Description of STS core capabilities (adapted from First Experiments Spallation Neutron Source Second Target Station)

1. INTRODUCTION

Neutron scattering and spectroscopy were initially developed in the 1940s and 1950s, and the 1994 Nobel Prize in Physics was awarded to Clifford G. Shull and Bertram N. Brockhouse for their pioneering efforts [Levi, 1994]. Over the past seven decades, neutron scattering has become a vital tool for studying materials across many scientific fields and applications, including automotive engines, batteries, data storage, geology, polymers, and biomedicine. The exceptional properties of neutrons provide unique insight into the structure and function of materials, as summarized below.

- *Materials structure and dynamics:* Neutrons have a broad range of useful wavelengths, allowing the examination of structures from the atomic level to the size of biological cells. (The achievable wavelength range is dependent on the design of the neutron source and neutron scattering instrument.) Neutron energies span a range that is ideal for studying the individual and collective atomic motions that determine the properties of materials. Differences in neutron energy can be measured to allow the dynamics of atomic and molecular processes to be followed on time scales ranging from fractions of a picosecond to microseconds—corresponding to vibrations in rigid lattices to the slow movements of large macromolecules.
- *Elemental and isotopic sensitivity:* Neutrons are scattered via interactions with atomic nuclei, which makes them sensitive to the identity of both the element and the specific isotope being studied. Hence, unlike other techniques that scatter from the electric charge density in atoms, neutron scattering can readily distinguish between some elements with similar atomic numbers and is sensitive to light elements such as hydrogen, even in the presence of heavy elements. Further, the neutron scattering response of some isotopes can vary, making differentiation of isotopes very distinct. This unique property of neutrons makes it possible to use isotopic substitution—for example, replacing hydrogen with deuterium—to study the role of hydrogen in catalytic processes or the association of water in protein complexes.
- *Magnetism:* Neutrons have a magnetic moment, but no charge. Thus, neutrons provide an exquisitely sensitive probe for the study of magnetic properties and dynamics in materials. This feature has been exceptionally valuable for the study of materials ranging from superconductors and quantum materials to computer storage media.
- *Penetrating power:* Neutrons readily pass through most materials, which makes it possible to study bulk materials and buried interfaces. Further, samples can be studied under realistic conditions, such as in situ and operando studies of catalytic processes in reactors, studies of geological processes under extremes of pressure and temperature, and observations of fuel injector performance in an operating automobile engine.

Today, more than a dozen major neutron scattering facilities exist worldwide, including both reactor-based and accelerator-based neutron sources [*Neutrons for the Nation,* 2018]. The STS will provide new capabilities that ensure US leadership in neutron scattering. In the United States, the Office of Science of the US Department of Energy (DOE) currently supports two major neutron scattering user facilities at Oak Ridge National Laboratory (ORNL): the High Flux Isotope Reactor (HFIR) and the Spallation Neutron Source (SNS) and the US Department of Commerce supports the National Institute of Standards and Technology (NIST) Center for Neutron Research (NCNR). Each year, more than a thousand researchers from nations around the globe use the two DOE neutron sources that are made available by the Office of Science user program ["Number of Users," 2019]. A brief summary of the characteristics of HFIR and SNS and how they compare to other leading neutron sources is presented here.

Operating at 85 MW, HFIR 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. Its thermal neutron flux is similar to that of the high-flux reactor of the Institut Laue-Langevin (ILL), the premier European reactor-based neutron source, and neutron scattering instruments at HFIR and ILL address similar scientific questions.

The First Target Station (FTS) at SNS is presently the most powerful accelerator-driven neutron source in the world, operating at a power of 1.4 MW. It provides beams of neutrons in short pulses at a repetition rate of 60 Hz with the highest peak brightness in the world. When the 25 Hz pulsed neutron source at the Japan Proton Accelerator Research Complex (J-PARC) reaches its full power capability in in the near future, it will exceed the peak brightness of SNS. In addition, the European Spallation Source (ESS), now under construction in Sweden, will provide similar peak brightness once it begins operating at 2 MW in the mid-2020s, with a future upgrade path to 5 MW. ESS will deliver beams of neutrons in long pulses at 14 Hz, which will provide time-averaged fluxes of both cold and thermal neutrons comparable to those of a reactor-based source. The lower repetition rates of ESS and J-PARC compared to the FTS will allow the use of broader ranges of neutron energies in each pulse. Long-pulse spallation sources, such as the ESS, are highly flexible, and individual instruments can be optimized for experiments that require high peak brightness and a broad range of energies or for high time-averaged flux, essentially bridging between short pulsed sources and continuous neutron sources.

