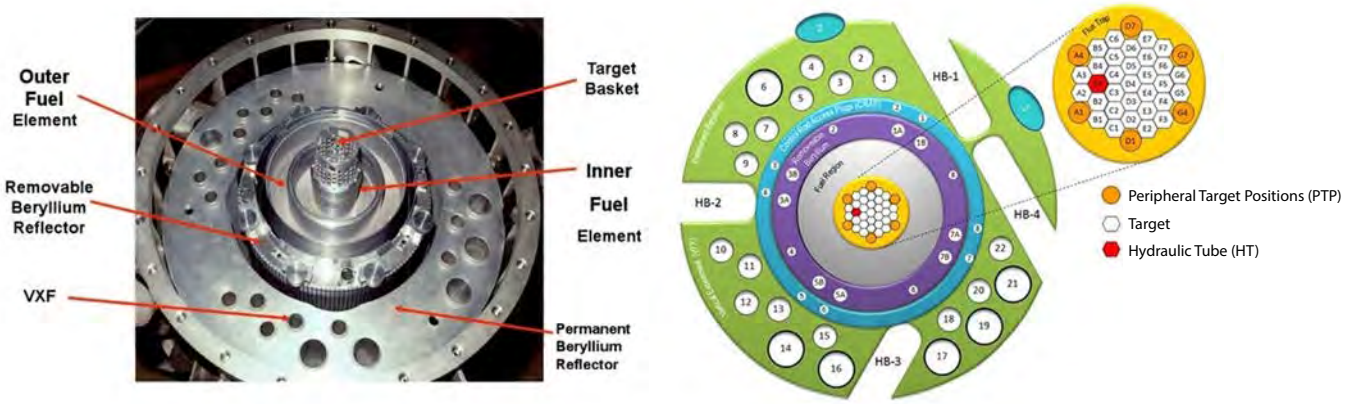

FIGURE A1.1. Photo and schematic of the HFIR core, showing the flux trap (yellow), fuel region (gray), and reflector (purple and green).

The various target positions for isotope production and materials irradiation are shown as well as the four horizontal beam tubes for neutron scattering (the cold source is incorporated in the HB-4 beam tube)

Source: Oak Ridge National Laboratory, U.S. Dept. of Energy

two concentric cylindrical fuel elements, each approximately 61 cm in height, surrounding a 12.7 cm diameter central flux trap. The fuel is contained in 171 inner and 369 outer aluminum-clad fuel plates curved in the shape of an involute to provide a constant cooling channel width between plates. HFIR currently uses highly enriched ^{235}U fuel and operates at a power level of 85 MWt.

The fuel region is surrounded by an annular beryllium reflector approximately 30.5 cm thick. The beryllium reflector is in turn surrounded by a water reflector of effectively infinite thickness. The reactor core assembly is contained in a 2.44 m diameter pressure vessel located in a 5.5 m diameter cylindrical pool of water. The pool walls are reinforced concrete with a stainless-steel liner.

The central flux trap includes 37 cylindrical target positions where multiple capsules can be irradiated in the highest-flux region of the reactor. There are an additional 42 target positions distributed in the beryllium reflector where the neutron fluxes are lower. Four horizontal beam tubes penetrate the reflector to transport beams of neutrons to 12 scattering instruments located outside the biological shield. One beam tube incorporates a liquid hydrogen cold source and transports cold neutrons to instruments in an adjacent guide hall, while the other beam tubes transport thermal neutrons to instruments outside the reactor shielding in the beam room. Two pneumatic tubes provide access for neutron activation analysis, and four slant tubes are available for engineering studies.

In addition to having the highest thermal neutron flux, the HFIR complex includes a unique capability for radioisotope separations, the Radiochemical Engineering Development Center (REDC). REDC is essential to the chemical separation and purification of alpha emitting isotopes produced at HFIR, as well as other isotopes making up more than 400 radioisotope shipments annually to universities, hospitals, industry, and other research institutions. This HFIR/REDC complex (Figure A1.2) is essential to the DOE isotope mission and unique in the world.

User Communities

HFIR serves five distinct user communities, each with unique characteristics. They include neutron scattering, isotope production and research, materials irradiation and radiation effects research, neutron activation analysis, and neutrino research. The flexible design of HFIR allows these communities to be served simultaneously at the highest neutron fluxes with minimal interference. A summary of numbers of experiments, users, and publications for each of these communities is given in Table A1.2.

Neutron Scattering

HFIR and ILL in France produce the highest continuous neutron flux in the world for neutron scattering, a factor of two or more higher than any other facility. The brightness of the HFIR source for both cold and thermal neutrons slightly exceeds that of ILL, as shown in Figure A1.3. Table A1.1 provides a listing of

FIGURE A1.2. ORNL's High Flux Isotope Reactor (HFIR) campus including the Radiochemical Engineering Development Center (REDC)

Source: Oak Ridge National Laboratory, U.S. Dept. of Energy

TABLE A1.2.

HFIR Experiments, Unique Users, and Journal Articles (2017)

USER COMMUNITY	NUMBER OF EXPERIMENTS	UNIQUE USERS	JOURNAL ARTICLES
Neutron scattering	561	561[a]	192[a]
Isotopes	~50[b]	~50[c]	2
Materials irradiation	~400[d]	~50[c]	48
Activation analysis	~900[d]	~10[c]	1
Neutrino physics	1	14[e]	2
Other HFIR			10
Totals	1747	635	243

a. Unique users performing neutron scattering research on site at ORNL in 2018
b. Number of unique irradiation campaigns
c. Principal investigators and unique customers
d. Unique capsules
e. Consortium institutions

selected high-flux reactors in service today, including the number of scattering instruments at each facility with neutron scattering capability. Europe has twice as many scattering instruments at high-flux reactors as the United States.

HFIR is the highest flux steady-state neutron source for neutron scattering in the world, and is a key asset in providing the United States with this much needed tool for materials research. The U.S. competitive position in neutron scattering could be substantially strengthened by making improvements to HFIR instruments and related beam systems, expanding low-background experimental space, and increasing the number of instruments.[1] Reactor-based and pulsed neutron sources are complementary, with reactor-based sources preferred for experiments that require the highest neutron counts in specific, predetermined regions of experimental space. Both types of sources are needed for a globally competitive neutron scattering program.

Isotope Production and Research

HFIR, together with SM-3 in Russia, produces the highest thermal neutron flux for isotope production—more than a factor of two above any other facility worldwide. HFIR and SM-3 are the only facilities capable of producing milligram quantities of heavy actinides, including Cf-252. Californium-252 is widely used for industrial applications, with ~70% of the world's supply provided by HFIR. By-products of Cf-252 production, including Bk-249, Cm-248, mixtures of Cf-249, 250, and 251, Es-254, and Fm-257, are used for heavy element chemistry and for superheavy element research and discovery. Elements 115 and 117 were discovered using Bk-249 from HFIR, and HFIR isotopes have been involved in the discovery or confirmation of eight additional elements since 1970. Curium-248 from HFIR is currently being used in a discovery experiment for element 119, and mixed Cf recovered from HFIR Cf-252 sources is planned for use in the search for element 120. The very high flux of HFIR also enables the production of many other isotopes with the high specific activity that is often preferred in industry and medicine.

HFIR isotopes are processed in the adjacent REDC, a large complex that includes heavily-shielded hot cells for remote handling and chemical processing of highly

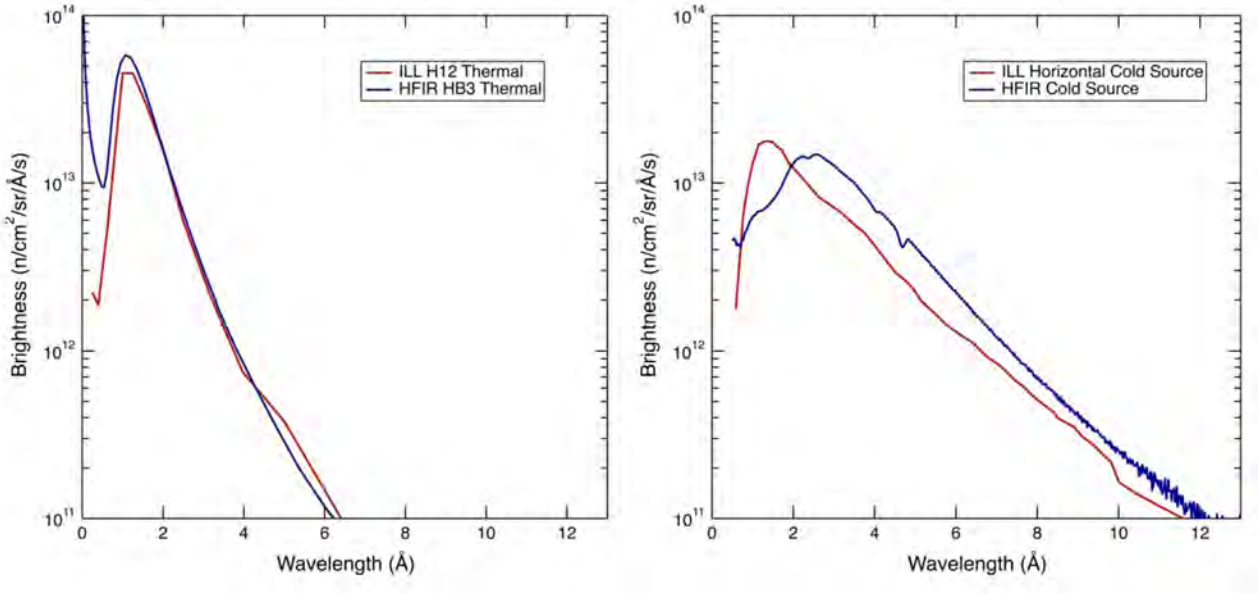

FIGURE A1.3. Source brightness for thermal and cold neutron scattering at HFIR and ILL
Source: Oak Ridge National Laboratory, U.S. Dept. of Energy

radioactive materials. HFIR isotopes are distributed to hundreds of research, medical, and industrial customers each year. Many of these isotopes are unique to HFIR and are incorporated into industrial and medical products with tens of thousands of end users. A list of HFIR isotopes currently in worldwide distribution is shown Table A1.3. In addition to the heavy actinides, unique and high-specific-activity isotopes from HFIR include Pu-238 (to power National Aeronautics and Space Administration deep space missions), Ac-227 (for targeted alpha therapy), Ni-63 (for luggage screening at airports), and Se-75 (for nondestructive testing of pipelines and other infrastructure).