HFIR and the FTS at SNS provide optimized beam characteristics that are used for specific studies of materials. Briefly, HFIR produces continuous beams of either cold or thermal neutrons that are typically monochromatic and are optimized for studies of materials over selectable but narrow ranges of length scale or energy. The FTS produces pulsed beams of neutrons with very short pulses and therefore high energy resolution. Its high (60 Hz) repetition rate allows for a medium bandwidth of neutron energies to be used, because neutrons of different energies are separated by their arrival time at the detector; a longer time between pulses therefore results in a broader energy bandwidth. The FTS is best optimized for thermal neutrons that are ideal for spatial resolutions on the atomic scale and fast dynamics studies of materials.

SNS is currently undergoing a proton power upgrade (PPU) to double its power capability to 2.8 MW. This upgrade, which will be completed in 2024, will deliver 2 MW of proton beam to the FTS, resulting in a significant increase in thermal neutron brightness to enable new capabilities for materials research in the thermal energy (shorter wavelength) range. The PPU will keep the FTS competitive with J-PARC and ESS for experiments that require beams of thermal neutrons with high peak brightness and high energy resolution and will ensure that researchers in the United States continue to have access to world-leading neutron scattering capabilities.

Even with these existing sources, there is a global need for a high-intensity cold neutron source that is able to simultaneously use a broad energy/wavelength range. Such a source would provide the research community with exciting new opportunities to explore a wide range of materials, including in situ and operando studies during synthesis and processing, nonequilibrium phenomena, and dynamics. This need will be partially addressed by ESS in Europe and J-PARC in Japan, as discussed above. The proposed Second Target Station (STS) at SNS will provide the US with a world-leading capability in high-brightness cold neutron beams with broad energy/wavelength ranges. The STS will complement existing US sources to ensure future state-of-the-art capabilities for the US research community.

SNS, which began operating in 2006, was designed with an accelerator capable of generating neutrons not only for the existing FTS, but also for a future second target station. The ongoing PPU project at SNS, described above, is designed to provide 0.7 MW of proton beam to power the STS (in addition to delivering 2 MW to the FTS). Construction of the STS will provide transformative capabilities that allow thousands of users to address grand scientific challenges [Hemminger, 2015], advance energy research [BES Workshop Reports, 2019], and accelerate industrial innovations through the combination of:

- Cold (long-wavelength) neutrons of unprecedented peak brightness (1.5×10^{15} n/s/cm^2/Å/ster at $\lambda = 3$ Å)
- Short pulses containing neutrons with broad ranges of usable wavelength or energy ($\Delta\lambda = 13.2$ Å at 15 Hz at a distance of 20 m from the source)

This unique combination of neutron beam characteristics will open new avenues for examining materials and systems over greatly increased length, energy, and time scales. These characteristics—in combination with a proposed suite of new instruments (capacity of 22 instruments) and sample environments, advances in neutron optics and detectors, and new computational methods—will make it possible to conduct a wide range of experiments that are not now possible anywhere in the world. Specifically, the STS will provide unique capabilities for experiments that require:

- Time-resolved or cinematic (i.e., "movies") measurements of kinetic processes and beyond-equilibrium matter
- Simultaneous measurements of hierarchical architectures across unprecedented length scales, from the atomic scale to the micron and beyond
- Smaller sample and beam sizes needed for characterization of new materials
- Special environments for exploring new frontiers in materials at extreme conditions

The revolutionary increase in cold neutron peak brightness at the STS is made possible by combining recent innovations in neutron production technologies that allow (1) neutron production in a more compact volume by focusing the incident proton beam on a smaller area of the target; (2) using a solid, rotating tungsten target that can accommodate higher proton flux; (3) locating the cold moderators that are used to tune neutron energy as close as possible to the compact neutron production zone; and (4) a compact cold moderator geometry that can increase neutron brightness. These advances, together with proton pulse compression in the existing SNS accumulator ring, will produce sharp, cold neutron pulses with unprecedented peak brightness, as described in Sect. 2.

The experiments outlined in this report serve as examples of how the STS will provide wholly new capabilities that both complement and substantially extend this nation's current resources for neutron scattering. The STS has a pivotal role to play in extending the reach of neutron scattering to new and transformative opportunities for discovery science. These opportunities include studying the structure, dynamics, properties, and reactions of complex materials that have heterogeneity, interfaces, and disorder and conducting temporally resolved, in situ and operando studies of materials and chemical processes. In addition, they include studies of materials systems across larger length scales—from the atomic scale to the micron scale and beyond—revealing how materials self-assemble into hierarchical structures or molecules interact in living biological cells.

As highlighted in the report *Neutrons for the Nation* [2018], the United States is in need of additional neutron scattering facilities, especially at long wavelengths. The STS addresses the research community's need for bright beams of cold neutrons and provides US users with three DOE-sponsored facilities that offer distinctly different capabilities—the STS, the FTS, and HFIR—in addition to other facilities, such as the NCNR. The STS will furnish wholly new experimental capabilities needed to address future critical questions across a wide range of scientific areas and to drive the development of the technologies of tomorrow.

References for Sect. 1

BES Workshop Reports, 2019. Series of reports available at https://science.osti.gov/bes/Community-Resources/Reports (accessed May 30, 2019).

Hemminger, J. C. (chair). *Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science: A Report from the Basic Energy Sciences Advisory Committee,* U.S. Department of Energy, November 2015. Available at https://science.osti.gov/-/media/bes/besac/pdf/Reports/Challenges_at_the_Frontiers_of_Matter_and_Energy_rpt.pdf (accessed June 8, 2019).

Levi, B. G. *Phys. Today* **1994,** *47* (12), 17.

Neutrons for the Nation: Discovery and Applications while Minimizing the Risk of Nuclear Proliferation, American Physical Society, College Park, MD, July 2018.

"Number of Users Reported by BES User Facilities," https://science.osti.gov/-/media/bes/suf/pdf/BES_Facilities_Number_of_Users.pdf (accessed May 30, 2019).

2. Overview of STS Neutron Beam Production

The proposed Second Target Station (STS) is designed to produce beams of cold (long-wavelength) neutrons in short pulses with high peak brightness. High brightness will be achieved by employing three coupled processes. First, the cross section of the incoming proton beam at the target will be compressed by >50% relative to the First Target Station (FTS) at the Spallation Neutron Source (SNS). Second, the STS will be equipped with a solid rotating tungsten target that can support the higher proton flux. Finally, novel compact moderator designs will be optimally coupled to the target. This source design, coupled with a short proton pulse that produces neutrons in a short period of time, results in world-leading neutron peak brightness. The short proton pulse is made possible by using the existing accumulator ring to compress the train of long pulses produced by the SNS linear accelerator. The STS will receive proton pulses from the accumulator ring at 15 Hz, allowing the use of a very broad range of neutron energies. This section presents an overview of how the STS has been designed to provide the unique beams of neutrons.

2.1 Production of Proton Pulses

A schematic layout of the SNS complex, including the proposed STS, is shown in Fig. 2.1. The accelerator comprises a negative hydrogen (H^-) ion injector (also called the front-end system), a 1 GeV linear accelerator (linac), an accumulator ring, and associated beam transport lines. The injector consists of an H^- ion source, a low-energy beam transport (LEBT) system that provides initial acceleration to 65 keV and electrostatic chopping of the 1 ms pulses that are produced at a rate of 60 Hz, a 402.5 MHz radiofrequency quadrupole (RFQ) that accelerates the beam to 2.5 MeV and imposes the radiofrequency (RF) time structure, and a medium-energy beam transport (MEBT) line. The linac consists of permanent quadrupole magnets in drift tube assemblies that transversely focus the H^- ion beam and superconducting cryomodules that generate RF standing waves that further accelerate the beam to 1 GeV. The ongoing proton power upgrade (PPU) project will install additional superconducting cryomodules and upgrade the RF systems so that the final energy of the beam can be increased to 1.3 GeV. Together with increased H^- ion current output from the front-end system, these changes will increase the power capability of the linac from 1.4 MW to 2.8 MW.