Materials Irradiation and Radiation Effects Research

HFIR provides the highest fast-neutron damage rate in the world for materials research in areas such as accident-tolerant nuclear reactor fuels and materials for future fusion reactors. Hundreds of specimens are irradiated each year for multiple DOE programs and other sponsors. More than 30 positions are available in the central flux trap of HFIR for high-flux experiments involving a total of up to 200 individual capsules. Neutron irradiation capabilities include neutron flux tailoring and temperature control for many experiments; more than 400 unique neutron irradiation experiments were performed at HFIR in FY 2017. This represents several thousand individual specimens ranging from fundamental irradiation effects to qualification of advanced materials supporting dozens of sponsors.

A gamma irradiation facility is also available that produces the highest dose rate for gamma radiation damage to understand materials behavior and qualify materials in high-gamma radiation environments (such as in nuclear reactors).

Neutron Activation Analysis

HFIR neutron activation analysis capabilities are the best in the world, providing the highest-sensitivity trace analysis for national security programs, international treaty verification, environmental compliance, and other applications. Two pneumatic tubes, one leading to a higher flux region of the reflector and the other to a lower-flux region, transport samples to the reactor for irradiation and then on to shielded counting stations. Primary customers include the International Atomic Energy Commission and DOE and National Nuclear Security Administration sponsors. More than 900 samples were analyzed in 2018.

Neutrino Research

The combination of a very high neutrino flux and the capability of locating a neutrino detector close to the reactor make HFIR uniquely attractive for reactor-based neutrino research. In 2015, 14 universities led by Yale University formed a consortium with ORNL to design, build, and operate a neutrino expe-

TABLE A1.3. Medical, Industrial, and Research Use of Selected HFIR Isotopes

HFIR produces more than 50 different isotopes for hundreds of customers that supply products to tens of thousands of end users each year. Selected examples of isotopes currently in high demand are shown.

ISOTOPE	DESCRIPTION	APPLICATION	UNIQUENESS TO HFIR
Californium-252 (Cf-252)	Compact neutron source	Nondestructive analysis of nuclear fuel rods; Analysis of product streams in mining and cement industry; Oil well logging; Safe reactor startup	HFIR supplies 70% of global demand (only other source of Cf252 is in Russia)
Plutonium-238 (Pu-238)	Radioisotope power source	Power and heating systems for NASA deep space and outer planet missions	HFIR (supplemented by Idaho National Lab) is the sole supplier for NASA
Nickel-63 (Ni-63)	Compact irradiation source	Security screening of luggage at most airports	HFIR is sole supplier outside Russia
Actinium-227 (Ac-227)	Alpha radiation source together with its daughter Ra-223	FDA-approved for targeted alpha therapy of advanced cancers	Can only be produced in HFIR; demand growing with >$1B in private sector investment
Barium-133 (Ba-133)	Gamma radiation source	Specific oil well logging applications; calibration source for medical imaging devices	Produced only in HFIR at desired specific activities and quantities
Selenium-75 (Se-75)	Gamma radiography source	Nondestructive testing of welds in bridges, shipbuilding, and other infrastructure	HFIR produces very high specific activity Se-177 widely preferred in industry
Other heavy actinides (byproducts of Cf-252 production)	Berkelium-249, Einsteinium-254, etc.	New element discovery (including elements 117 and 115); heavy element chemistry	Actinides from HFIR currently being used in searches for elements 119 and 120
Lutetium-177 (Lu-177)	FDA approved for treatment on neuro-endocrine cancers	Multiple clinical trials for other advanced cancers; >$1B in private investment	HFIR uniquely capable to produce with minimal impurities at high specific activity

riment at HFIR (the Precision Reactor Oscillation and SPECTrum Experiment, or PROSPECT[2]). The goal is to measure short-baseline neutrino oscillations with implications for fundamental nuclear physics and the standard model. Related advances in neutrino detection and properties offer potential for the development of stand-off reactor monitoring.

HFIR in the 21st Century

HFIR has been substantially refurbished and upgraded over the past two decades with new infrastructure, a high-brightness cold source, and a guide hall and new instruments. Continued operation of HFIR beyond mid-century will require replacement of the pressure vessel—an upgrade previously accomplished at several other research reactors. Pressure vessel replacement would extend HFIR operation into the next century and would provide options for significant mission-related upgrades.

HFIR was designed to facilitate the replacement of all reactor systems, including the pressure vessel. HFIR executes an extensive corrective and predicted maintenance program including more than 700 preventative tasks each year. Components that have been refurbished/replaced include primary and back-up pumps, the beryllium reflector, beam tubes, heat exchangers, cooling tower, control plates, and electrical and safety systems. The program also includes the fuel cycle, including offsite production of fresh fuel and fuel elements and disposition of spent fuel. The HFIR maintenance program is up-to-date and has supported an operational predictability exceeding 92% since 2007.

FIGURE A1.4. Original Installation of the HFIR Pressure Vessel The HFIR building and pool were designed to support pressure vessel replacement.
Source: ORO Construction Division, M.K. Ferguson Co.

Pressure Vessel

HFIR was designed for pressure vessel replacement. The existing crane used for vessel installation can be used for removal and replacement. The existing truck airlock can be used to admit the new vessel. A photograph from the original vessel installation is shown in Figure A1.4. There are only three welded pipe connections (all other connections are flanged), and the vessel can be disconnected and sectioned under water in the existing reactor pool. The vessel is less activated than other waste that is routinely disposed at HFIR. Vessel sectioning and replacement have been demonstrated in industry and at the ILL and Petten research reactors in Europe. A plan for vessel removal was developed for HFIR in the 1980s.

Replacement of the pressure vessel will be required by mid-century due to embrittlement, possibly earlier if embrittlement trends depart from theoretical predictions. A new vessel would allow return to HFIR's 100 MWth design power level and would enable mission upgrades, including larger beam nozzles for enhanced neutron scattering, vessel head changes to support the isotope and materials irradiation missions, and improved cold source design for up to a 50% increase in source brightness. These changes would also support additional scattering instruments, improved online insertion/removal of isotope production and materials irradiation samples, better temperature control and instrumentation for in-core experiments, and improved facilities for handling irradiated materials.

In 1987, it was discovered that the HFIR reactor vessel welds and base materials were embrittling due to irradiation damage at a faster rate than anticipated by the original designers, such that certain portions of the reactor vessel in the vicinity of the beam tube nozzles no longer met the American Society of Mechanical Engineers (ASME) Boiler and Pressure Vessel Code. In order to resume operations, reactor power was lowered to 85 MWth from 100 MWth, some operational parameters were changed, and a hydrostatic proof test of the reactor vessel was instituted to ensure vessel integrity. This test is performed every two effective full power years.

One of the corrective actions proposed at the time was to determine if the HFIR pressure vessel could be replaced with a new vessel. An engineering assessment was performed, and it was determined that the vessel could be replaced. This included removing the old vessel, cutting it up in the pool, disposing of the irradiated material in an appropriate DOE low-level waste facility, fabricating a new vessel with new materials that were known to resist radiation damage (304L stainless steel), and reconnecting all the piping and support structures.

In many ways, the reactor vessel restricts upgrades to the reactor because it is the most permanent fixture in the facility. The current vessel nozzle sizes are 8.0 in. ID for HB-1, HB-3, and HB-4, and 12.0 in. ID for HB-2. Increasing the HB-1, 3, and 4 nozzle sizes to the same as at HB-2 would allow larger beam tubes at these locations, enabling larger beams for neutron scattering. The vessel head design of the current reactor restricts easy access to certain locations in the permanent beryllium reflector that are used for material irradiation and/or isotope production. If vessel replacement is pursued, the vessel head and beam tube nozzles will be redesigned to improve mission performance.

The 1987 replacement study concluded that the vessel could be replaced on an accelerated schedule that took about 3 years at a cost of $18M. The results of the study included a new vessel engineering specification (replacement vessel shell and extension region only), and a set of preconceptual design drawings. With cost escalation from 1987 dollars, more recently in January

2020, it was estimated that the redesign/procurement of a new stainless steel reactor pressure vessel shell with new upper and lower head, seismic upgrades, associated minor upgrades, larger nozzles to allow larger beam tubes at HB-1, -3, and -4 (HB-2 equivalent size), and top head changes to better support isotopes and materials irradiation missions, would be $300M.

The complete replacement of a research reactor vessel has been previously accomplished at the Institut Laue Langevin (ILL) and Petten research reactors in Europe. In 1983–1985, the pressure vessel at the 45MWth High Flux Testing Reactor (HFR) at Petten was replaced. The Petten replacement study[3] contains a complete description of the replacement campaign for that reactor. In 1995, the reactor vessel at the 75 MWth ILL reactor was replaced. ILL has an aluminum vessel with a core region similar to HFIR. In addition, extensive experience exists for heavy component replacement at nuclear power plants.

Second guide hall

The APS report, *Neutrons for the Nation,*[4] makes the case that reactor-based neutron scattering continues to be essential for U.S. scientific competitiveness, and recommends a sharp increase in investments in neutron instrumentation. A revitalization of HFIR, with improvements to the reflector design and a new pressure vessel, presents an outstanding opportunity to improve the U.S. capabilities in materials research using neutrons. One of the main challenges at HFIR is the relatively cramped space and high fast neutron background in the existing thermal beam room. Thus, significant gains can be attained by adding a second guide hall. This would enable the construction of more instruments with great improvements in the signal-to-noise.

An additional guide hall at the HB-2 position with ten instruments would require the removal of three existing instruments for a net gain of six. With the possible addition of a couple of new instruments in the HB-4 guide hall, one can envision that an increase of instruments in the user program from 12 to 20 is possible. It must be recognized from the outset that the true benefits of improvements to the neutron source can only be realized if they are coupled with upgrading and constructing neutron scattering instrumentation to world competitive levels. Indeed, most of the improvements in neutron scattering over the past 50 years have been realized via enhancements in instrumentation.

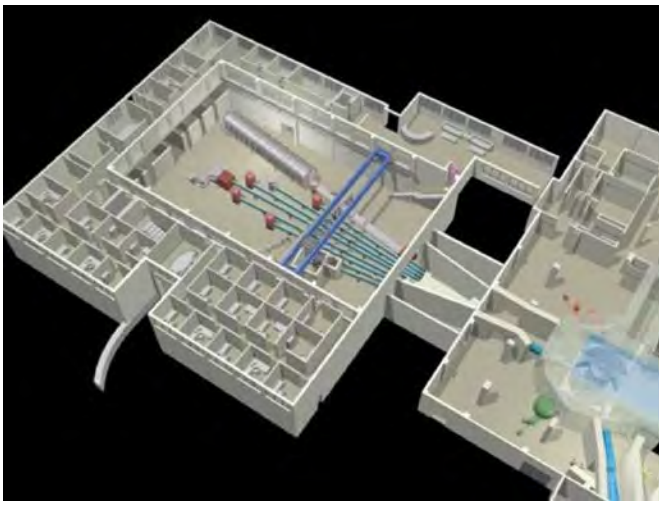

FIGURE A1.5. Early HB-2 Guide Hall Concept
Source: Oak Ridge National Laboratory, U.S. Dept. of Energy

With this in mind, several possibilities for a reconfiguration are possible. One model that has been discussed is to build a cold guide hall at HB-2, and recast the HB-4 guide hall as a thermal neutron facility. Moving thermal instruments into a guide hall enables significant improvements in signal to noise, and is essential for building the best instruments to complement the facilities envisioned at the SNS. Up to 20 world class instruments could be accommodated in this configuration.