The linac beam is transported via the high-energy beam transport (HEBT) line to the injection point in the accumulator ring, where the electrons are stripped off the H^- ions by passing through a diamond foil, converting the H^- ions to protons. The accumulator ring consists of magnets that circulate the protons during accumulation at a fixed energy. The 1000 “mini-pulses” contained in the 1 ms long pulses of

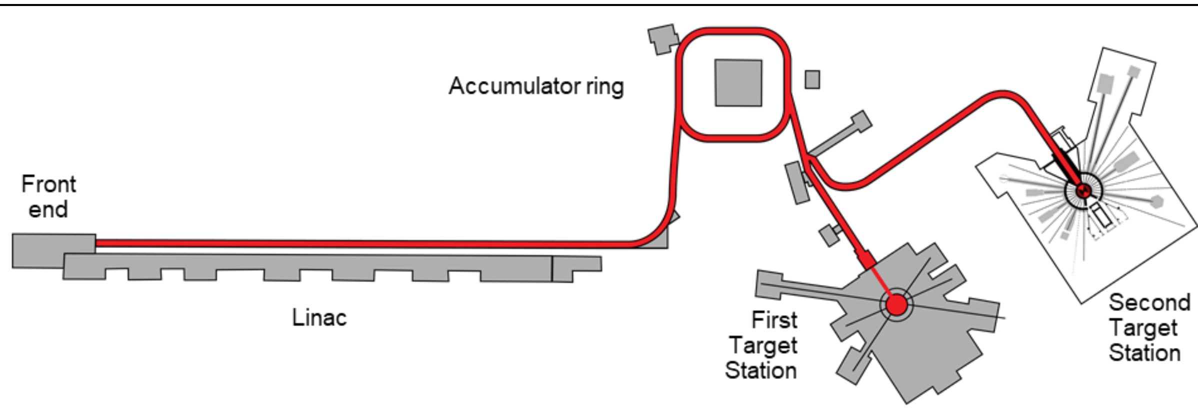

Fig. 2.1. Schematic layout of the SNS complex, including the proposed STS (at right). The beam path is shown in red. Image source: ORNL.

protons are “stacked” (accumulated) on top of one another in the ring to produce a 1 μs pulse, reaching an intensity of 1.5×10^{14} protons per pulse. When accumulation is complete, extraction kicker magnets fire during the 250 ns gap between pulses to remove the accumulated beam in a single turn and direct it into the ring-to-target beam transport (RTBT) line.

To support the STS, the kicker magnets will be programmed to redirect one out of every four proton pulses to a second RTBT line. The STS will therefore operate with a 700 kW beam of proton pulses with a frequency of 15 Hz, whereas the FTS will operate with a 2 MW beam of proton pulses with 45 pulses per second delivered at a frequency of 60 Hz. This design allows both target stations, the FTS and the STS, to be supported by the same accelerator, yet they will operate independently of each other.

In the selection of these operating power and frequency parameters, an important consideration was that the FTS was designed to receive a maximum power of 2 MW. The selected frequency allows the two target stations to use almost all of the power capability (2.8 MW beam power, with 46.7 kJ of energy per proton pulse) of the SNS accelerator after the PPU project has been completed. The lower frequency of the STS compared to the FTS will provide beams of neutrons that have a greater (4×) range of usable wavelengths. This increased wavelength range was an important requirement of the scientific case for STS. Alternative frequencies of 10 Hz and 20 Hz were considered; the recommendation from an external technical review was that 15 Hz provided a sufficiently broad range of neutron wavelengths to satisfy the science case while maximizing the power delivered to the STS target and therefore the neutron flux. In making this decision, the review team took into consideration the fact that operating the STS at 20 Hz would reduce the number of pulses that could be sent to the FTS to 40 per second. This would reduce the operating power of the FTS to below 2 MW. The team also took into consideration the fact that neutron instruments at the STS could be operated at 7.5 Hz by using choppers to remove every second neutron pulse, increasing the range of neutron wavelengths if required. In summary, an operating frequency of 15 Hz offers greatest flexibility while maximizing the power and performance of both the STS and FTS.

2.2 Compact Source Design

The STS neutron source will be designed to produce high-brightness cold neutron beams by employing three coupled processes. First, the incoming proton beam at the target will be compressed in size by more than 50% relative to the FTS to a cross section of ~62 cm^2. Second, a solid rotating tungsten target that can support the higher proton flux will be employed. Finally, novel compact moderator designs will be optimally coupled to the target. This source design, coupled with a short proton pulse that produces neutrons in a short period of time, results in world-leading neutron peak brightness.

The proton pulses transported to the STS from the accumulator ring will impact the outer edge of the rotating tungsten target to spall neutrons that will be directed to instruments. The target is approximately 1.1 m in diameter and 6 cm thick. Figure 2.2 shows the STS target and moderator design.