In 2003, a cold guide hall for HB-2 was among the long-term priorities outlined in the DOE Office of Science report, *Facilities for the Future of Science: A Twenty-Year Outlook*.[5] A cut-away view of the instrument level of HB-2 Guide Hall as envisioned at that time is illustrated in Figure A1.5. The preliminary design made use of the perceived wisdom that the performance of the instrument suite is greatly improved if essentially all instruments occupy end-of-guide positions. It was envisioned that up to 10 new instruments could be constructed in the guide hall. Adequate allowance was made for the requirement of the ancillary laboratories and office space needed to make the best use of these instruments. The estimated cost of constructing the HB-2 facility, including the cold source, guide system, instruments, guide hall, project management, and 20% contingency was just under $100 million dollars (in constant 2003 dollars) over a 5-year period. An additional examination of the HB-2 cold source possibility was carried out in 2012 and confirmed a new cold source at HB-2 could easily be 50% brighter than the more compact cold source extant

at HB-4. A more recent examination presented to the BESAC Subcommittee on High-Performance Reactor-based Research Facilities in January 2020 estimated the cost $375M.

New reflector

In the past, the possible instrumentation upgrades for HFIR have been considered under the assumption that the essential configuration of the reactor pressure vessel and Be reflector would remain unchanged. A new reflector would be particularly advantageous for a cold source in the HB-2 location. Changing a major component of the reactor can affect several aspects of operation, including cycle length, as discussed elsewhere. Many options are under consideration and much optimization may be possible. To get a general idea of the possible effects of a new moderator on the brightness delivered to neutron instruments, it is worthwhile to examine the gain factors obtained simply by replacing the Be reflector with a D_2O reflector. The net result is that brightness of cold and thermal neutrons is increased by 30–40%, while the fast neutron background is reduced by a similar amount, suggesting that the signal to noise can be improved by roughly a factor of two, independent of other improvements.

The HFIR beryllium reflector is composed of three regions including, in order of replacement frequency and distance from core centerline, the removable beryllium reflector, the semi-permanent beryllium reflector, and the permanent beryllium reflector. The expected lifetimes of these components are approximately 83.7, 167.4, and 279 GWd, respectively (or approximately 6, 12, and 20 years). In preparation for the HFIR permanent beryllium change-out in 2024, ORNL redesigned the permanent beryllium reflector to include six additional irradiation sites, be more versatile with respect to irradiation and scattering experiments, and enhance its thermal-structural performance. The new design increases the number of vertical experiment facilities from 22 to 28, and arranges them in a way to maximize their availability for radioisotope production (e.g., ^{238}Pu production targets) and materials irradiation experiments without interfering with the neutrons delivered to the cold and thermal neutron scattering instruments.

Replacing HFIR's beryllium reflector with heavy water (D_2O) offers the potential to further enhance neutron scattering performance. The D_2O could be introduced as either a physical tank located within the pressure vessel, or as the coolant beyond the control element region. The absorption cross section and thermal diffusion length of D_2O are much less than those of beryllium; thus, the neutron mean free path in D_2O is much longer. Consequently, a D_2O tank has the possibility to significantly increase the reflector region's volume-averaged neutron flux and provide a more constant flux profile across its radius in comparison to the beryllium reflector. This enhancement could result in increased neutron fluxes on scattering samples, and additional space for larger beam tubes. However, the direct change from beryllium to D_2O results in reactivity and cycle length degradation due to the change in neutron reflection properties. Thus, a combination of beryllium and D_2O reflectors may provide optimal performance.

At a minimum, conversion to a D_2O reflector would require:

1. an initial study to better characterize the performance impacts of the change
2. an evaluation of potential impacts to the safety basis
3. an engineering evaluation and design
4. as-required safety basis evaluations/calculations and updates to the documented safety analysis (DSA) with U.S. DOE approval
5. construction of the designed system, and
6. startup testing.

The DSA would need to be evaluated to determine safety aspects that would need to be removed, updated, or added as a result of the modification. The nuclear design aspects of the reactor including power distributions, shutdown margin, and reactivity coefficients would need to be addressed. Additionally, tritium produced via nuclear activation of the D_2O would need to be managed.

Fuel cycle

The HFIR fuel cycle can be broken down into five separate phases: HFIR Uranium Oxide Production, HFIR Fuel Assembly Fabrication, HFIR Fuel Production Equipment Upgrades, fresh and irradiated fuel shipment, and HFIR Spent Fuel Storage and Disposal.

HFIR's uranium oxide is provided from feedstock at the Y-12 National Security Complex. The oxide processing takes place at Y-12's 9212 Facility. This antiquated facility is scheduled to be decommissioned in the middle to late 2020s and will be replaced by a new

facility, the Uranium Processing Facility (UPF), currently under construction at Y-12. HFIR fuel elements are fabricated and assembled at BWXT in Lynchburg, Virginia.

HFIR recently experienced a fuel deformation event that caused a manual shutdown due to increased radiation readings in the primary coolant system in November 2018. Upon opening the reactor vessel, fuel plate deformation on outer fuel element O-488 was observed. The cause of the fuel deformation has been attributed to machining errors on the outer side plate and subsequent fuel element assembly issues that led to inadequate welding and attachment of the fuel plates to the inner side plate. Enhancements to HFIR operations are underway to address potential vulnerabilities noted from the event.

HFIR restarted in October 2019 following completion of corrective actions that were made as a result of the fuel deformation event. The restart of the fuel element manufacturing and assembly processes at BWXT is planned for 2020.

LEU conversion

ORNL is funded by the U.S. DOE NNSA's Office of Material Management and Minimization to perform HFIR HEU to LEU conversion studies as part of their nuclear nonproliferation mission. HFIR is one of six domestic high-performance research reactors (USHPRRs) that cannot be converted with existing LEU fuel forms and corresponding qualification envelopes. HFIR is committed to converting to LEU once a fuel form capable of ensuring that operations will continue at the current functional, scientific performance level in a safe, reliable, and affordable manner.

HFIR LEU conversion will take place in five phases with the appropriate safety basis preparation by ORNL and U.S. DOE SC approval for each.

- The first phase is to present U.S. DOE SC with a Preliminary Documented Safety Analysis (PDSA) in the early 2020s.
- The second phase consists of running at least one cycle with the current HEU fuel at the higher power required for LEU conversion (e.g., 95 MW) to demonstrate the ability of the reactor cooling systems to remove the higher heat load.
- Third, in-vessel, low-power tests of the LEU lead test core (LTC) will be conducted to confirm calculated neutronic parameters.
- Then, a single cycle with the LTC will be run at the higher power to demonstrate continued ability to perform HFIR's scientific mission safely.
- The fifth and final phase consists of operating HFIR long-term with LEU fuel at the higher power following conversion. The low-power LTC tests and conversion to LEU are currently scheduled for 2030 and 2033, respectively.

Fuel design studies have been conducted by ORNL to evaluate performance and safety metrics for two proposed fuel systems for HFIR: uranium-molybdenum monolithic alloy fuel (U-10Mo) and uranium-silicide dispersion fuel (U_3Si_2-Al). Although the other five USHPRRs are planning to be converted with the U-10Mo monolithic fuel system, due to the complex nature of the HFIR fuel system (e.g., radially contoured fuel zone), it was anticipated that the fuel manufacturing R&D process for HFIR U-10Mo monolithic fuel would be long and expensive and might not deliver a manufacturing process with adequate yields to maintain an economically viable fuel. Therefore, in 2017, the conversion program asked ORNL to evaluate U_3Si_2-Al dispersion fuel systems[6] because the fuel manufacturing R&D effort was believed to be shorter and less expensive, and the resulting manufacturing process was thought to be capable of higher yield/lower cost than U-10Mo monolithic fuel.

Advantages of the silicide dispersion fuel over monolithic are that it:

1. has been fabricated for several years by several vendors using a process that is similar to the one currently used to fabricate the complex fuel design of the HFIR HEU U_3O_8-Al dispersion fuel
2. was qualified and approved by the U.S. Nuclear Regulatory Commission for use in medium-power research reactors (NUREG-1313, 1988), and
3. offers better uranium utilization (i.e., less uranium required per day of operation).

However, fabrication of fuel plates with the complex HFIR design features has yet to be demonstrated and additional irradiation testing is required to qualify this fuel system for use in HFIR.

BWXT is currently developing U_3Si_2-Al fuel plates for the HFIR-FUTURE irradiation tests to be performed in the SCK-CEN BR2 reactor. Fabrication is expected to be completed in late 2020, with irradiation to follow shortly thereafter. Results from these tests

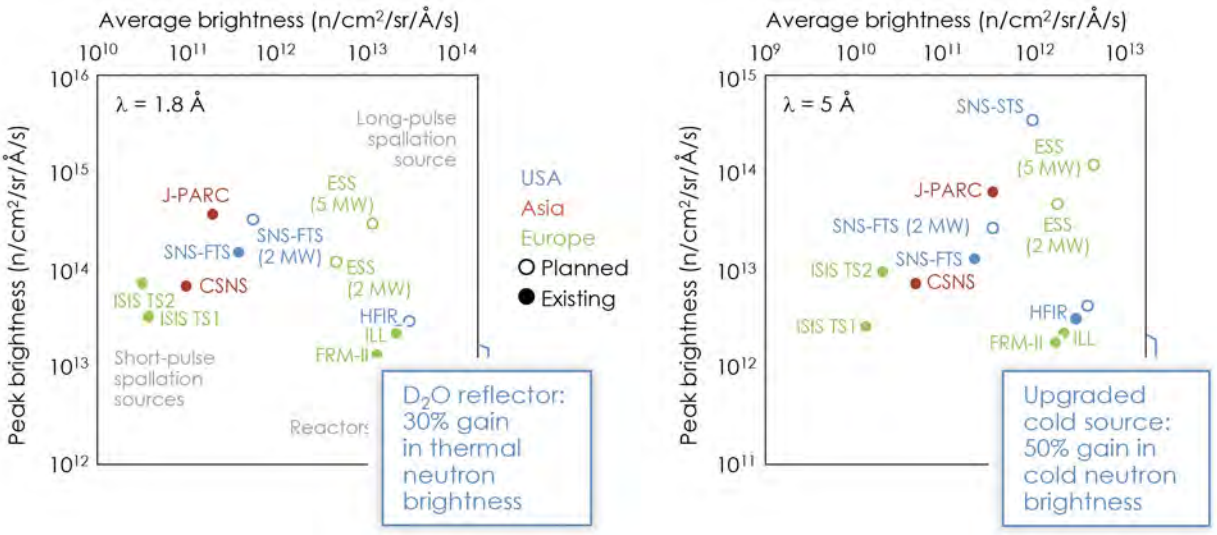

FIGURE A1.6. The Upgraded HFIR Will Provide World-leading Time-averaged Brightness for Both Cold and Thermal Neutrons

Source: Oak Ridge National Laboratory, U.S. Dept. of Energy

will help provide input to subsequent fabrication and irradiation phases, which will consist of fabrication down-selections, plate demonstrations, full-size HFIR plate irradiations, fuel assembly fabrication demonstrations, design demonstration element testing, LTC fabrication and testing, and HFIR conversion.