The target consists of 21 separate stainless steel segments, each housing a solid 6 cm thick tungsten block that is encased in a layer of tantalum to protect the tungsten from contact with cooling water. The stainless steel segments are welded to a central hub at the end of a 4 m long shaft that extends above the target monolith. This shaft is connected to a drive system that rotates the target at ~42.9 rpm, so that it completes one rotation every 1.4 s. The target is rotated to spread the power load on the target and therefore simplify the cooling requirements. The target is cooled by water conveyed through the shaft and directed through the stainless steel housings around the tantalum-clad tungsten blocks. This design allows the incident proton energy to be spread across the 21 target blocks, so that each block receives the equivalent of ~33 kW (700 kW distributed over 21 blocks) of proton beam power. With a stationary target, further segmentation of the tungsten would be needed to allow for greater water cooling; this would reduce the average density of the target material in the neutron production zone and consequently decrease neutron production in the vicinity of the moderators. Thus, the rotating target design enables a brighter neutron source.

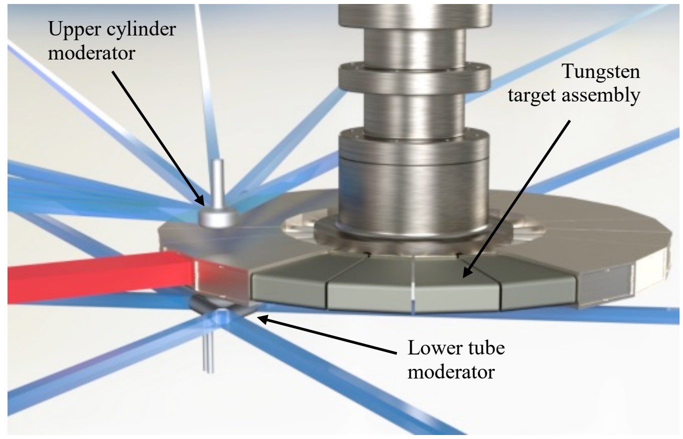

Fig. 2.2. Rotating tungsten target and moderator configuration. The outer diameter of the target assembly is 1.1 m. The red beam illustrates the incident proton beam coming from the accelerator, while the blue beams represent the outgoing neutron beams emitted from the two moderators. The neutron beam size is shown as 3 × 3 cm^2. Image source: ORNL.

The spalled neutrons are then moderated (reduced in energy) by a pair of compact moderators (~30 mm tall), located above and below the target, to optimize the production of high-brightness cold neutrons. Neutrons collide with hydrogen molecules in these moderators, thereby reducing their energy. They are surrounded by 20 mm of light water, which acts as a pre-moderator. The moderators are operated at a temperature of 20 K and with high-purity *para*-hydrogen i.e., molecules of hydrogen with aligned spins.

The upper moderator is a vertical cylinder (3 cm high, 8.2 cm in diameter) that emits neutrons; these neutrons then enter guides and are delivered to 16 instruments (for clarity, only 8 of the 16 emitted neutron beams/instrument paths are shown in Fig. 2.2). This upper moderator has a narrower neutron pulse width for better neutron wavelength resolution. The lower moderator consists of three horizontal tubes (14–16 cm long, 3 cm in diameter) that are connected to form a triangle; the neutrons enter along the length of each tube and are emitted from the 3 cm diameter ends of these tubes to illuminate six beam lines. The lower moderator has the same peak brightness as the upper moderator but produces somewhat broader neutron pulses with a correspondingly higher time-integrated brightness. Instruments that require better resolution will view the upper cylindrical moderator, while those that require lower resolution will view the lower moderator and benefit from receiving more neutrons. Both moderators are far smaller than the 120 mm tall moderators at the FTS; this results in much brighter beams of neutrons, as discussed below.