Seismic upgrades

Seismic upgrades for the reactor building could be accomplished at the same time as the vessel replacement. These upgrades are required to meet current seismic standards for the building—the reactor itself meets current seismic standards including reactor safety in the event of a building collapse. The upgrades primarily involve reinforcement of several columns and roof beams using technology that has been successfully demonstrated at other facilities.

Enhanced Mission Performance

The improvements and upgrades described above offer opportunities to substantially enhance the mission performance of HFIR. The new pressure vessel will support larger beam tubes and an improved cold source, strengthening and expanding neutron scattering capabilities. The redesigned pressure vessel head will enable improved access for isotope production and materials irradiation. The new pressure vessel will also allow a return to 100MWt operation, providing an immediate ~20% increase in neutron flux. The higher power level will also be essential for maintaining current performance levels with low enrichment fuel should a suitable fuel technology become available.

In Figure A1.6, the average neutron brightness and peak brightness are compared for leading steady-state and spallation neutron sources worldwide. The upgraded HFIR will have world-leading time-averaged brightness for both thermal and cold neutrons. The high average steady-state brightness complements the intense peak brightness available at pulsed spallation sources, with the steady-state sources providing distinctive advantages for neutron scattering studies at specific length and time scales. The very high cold and thermal neutron fluxes at the upgraded HFIR will extend experiments to new frontiers, particularly for weak scattering systems and samples available only in smaller sizes.

The second guide hall will provide an opportunity to increase the number of instruments from the current 12 to 20. All instruments will be state-of-the-art, and fed by world-leading cold and thermal neutron beams. Particular instrument choices and designs will be developed with broad community input. A new cold source will provide a ~50% boost to cold neutron brightness, and improved beam systems will increase available flux at cold and thermal instruments by factors of two or more. Low backgrounds in the guide halls will increase measurement sensitivity enabling faster data acquisition and detection of weaker signals. This will enable

new and better experiments to probe the structure and dynamics of materials that will drive future energy technologies, including energy storage materials, catalysts for production of fuels and chemicals, structural materials for transportation, next generation polymers, and quantum materials. Moreover, these instruments will provide the highest resolution for phase transitions at extreme conditions of magnetic field and temperature, quantum phenomena, residual stress mapping of engineered systems, and imaging of operating systems including batteries, fuel cells, and engines.

The increased neutron flux enabled by the new pressure vessel will provide a corresponding increase in isotope production and damage rates for materials irradiation experiments. In addition, the changes to the reactor vessel head will facilitate introduction and removal of capsules, including during reactor operations. This will allow increased isotope production, especially for short-lived isotopes, such as Pt195m, Lu-177, W-188/Re-188, and Sr-89 for medical applications, Se-75 for radiography, and Es-253 for heavy element chemistry. The improved access will also enable a significant increase in instrumented materials irradiation experiments to advance radiation effects research, including the development of accident-tolerant fuels and fusion reactor materials.

For over 50 years, HFIR has addressed important and often unique missions supporting the DOE Office of Science and the Nation. The proposed upgrades will significantly enhance the value of the reactor in carrying out these missions, and ensure its continued availability for the foreseeable future. Preliminary estimates indicate that the vessel replacement and improvements described above could be accomplished in a multi-year effort including a reactor outage of approximately two years. New scattering instruments would come online in stages following the outage. The upgraded HFIR will offer new and expanded state-of-the-art capabilities for cold and thermal neutron scattering, isotope production and research, and materials irradiation using the world's most intense steady-state neutron beams. Preliminary estimates indicate that the full HFIR upgrade project including pressure vessel, top and bottom head, reflector, cold source, redesigned nozzles and beam tubes, second guide hall, guides, instruments, building seismic upgrades, and various life extension projects would be in the general range of $500–800M, including contingency.

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APPENDIX 2. The Global Effort to Convert Research Reactors to Low Enriched Uranium Fuels

The U.S. technical effort to replace the use of High Enriched Uranium (HEU, U-235 enrichment ≥ 20%) fuel with Low Enriched Uranium (LEU, U-235 enrichment < 20%) fuel began in 1978 as the Reduced Enrichment for Research and Test Reactors (RERTR) program, immediately working as a global community of reactor operators, fabricators, and their governments. From the first RERTR International Meeting in 1978, the program has been focused upon preservation of reactor mission capability as a central tenet of the conversion program. Indeed, the reason the program continues forty years later is because the community continues to collaborate on projects to preserve mission capability, rather than forcing degradation of performance. The RERTR program management within the Department of Energy matured to the Global Threat Reduction Initiative (2004-2015) and now the National Nuclear Security Administration (NNSA) Office of Material Management and Minimization (M3, 2015-present).

As indicated in Figure A2.1, there has been a great deal of success converting reactors around the world. A total of 71 reactors converted from Highly Enriched Uranium (HEU) fuel to Low Enriched Uranium (LEU) fuel in the period 1978-2019, and an additional 31 reactors that used HEU fuel have been confirmed permanently shutdown. Table A2.1 lists the reactors with a peak thermal flux > E14 n/cm²/s that converted in the period 1978-2019. The list includes many high impact reactors that represent a wide variety of scientific and isotope production capabilities. Table A2.2 indicates the variety of research reactor fuels used in reactors that have converted or that are under development and qualification for conversion of the remaining reactors.

Overview of U.S. and European High Flux Reactor Conversion Efforts Since 2005

Though the global community has converted 24 reactors with high flux, unique challenges remain for a group of highly optimized HEU reactors in the U.S. and Europe. The U.S. High Performance Research Reactors (USHPRR) and European High Flux Reactors (EUHFR) are each quite distinct, but have less fuel assembly design and/or grid-plate flexibility than prior conversions; high power density in the fuel in order to provide the intense experimental fluxes; and high burnup in those reactors that reload fuel in order to minimize fuel costs. This Appendix describes many of the details of the efforts to convert the USHPRR and EUHFR reactors. The aspects of that effort that are most relevant to the capabilities of HFIR are described in the HEU-LEU Conversion section, whether

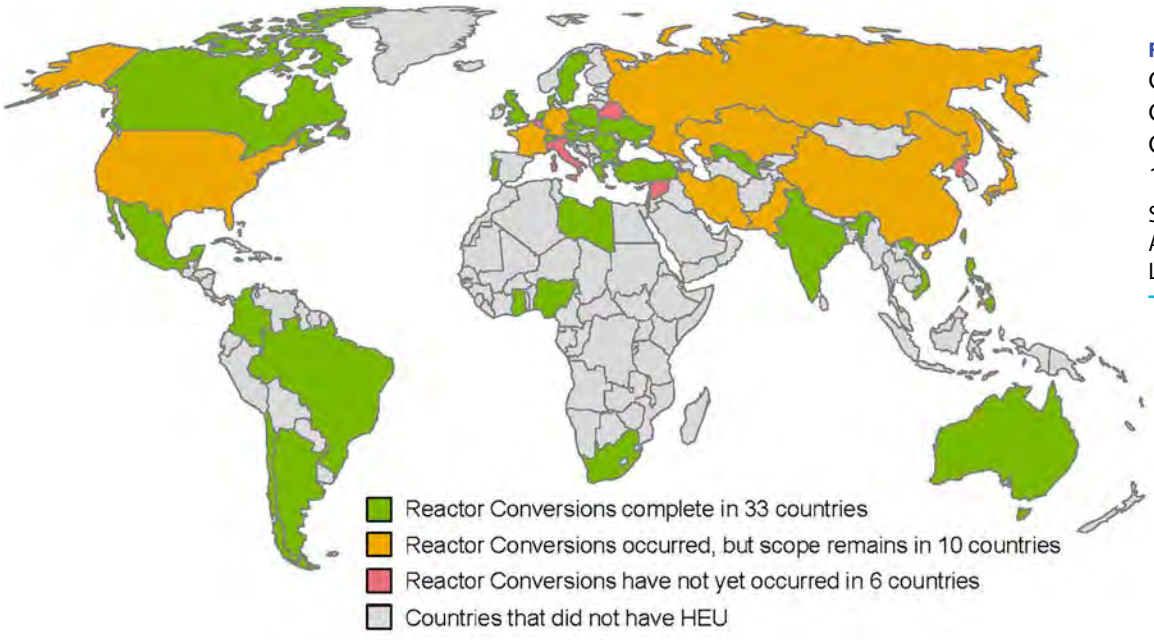

FIGURE A2.1
Geography of the Global Reactor Conversions, 1978–2019

Source: John Stevens, Argonne National Laboratory

TABLE A2.1. High Flux Reactors Converted to LEU 1979–2019 (i.e., peak thermal flux > E14 n/cm2/s)

COUNTRY	FACILITY NAME	TYPE	STATUS	CONVERTED	THERMAL POWER (MW)
Canada	NRU	HEAVY WATER	PERMANENT SHUTDOWN	1992	135
China	HFETR	TANK	OPERATIONAL	2007	125
France	OSIRIS	POOL	UNDER DECOMMISSIONING	1979	70
Sweden	R2	TANK	UNDER DECOMMISSIONING	1990	50
Japan	JMTR	TANK	PERMANENT SHUTDOWN	1993	50
Netherlands	HFR	TANK IN POOL	OPERATIONAL	1998	45
Poland	MARIA	POOL	OPERATIONAL	2012	30
South Africa	SAFARI-1	TANK IN POOL	OPERATIONAL	2008	20
Romania	TRIGA II PITESTI - SS	TRIGA	OPERATIONAL	1992	14
Czech Republic	LVR-15 REZ	TANK WWR	OPERATIONAL	2010	10
Germany	BER-II	POOL	PERMANENT SHUTDOWN	1997	10
Hungary	BUDAPEST RR	TANK WWR	OPERATIONAL	2009	10
Pakistan	PARR-1	POOL	OPERATIONAL	1991	10
Ukraine	WWR-M KIEV	TANK WWR	OPERATIONAL	2008	10
Libya	IRT-1	POOL, IRT	TEMPORARY SHUTDOWN	2006	10
Uzbekistan	WWR-SM TASHKENT	TANK WWR	OPERATIONAL	2008	10
Austria	ASTRA	POOL	DECOMMISSIONED	1983	10
Denmark	DR-3	HEAVY WATER	UNDER DECOMMISSIONING	1988	10
Switzerland	SAPHIR	POOL	DECOMMISSIONED	1990	10
Australia	HIFAR	HEAVY WATER	PERMANENT SHUTDOWN	2004	10
Germany	FRG-1	POOL	UNDER DECOMMISSIONING	1991	5
United States	GTRR (Georgia Tech)	TANK	DECOMMISSIONED	1997	5
Greece	GRR-1 (Demokritos)	POOL	EXTENDED SHUTDOWN	1999	5
Canada	MNR MCMASTER	POOL, MTR	OPERATIONAL	1999	3

Note that that the Conversion Program addresses actual performance metrics rather than simple flux values. The data presented in this table is from the IAEA database on 22 April 2020, https://nucleus.iaea.org/RRDB/RR/ReactorSearch.aspx

as a HFIR LEU conversion or a refurbished HFIR with LEU fuel.

In 2005, the NNSA Reactor Conversion Program formed the USHPRR sub-program to maximize synergy during conversion of the five U.S. reactors using HEU to meet their high flux, high national impact missions: The MITR at Massachusetts Institute of Technology in Cambridge, Massachusetts; the MURR at University of Missouri in Columbia, Missouri; the NBSR at the National Institute of Standards and Testing (NIST) in Maryland; the ATR at the Idaho National Laboratory (INL); and the HFIR at Oak Ridge National Laboratory (ORNL) in Tennessee. (The ATRC critical facility will also be converted to remain appropriate for the ATR reactor programs). The NNSA USHPRR sub-program has assembled expertise from nine national laboratories and sites (Argonne, Brookhaven, Idaho, Los Alamos, Oak Ridge, Pacific Northwest, Sandia, and Savannah River national laboratories and the Y-12 national security complex) as well as the reactor operating institutions, fuel fabricator BWXT, and the U.S. Nuclear Regulatory Commission (NRC).

In parallel to the USHPRR effort, the NNSA Reactor Conversion Program has been collaborating with the EUHFR and their fabricator CERCA as a group since 2008 to develop and qualify the high density LEU fuel that will allow conversion of the EUHFR reactors: the BR2 at SCK CEN in Mol, Belgium; the RHF at Institut Laue-Langevin (ILL) in Grenoble, France; and the JHR under construction at the French Alternative Energies and Atomic Energy Commission (CEA) in Cadarache, France. The U.S. technical effort to support the EUHFR conversion has always involved a team of Argonne and Idaho National Laboratories, under the International Reactor Conversion sub-program at NNSA. The Y-12 national security complex has been instrumental for fresh uranium supply and transport. Savannah River National Laboratory provides strategic assistance.

USHPRR Feasibility Studies conducted in 2005-2009 developed conceptual LEU designs for each of the reactors to preserve their mission capabilities with a revolutionary high-density LEU fuel, U-10Mo monolithic fuel. This monolithic fuel form is a foil of

TABLE A2.2. Uranium Density of Research Reactor Fuels Qualified and Under Qualification

	URANIUM LOADING DENSITY (GU/CM³)			
	1978[1]	NOW[2]	IN PROGRESS	
TRIGA UZrH Pins	0.5	2.1	—	30/20 qualified in NUREG-1282 (1987)[3]
UO_2 Pins	9.3	—	—	not fabricable for plate geometry
UAl_x-Al Dispersion	1.7	2.3	—	HEU fuel in use at MITR, MURR, ATR, BR2, RHF
U_3O_8-Al Dispersion	1.3	3.2	—	HEU fuel in use at NBSR and HFIR
U_3Si-Al Dispersion	—	6	—	only suitable for limited irradiation conditions
U_3Si_2-Al Dispersion	—	4.8	—	Qualified fuel in NUREG-1313 (1988), but at much lower power density than USHPRR and EUHFR[4]
	—	—	4.8–5.6	HERACLES/LEU FOREvER at EUHFR Conditions (experiment irradiated, awaiting PIE)[5]
	—	—	5.3	SCK COBRA EUHFR Conditions including Gd integral burnable absorber (irradiation in progress)[6]
	—	—	4.8	USHPRR HFIR-Relevant Conditions (experiment being fabricated)[12]
UO_2-Al Dispersion	—	2.5	—	WWR-M2 Qualified (2002)[7]
	—	2.8	—	VVR-KN Conversion (2013) Coextruded tubes[8]
	—	3.0	—	IRT-4M Qualified (2002) Coextruded tubes[9]
UMo-Al Dispersion	—	5.4	—	IRT-3M Qualified (2016) Coextruded tubes[10]
	—	—	8	KJRR LTA (2 LTAs irradiated, PIE in progress)[11]
	—	—	8	HERACLES/US[5,6] (EUHFR experiments irradiated, PIE in progress)
UMo Monolithic	—	—	15.3	USHPRR HIP Clad Process (in qualification phase of experiments)[12-15]
	—	—	15.3	HERACLES C2TWP Clad Process (in development, miniplates irradiated)[5,16]

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FIGURE A2.2. The Concepts of Dispersion and Monolithic Fuel Plates

Source: Kim, Y.S. and Hofman, G.L., Journal of Nuclear Materials, Volume 419, Issues 1–3, December 2011, Pages 291 -- 301.

uranium-molybdenum (UMo) alloy (U-10Mo indicates an alloy with 10% molybdenum by weight) coated by a zirconium diffusion barrier, then clad in aluminum alloy by hot isostatic pressing. The U-10Mo monolithic fuel offers exceptional uranium density of approximately 15.3 gU/cm^3 of foil. The U-10Mo fuel is often termed *revolutionary* since multiple fabrication techniques necessary for consistent production are new to commercial production of research and test reactor fuel.

EUHFR Feasibility Studies conducted in 2008-2010 developed conceptual designs for BR2 and RHF to preserve their mission capabilities with an evolutionary high-density LEU U-7Mo dispersion fuel, since the JHR being constructed in France was designed to deploy LEU U-7Mo Dispersion Fuel that was under development. The dispersion fuel form is a mixture of particles of uranium-molybdenum alloy (U-7Mo indicates an alloy with 7% molybdenum by weight) mixed with an aluminum powder matrix and compacted to form the "fuel meat". That fuel meat is then clad in aluminum alloy by a rolling process. The U-7Mo dispersion fuel offers high density of approximately 8 gU/cm^3 of fuel meat (where the uranium density can be adjusted by altering the volume ratio of fuel particles and the aluminum matrix). The 7% Mo level was chosen for the dispersion fuel in order to balance the fission gas retention benefit of Mo in the alloy against the reduction in uranium loading density as the Mo weight fraction is increased. The U-7Mo fuel is often termed *evolutionary* since most fabrication techniques necessary for consistent production are consistent with the existing qualified dispersion fuels (UAl_x, U_3O_8, and U_3Si_2).

Early testing of UMo fuel systems indicated creation of an amorphous intermetallic interaction layer between the UMo alloy and aluminum. That interaction layer allowed fission gas bubbles to grow and interconnect, leading to a problematic level of plate swelling, or failure by "pillowing" or "delamination" if the interconnected bubble region reached a scale at which material strength was compromised.

For dispersion fuel, the addition of silicon to the aluminum matrix was effective at controlling the interaction between UMo and the matrix for experiments irradiated at moderate power to full burnup. Tests of the U-7Mo with silicon in the matrix performed well for moderate-power experiments including miniplates in ATR, pin experiments at HANARO, full-size plate experiments in ATR, and the KJRR Lead Test Assembly elements at the ATR. However, the fuel irradiation efforts of the EUHFR collaboration between 2008 and 2013 (during which the international team was named LEONIDAS) exposed continuing irradiation performance problems with the Uranium-Molybdenum (U-7Mo) dispersion fuel product subject to the combination of high power density and high burnup required for the EUHFR application. Two irradiation tests during that time frame (E-FUTURE and E-FUTURE-II) that used silicon in the fuel matrix to mitigate the interaction between the U-7Mo alloy and the aluminum matrix failed to meet the burnup required for EUHFR application.

For monolithic fuel, a zirconium layer between the UMo foil and the aluminum alloy clad proved highly effective at avoiding the interaction layer. Between 2007 and 2011, the USHPRR program conducted seven irradiation campaigns consisting of 14 large size plates and over 60 mini plates with U-10Mo fuel with a zirconium interlayer. Those tests included power densities and burnups to envelop the NRC-regulated USHPRR (MITR, MURR, and NBSR) and significant portions of the ATR and HFIR envelopes. Unfortunately, in the same time period, the USHPRR Fuel Fabrication effort had experienced significant challenges with fabrication scale-up of the novel U-10Mo monolith fuel form for full-size plate experiments and increased rates, with very low yields that caused many long delays and did not seem to be converging toward a sustainable cost.

Thus, in 2012-2013, NNSA Reactor Conversion fuel development and qualification efforts were significantly restructured for both the USHPRR and

EUHFR. The European collaborators also restructured their approach, evolving LEONIDAS into the HERACLES Consortium by the addition of the FRM-II reactor of Technical University of Munich (TUM) in Garching, Germany, and engagement with EURATOM Framework funding mechanisms.

The USHPRR and EUHFR teams learned from each other regarding the 2008-2013 challenges encountered. The EUHFR team adopted the diffusion barrier and heat treatment approaches that had proven vital for excellent irradiation performance of the U-10Mo monolithic fuel. The USHPRR team adopted inclusion of a commercial fuel fabricator and pilot-line-production that had proven predictable and effective for EUHFR experiment fabrication. Both teams slowed the pace of irradiation experiments to assure that maximum data value would be generated by each experiment, in terms of both fabrication data and irradiation performance data. In addition, both teams have had independent expert reviews to assure appropriate creativity, transparency, and rigor.

The independent expert review of the EUHFR plan in 2015 suggested that the EUHFR pursue U_3Si_2 dispersion fuel as a backup to their work on U-7Mo dispersion. Though the uranium density of U_3Si_2 is considerably lower than U-7Mo, three attributes were of interest to the EUHFR as a backup. First, U_3Si_2 dispersion was qualified for modest power densities in 1988 and has since been used to convert many research reactors and has been deployed in several new reactors, including a number with peak fluxes above E14 n/cm^2/s (such as HFR Petten, SAFARI, MARIA, and OPAL). The JHR in France will begin operations with U_3Si_2, and the CEA completed the high-power-density EVITA experiments at the BR2 reactor in Belgium to support fuel qualification for the JHR. (Unfortunately, EVITA results are not available outside of the JHR project since the fuel qualification case is still being reviewed by the French regulator.) Second, the fabrication of U_3Si_2 is well established and will be simpler than the U-7Mo dispersion fabrication. Thus, fuel cost per element should be lower, even if more elements are needed each year due to lower density. Third, Orano has recently deployed a backend solution for U_3Si_2 fuel, while the backend for U-7Mo dispersion fuel would require development and deployment.