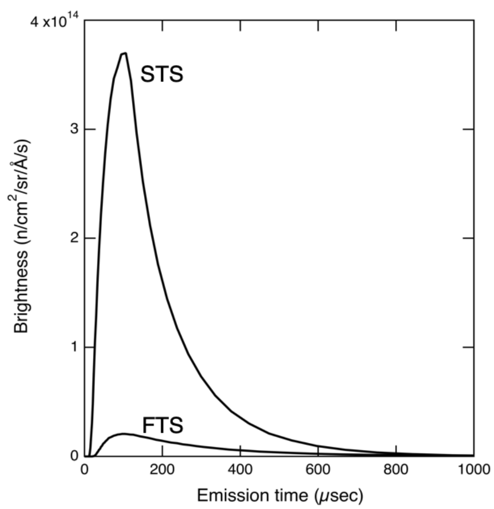

Fig. 2.3. Pulse shapes emitted from FTS and STS cold, coupled moderators at a wavelength of 5 Å (a typical benchmark for cold neutrons). Calculations are for STS operation at 15 proton pulses per second and 700 kW and for FTS operation at 45 proton pulses per second and 2 MW. Image source: ORNL.

Figure 2.3 shows the expected neutron brightness that will be emitted from the STS coupled moderator design, compared to that at the FTS. Here we define the brightness of a beam of neutrons as the number of neutrons of a certain wavelength (i.e., per angstrom) that pass through an area of 1 cm^2 in 1 s and are traveling in a direction within a solid angle of 1 steradian (i.e., $n/s/cm^2$/Å/ster). Brightness thus differs from source flux, a quantity that does not depend on the solid angle (divergence) of neutrons within the beam. For many experiments, brightness is a more important beam property than flux because higher brightness directly translates into more neutrons on the sample. This is the foundation for delivering the multiple orders of magnitude gains in instrument performance required to address the science challenges envisioned for the STS.

In Fig. 2.3, the height of the pulse shapes is the peak brightness; the integral under the curve multiplied by the number of proton pulses per second (15 and 45 for the STS and the FTS, respectively) is the time-averaged brightness. Instrument performance scales with peak brightness if the width of the pulse is broad enough to deliver the wavelength resolution desired, which is true for most of the instruments envisioned for the STS. This means that the higher the peak brightness, the better the performance of instruments at the STS.

Figure 2.4 compares the peak brightness and the time-averaged brightness of major current and planned neutron sources; this comparison shows that the STS will provide beams of cold neutrons with the world's highest peak brightness.

The FTS will remain the source of choice for many important classes of experiments, especially for experiments requiring thermal neutrons to examine materials on the atomic scale and for fast dynamics of materials.

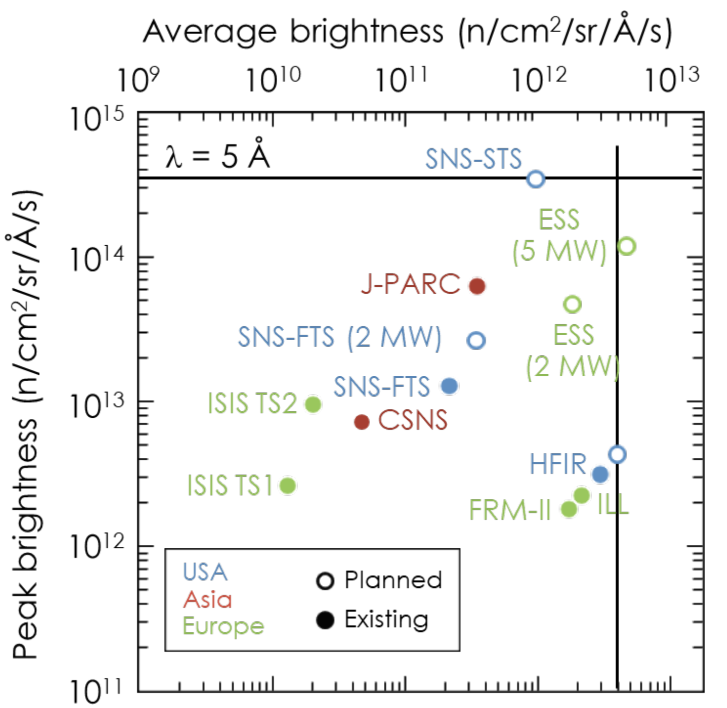

Fig. 2.4. Peak and time-averaged brightness of current (closed circles) and planned (open circles) neutron sources, illustrated at 5 Å. CSNS: China Spallation Neutron Source, China; ESS: European Spallation Source, Sweden; FRM-II: Forschungsreaktor München II, Germany; ILL: Institut Laue-Langevin, France; ISIS: ISIS Neutron and Muon Source, UK (TS: Target Station); J-PARC: Japan Proton Accelerator Research Complex, Japan. Image source: ORNL.