SCK CEN reconsidered their BR2 fuel element plate thickness and radius constraints, and determined that a modified geometry would allow preservation of mission capabilities with an LEU 5.3 g/cm^3 U_3Si_2 dispersion fuel incorporating gadolinium as an integral burnable absorber.

Since the promising results for LEU U_3Si_2 application to a redesigned BR2 fuel element, the conversion design teams for HFIR and the RHF reactor at ILL in France have both reconsidered geometric constraints and have developed design candidates for variants of U_3Si_2 details that would preserve mission capability.

In the case of HFIR, U_3Si_2 is not the backup solution, but was established as the baseline solution in 2019.

Notable USHPRR and EUHFR deliverables since the 2016 NAS study was published include:

U-10Mo Monolithic Fuel

- U-10Mo Monolithic Fuel Fabrication Pilot Line was deployed and commissioned at commercial fabricator BWXT in Lynchburg, Virginia.
- The BWXT Pilot Line was used to make the USHPRR monolithic fuel miniplates for the MP-1 qualification experiment from full-size foils. After completing two irradiation cycles, the irradiation of MP-1 fuel was stopped during the third cycle. A small number of miniplates for MP-1 that were made utilizing laboratory-scale equipment experienced performance issues, while all of the BWXT-made miniplates performed as expected.
- Preliminary safety analyses for all three NRC-regulated USHPRRs (MITR, MURR, NBSR) have been performed that establish a safety case for each LEU design and operating plan that preserves the mission capabilities of the reactors. The USHPRR sub-program is working with the NRC to receive feedback on these analyses. (The preliminary designation acknowledges that the U-10Mo monolithic fuel qualification is still in progress, and the fabrication tolerances of the final fuel products are subject to change.)
- A Preliminary Report on U-Mo Monolithic Fuel for Research Reactors submitted to the NRC for review. The report provides a comprehensive account of the research and development (R&D) performed by the USHPRR sub-program and signifies the shift from

R&D to the implementation phase of U-10Mo fuel. The report summarizes characterization and irradiation performance data that was obtained from early scoping and development irradiation campaigns and demonstrates that the U-10Mo monolithic fuel system is suitable for fuel qualification.

- The ATR conversion team has completed a conceptual fuel design and is preparing a Safety Analysis Report addendum to test first LEU element.
- Within the HERACLES Consortium TUM, CEA, and CERCA are pursuing a European variant of the U-10Mo monolithic fuel. Their "C2TWP" approach applies the zirconium diffusion barrier by Physical Vapor Deposition and then rolls the coated foil and clad to bond them. The first mini-plate samples of C2TWP product were irradiated in the EMPIrE experiment at ATR.

U-7Mo Dispersion Fuel

- EMPIrE Fabrication and Irradiation Condition Parametric Miniplate Experiment fabricated at CERCA and irradiated at the ATR at conditions that included the envelope of BR2 and RHF. EMPIrE irradiated 48 miniplates to explore the impacts of variations in both fabrication and irradiation conditions. Non-destructive PIE indicates good performance for nearly all variants examined, with no failures. Destructive PIE is in progress. CERCA is installing pilot devices capable of fabrication variants in order to respond efficiently if EMPIrE destructive PIE shows an advantage of one variant over the other.
- SEMPER FIDELIS Full-Size Plate Experiment fabricated at CERCA and irradiated at the BR2. The experiment did suffer from a faulty irradiation device design that led to damage of a number of the plates before they reached their target burnups. However, one plate was irradiated successfully to more than 80% local burnup at power levels that envelope BR2 and RHF. The plates that were damaged are still yielding significant data about how fuel performance evolves at different power densities to different burnups. Initial destructive examination is favorable for the plate that reached 80% burnup. The PIE continues for the overall experiment.
- The HERACLES Consortium has been developing scaled-up fabrication capability at CERCA in parallel with the Comprehension Phase SEMPER FIDELIS and EMPIrE experiments. Pilot devices for UMo powder atomization, heat treatment, and coating are being deployed in the CERCA R&D Facility at their Romans site. The fuel meat compaction, rolling to apply clad, and fuel element assembly all use standard equipment of the CERCA fabrication facility.

U_3Si_2 Dispersion Fuel for High Power/High Burnup Applications

- BR2 has qualified and deployed a modified element design (named COBRA) with HEU fuel fabricated by BWXT. The modified geometry will allow preservation of mission capabilities with an LEU 5.3 g/cm3 U_3Si_2 dispersion fuel with gadolinium as an integral burnable absorber.
- The COBRA-FUTURE Full-Size Plate experiment at BR2 to test the proposed LEU fuel meat at BR2 irradiation conditions has been fabricated at BWXT and irradiation is in progress. Three nominal cycles were completed by May 2020. A final bounding irradiation cycle will begin in August 2020.
- The HiPROSIT Full Size Plate experiment at BR2 to test U_3Si_2 fabricated by CERCA at EUHFR irradiation conditions with loadings of 4.8 gU/cm^3, 5.3 gU/cm^3, and 5.6 gU/cm^3 was fabricated and irradiated. The plates should have achieved local burnups greater than 80%. PIE will commence in 2020 after cooling.
- Initial HFIR silicide design options have been completed that preserve full mission capability.
- LEU fabrication demonstrations for HFIR U_3Si_2 design options are underway at BWXT.
- The FUTURE HFIR experiment at BR2 to test U_3Si_2 with fuel meat characteristics and irradiation conditions relevant to HFIR is has been designed and is being fabricated.

LEU Fuel Cost Projections

- Fabrication yields have been dramatically improved since the 2015 NAS review.
- USHPRR cost projection modeling has been improved based on a Process Flow Diagram that details each fabrication step at BWXT.
- As of January 2020, LEU U-10Mo monolithic fuel is projected to cost more than the current HEU fuel, but the increase should be less than 40%.
- The initial cost projection for HFIR LEU U_3Si_2 dispersion fuel is that the fuel costs will be similar to current HEU costs since U_3O_8 powder production will no longer be needed.

Remaining Work Needed to Support LEU Fuel Qualification

A number of irradiation tests are still required to qualify the high-density U-10Mo monolithic and U-7Mo dispersion for application in research and test reactors, and U_3Si_2 dispersion fuels for application to reactors with high power density. Furthermore, reactor-specific irradiations are required for each of the USHPRR and EUHFR reactors due to the scale and distinct complexity of each of those reactors.

The USHPRR program U-10Mo monolithic fuel is in the qualification phase rather than fuel development phase. The program is no longer investigating process changes to baseline production of the U-10Mo monolithic fuel. It will be Vacuum Induction Melt (VIM) Cast, Hot Rolled to bond the zirconium diffusion barrier to the U-10Mo, Cold Rolled to desired foil thickness, then Hot Isostatic Pressed (HIPed) to bond the aluminum clad. Two miniplate tests will provide samples with a variety of variations and irradiation conditions in order to allow PIE data showing that the fuel behavior as fabricated by BWXT is predictable and stable. The MP-1 test began irradiation in 2018 and has been completed. The MP-2 test will follow MP-1. The FSP-1 full-size plate experiment will also follow MP-1, in order to demonstrate consistent performance of miniplates and full-size plates as fabricated by BWXT. A series of reactor-specific tests will follow FSP-1 to demonstrate the acceptability of the specific geometry in the LEU-design irradiation conditions.

The HFIR U_3Si_2 dispersion fuel qualification plan will move through a series of tests at BR2 and ATR to address the distinct fuel configuration and irradiation conditions of the inner and outer cores of HFIR fuel. The HFIR qualification may be adapted depending on the path forward selected by BR2 and RHF, to the degree that U_3Si_2 experimental synergies might accelerate the three conversions.

Within the EUHFR collaboration, BR2 and RHF plan to downselect either U-7Mo dispersion or U_3Si_2 during 2021 based upon completion of the HERACLES Consortium U-7Mo Comprehension Phase and the PIE results of the EMPIrE, SEMPER FIDELIS, HiPROSIT, and COBRA-FUTURE experiments. After the downselection, there will be at least one full-size plate experiment and one full-size, curved and constrained plate experiment pursued by the consortium in parallel with CERCA fabrication industrialization. The BR2 will irradiate Lead Test Assemblies (LTAs) with the downselected fuel fabricated by the industrialized processes. RHF will then irradiate a Lead Test Core.

TUM plans to pursue the European U-10Mo monolithic approach in a manner analogous to the HFIR experimental plan since it is an involute-plate reactor like HFIR.

In the case of each of the fuels, modeling will continue to evolve as new PIE data becomes available in order to document and demonstrate a thorough understanding of the fuel behavior to the regulators.

The LEU fuel development for conversions will undoubtedly be useful for new research reactor builds. Prior U_3Si_2 qualification facilitated deployment of the ETRR-2 reactor in Egypt and the OPAL reactor in Australia by Argentina's INVAP and National Atomic Energy Commission (CNEA). Argentina, Brazil, and the Netherlands are all currently pursuing INVAP U_3Si_2 reactors (RA-10, RMB, and PALLAS reactors, respectively). KAERI of Korea deployed the JRTR in Jordan with CERCA U_3Si_2 fuel, and is constructing the KJRR reactor in Korea to use U-7Mo dispersion fuel. Indeed, KJRR is expected to be the first research and test reactor to qualify UMo fuel since their recent Lead Test Assembly irradiations at the ATR were successful.

Acronyms

APS: American Physical Society

ATR: Advanced Test Reactor at the Idaho National Laboratory

ATRC: Advanced Test Reactor Critical facility at the Idaho National Laboratory

BR2: Belgium Reactor 2 at SCK CEN in Mol, Belgium

BWXT: BWX Technologies, the research reactor fuel manufacturer in the U.S.

C2TWP: CEA CERCA TUM Welding Process (a process to bond layers of nuclear fuel and clad)

CEA: French Alternative Energies and Atomic Energy Commission (operators of JHR)

CERCA: Research reactor fuel manufacturing unit with Framatome of France

EMPIrE: A U.S./HERACLES joint mini-plate irradiation experiment

EUHFR: European High Flux Reactors (BR2, FRM-II, JHR, RHF)

FRM-II: Research Neutron Source Heinz Maier-Leibnitz (FRM-II) at Technical University of Munich in Garching, Germany

GTRI: Global Threat Reduction Initiative within NNSA, the U.S. conversion program 2004-2015

HALEU: High Assay Low Enriched Uranium (i.e., uranium with between 5% and 20% U-235)

HERACLES: Consortium of Europe's High Performance Research Reactors to support the worldwide non-proliferation efforts by minimizing their usage of HEU material HEU: High Enriched Uranium (i.e., 20% or more of uranium is U-235)

HFIR: High Flux Isotope Reactor at the Oak Ridge National Laboratory in Tennessee

HIP: Hot Isostatic Pressing (a process to bond layers of material, such as nuclear fuel and clad)

ILL: Institut Laue-Langevin (operators of RHF)

INVAP: Argentine research reactor vendor

JHR: Jules Horowitz Reactor under construction at the CEA's Cadarache research center in France

KAERI: Korea Atomic Energy research Institute

KJRR: Kijang Research Reactor under construction by KAERI

LEU: Low Enriched Uranium (i.e., less than 20% of uranium is U-235)

M3: Material Management and Minimization within NNSA, the U.S. conversion program 2015–present

MITR: Massachusetts Institute of Technology Reactor in Cambridge, Massachusetts

MURR: Missouri University Research Reactor in Columbia, Missouri

NAS: National Academies of Sciences, Engineering and Medicine

NBSR: National Bureau of Standards Reactor in Gaithersburg, Maryland

NNSA: National Nuclear Security Administration

RERTR: Reduced Enrichment for Research and Test Reactors, the U.S. conversion program 1978–2004

RHF: Reactor a' Haut Flux at the Institut Laue-Langevin in Grenoble, France

SCK CEN: Belgian research foundation (operators of BR2)

SEMPER FIDELIS: A HERACLES/U.S. joint full-size plate irradiation experiment

TRIGA: Training, Research, Isotopes, General Atomics, a UZrH pin-type fuel deployed by General Atomics

TUM: Technical University of Munich (operators of FRM-II)

U_3Si_2: Uranium Silicide alloy

UMo, U-7Mo, U-10Mo: Uranium Molybdenum alloy, where U-xMo notation indicates the weight percentage that is molybdenum

USHPRR: United States High Performance Research Reactors (ATR/ATRC, HFIR, MITR, MURR, and NBSR)

APPENDIX 3. HFIR, SNS, and NIST User Data

FIGURE A3.1. HFIR Facility GU Days Requested and Days Delivered

Source: Oak Ridge National Laboratory
Note: Number of GU days requested in GU Proposal Calls and number of actual GU days run in that calendar year.

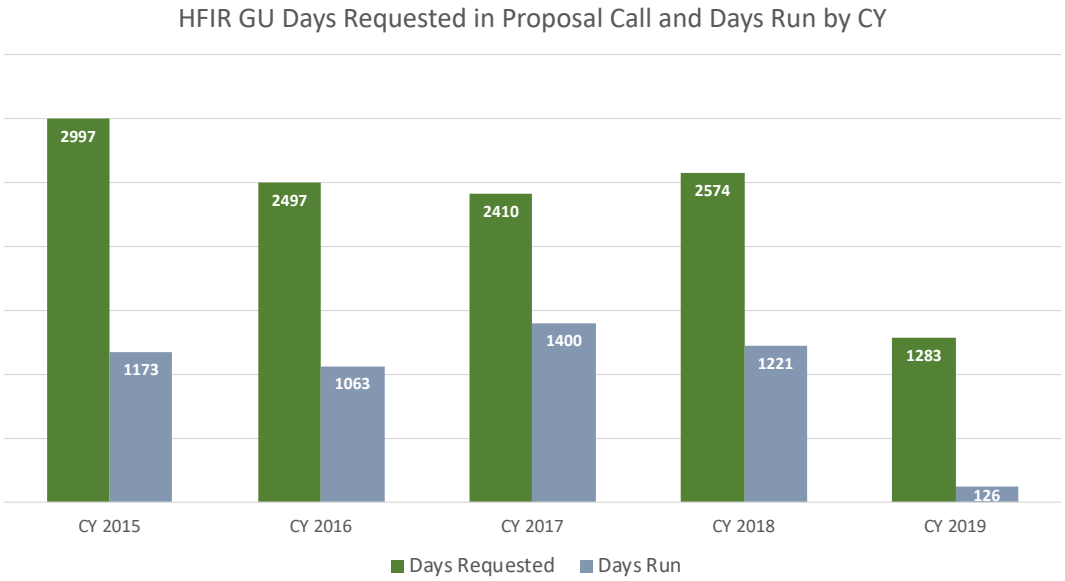

FIGURE A3.2. NIST Beamtime Between January 2015–January 2020

Source: National Institute of Standards and Technology
Note: Oversubscription values (defined as total days requested/total days offered) shows above, Days Requested

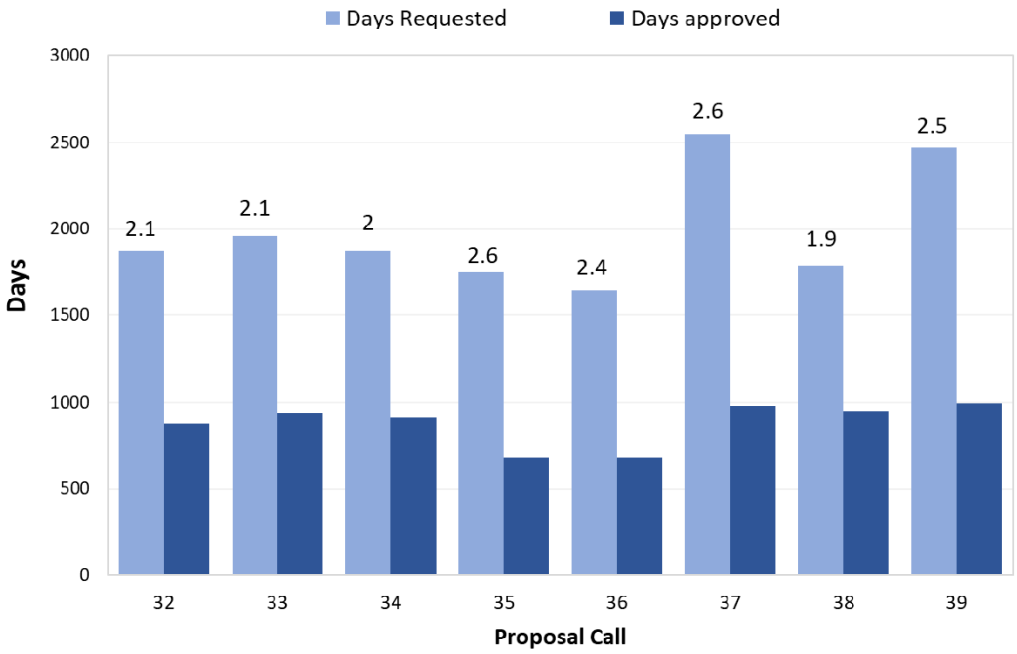

FIGURE A3.3. 32% of HFIR Proposals Rated ≥3 Are Not Awarded Beamtime

Source: Oak Ridge National Laboratory
Note: Proposals are rated by an external Science Review Committee using a rating system of 1 to 5, lowest to highest. Data includes most recent 6 HFIR proposal calls.

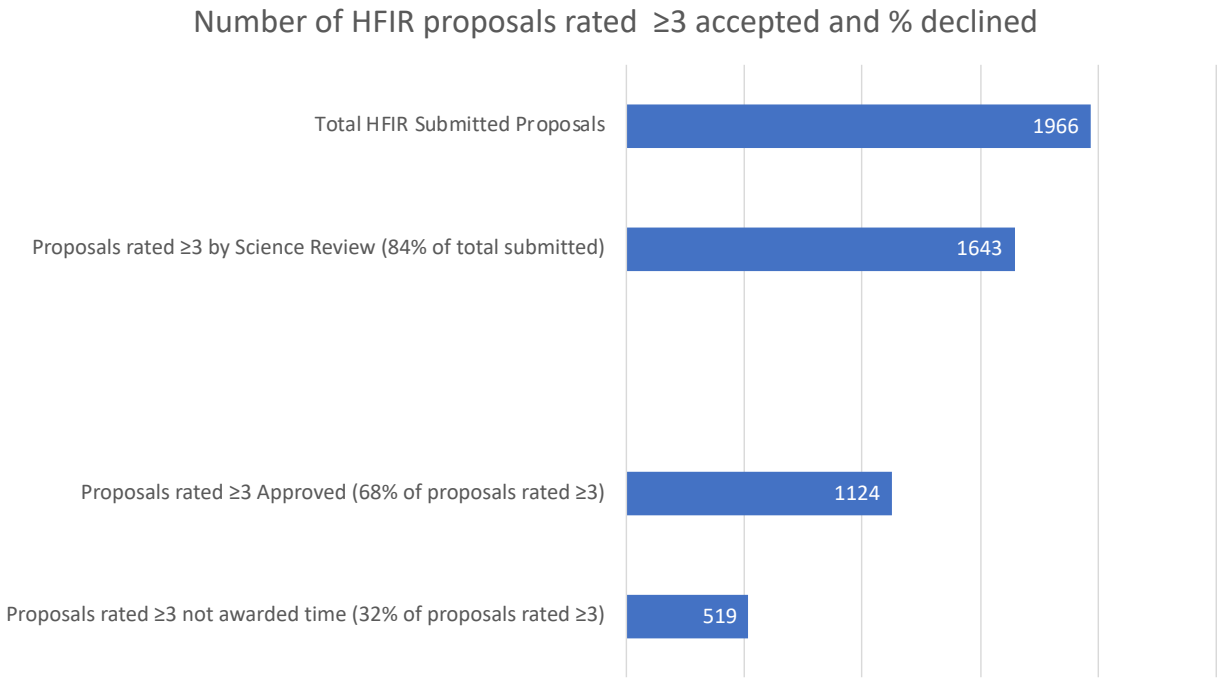

FIGURE A3.4. Oversubscription Rate Over Time

Source: Oak Ridge National Laboratory
Note: Subscription Rate = number of days requested divided by the number of days available in the General User Program.

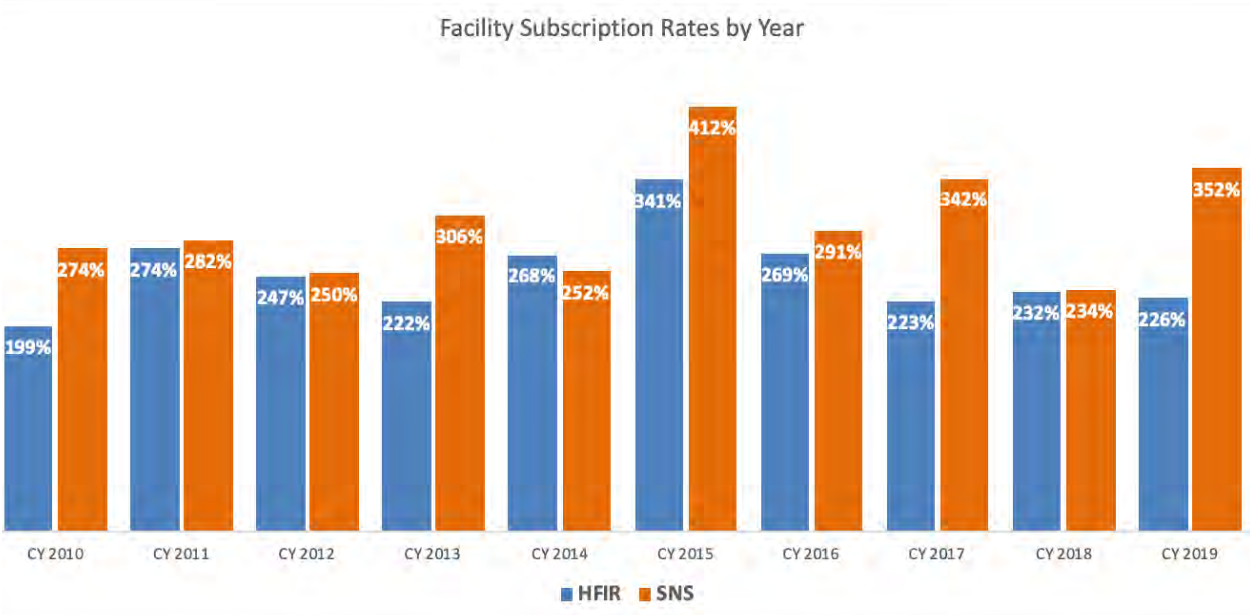

FIGURE A3.5. Number of SNS and HFIR Users by Fiscal Year

Source: Oak Ridge National Laboratory
Note: In FY2019, the User Program at HFIR was not operating.

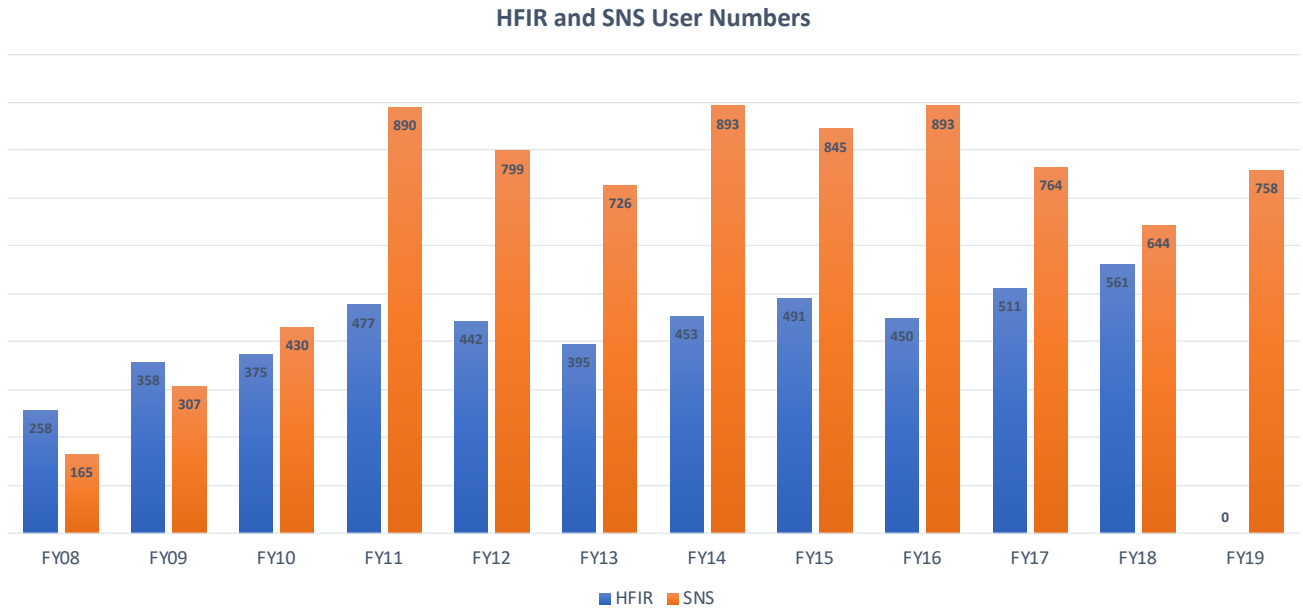

FIGURE A3.6. HFIR Subscription Rate by Field Over Recent 5-Year Period

Source: Oak Ridge National Laboratory
Note: Subscription rate by field: Researchers are asked to indicate one or more research areas when they submit a proposal, which we combined into these larger fields. The "subscription rate by field" shown in this chart is calculated as the number of received proposals that indicate a research field, divided by the number of proposals allocated that indicate the same field.

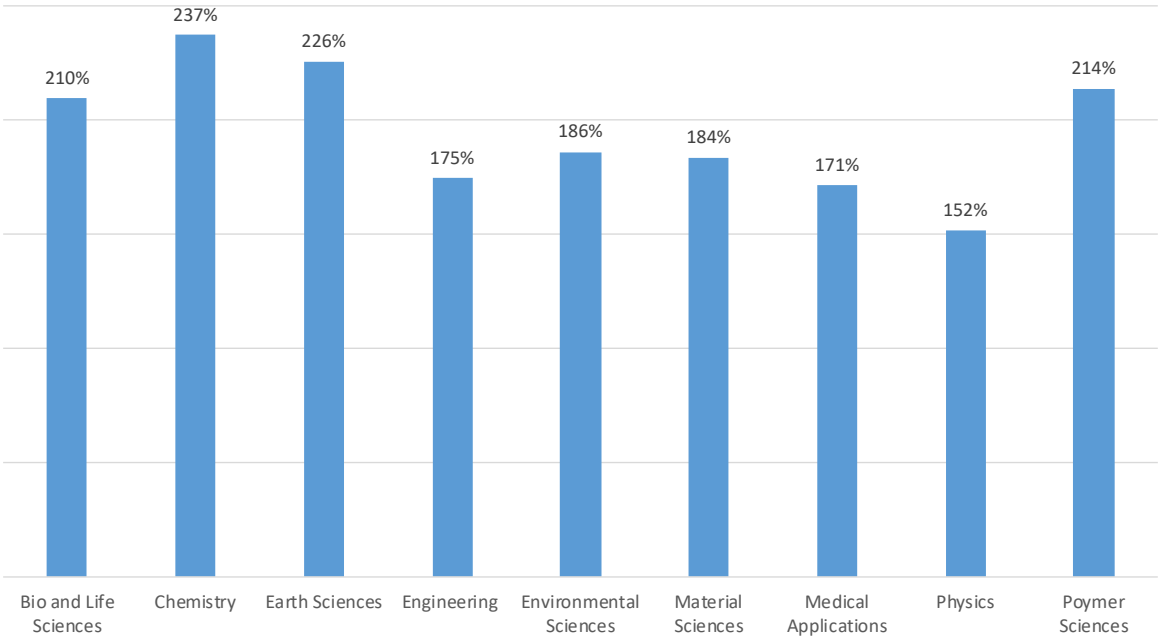

FIGURE A3.7. HFIR Instrument General User Proposal Metrics
Source: Oak Ridge National Laboratory

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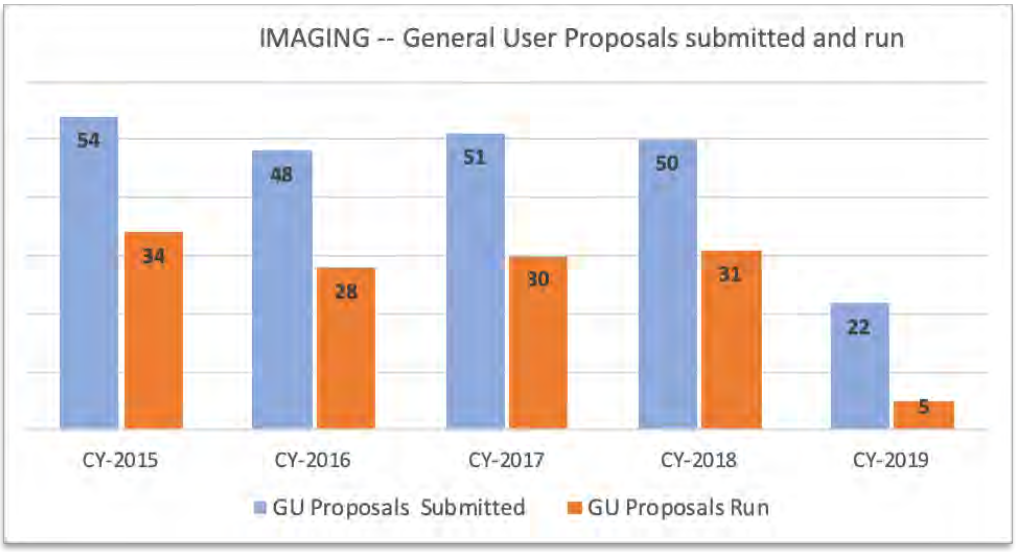

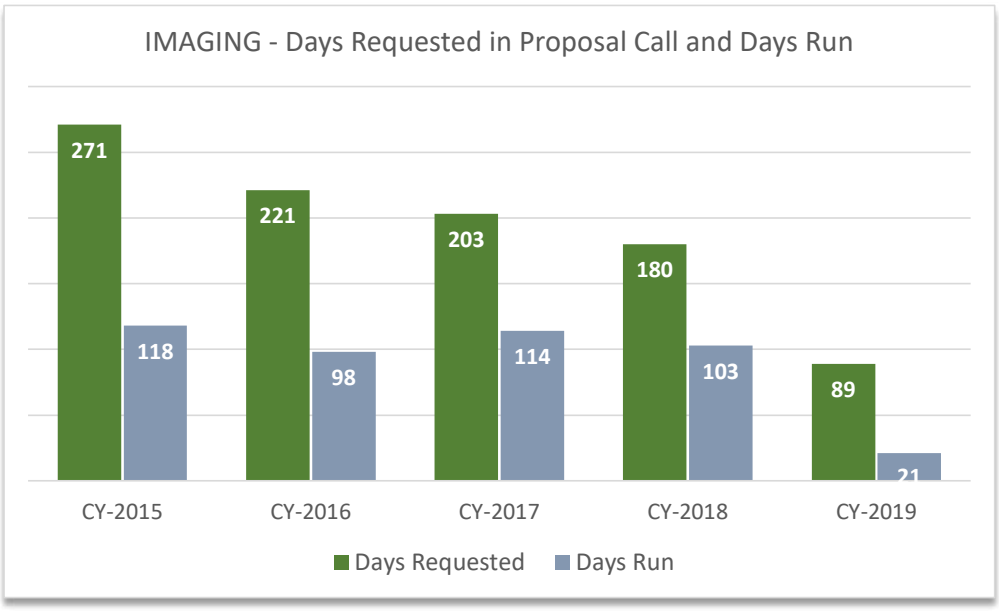


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