

## Neutron Delivery Systems Design of the Proposed NIST Neutron Source

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### INTRODUCTION

In order to meet the diverse needs of the neutron beam research community, an essential aspect of the proposed NIST Neutron Source (NNS) user facility [1] is the provision of cold and thermal neutron beams as well as several in-core irradiation positions, with a primary focus on neutron beam experiments. We refer to cold neutrons as those having energies below about 5 meV [2]. The wave-particle duality of the neutron allows this range to be described by neutron wavelengths,  $\lambda$ , greater than about 0.4 nm. This means that the wavelengths and energies of thermal and cold neutrons correspond closely to atomic and molecular length scales and the energies associated with atomic motions of condensed matter, allowing their simultaneous measurement and their non-destructive nature is advantageous for sensitive samples. The neutron's electrical neutrality, magnetic moment, and isotope-dependence of nuclear scattering, particularly with hydrogen and deuterium, provide undisputedly unique measurement possibilities and complementarity with x-ray, NMR, and other techniques. The challenge for neutron sources is to furnish adequate numbers of collimated neutron beams of sufficient intensity to satisfy the demand for experimental throughput. The NNS intends to provide not only a replacement for an aging facility but aims to offer significantly increased scientific output through enhanced beam intensity and an expansion in the number of experimental stations available.

Increased intensity also means that tighter beam collimation, narrower bandwidths, and higher spatial resolution detectors are tolerable, which in turn reduce the uncertainty of the inferred neutron energy and momentum exchanges between the neutron and the sample. Therefore, increasing the source flux per steradian (brightness) naturally leads to the revelation of new phenomena via improved data quality with less reliance on data corrections. This paper provides a general review of the neutron delivery systems design of the proposed NIST neutron source.

### MITIGATION OF FAST NEUTRON AND GAMMA CONTAMINATION

The neutron beams may be considered as desirable leakage from the reactor core. They employ evacuated (or possibly helium-filled) beam tubes in the reflector that penetrate the

reactor shield and define the leakage path. Just as it is important to provide the number of experimental stations and neutron beam intensity required for rapid throughput, it is equally important that the beams have low fast-neutron and gamma-ray contamination.

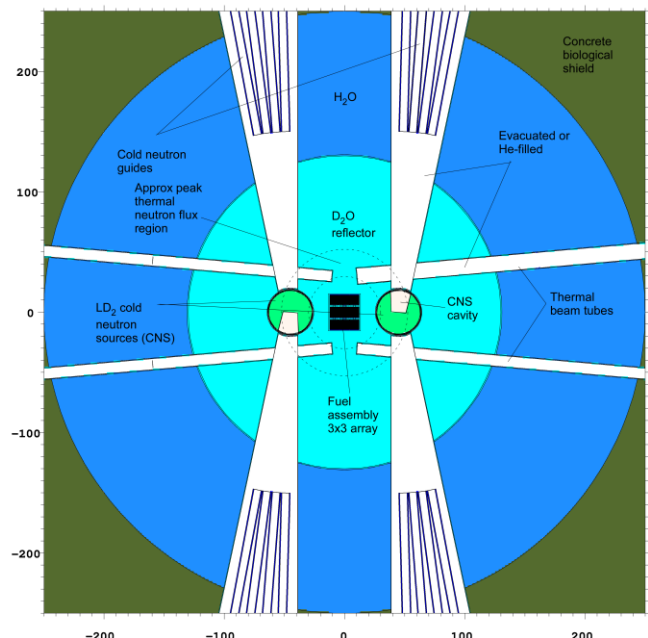


FIGURE 1: Schematic showing the layout of the two cold neutron sources and the tangential thermal and cold neutron beam tube arrangement (the latter containing cold neutron guides). Additional thermal beam tubes may be added and their precise locations will be optimized.

Fast neutrons penetrate instrument shielding, reduce their energy by multiple scattering, and contribute to a highly undesirable and indistinguishable background of neutron events of unknown history and origin, significantly compromising data quality. In so-called neutron “time-of-flight” measurements, these background neutrons tend to constitute a time-independent or a weakly time-structured background underlying the thermal or cold neutron pulse structure. Gamma-rays may also cause “false” events in neutron detectors, and both fast neutrons and gamma-rays in large numbers near the experimental areas can lead to

significant radiation shielding challenges, both for personnel and instrumentation.

The best course of action is to eliminate these contaminants close to the source. The compact reactor core results in an unperturbed thermal neutron flux that peaks in the D<sub>2</sub>O reflector surrounding the fuel. Initial background mitigation is performed by placing the beam tubes tangentially to the fuel so that they view the peak thermal flux region whilst excluding a direct sight of the fuel elements within their solid angle of acceptance. Thus neutrons traveling along the beam tubes have to have performed one or multiple collisions in the reflector with the associated softening of the emerging neutron spectrum. Likewise, a direct view of the intense gamma-rays emitted by the fuel is avoided.

## COLD NEUTRON PRODUCTION

Cold neutron generation requires a dedicated Cold Neutron Source (CNS). The CNS comprises a localized region of cryogenically-cooled moderator placed in or near the peak of the unperturbed thermal neutron flux [3,2,4]. Its purpose is to shift the neutron flux distribution towards lower energies via elastic collisions. If the CNS is positioned and sized appropriately, the neutrons approaching thermal equilibrium become characterized by a Maxwell-Boltzmann distribution with the lower effective temperature of the cold moderator. The current design concept has two liquid deuterium (LD<sub>2</sub>) moderators (typically operating between 23 K and 25 K) [5-8]. The ground state of the D<sub>2</sub> molecule is ortho, so the desired neutron energy loss process is an ortho-to-para spin-flip, favoring a high ortho-D<sub>2</sub> fraction. The overall performance of the CNS has been estimated from MCNP [9,10] particle transport calculations using ENDF/B-VII T=19 K neutron scattering kernels for LD<sub>2</sub> [11] with an assumed LD<sub>2</sub> void fraction of about 10%. However, the use of natural thermosyphon would increase the deuterium temperature to about 23 K. The ortho-para ratio assumed in the NNS MCNP model is 2:1, based on measurements under radiation performed at the Paul Scherrer Institute spallation neutron source in Switzerland [12], which also coincides with the high-temperature quantum mechanical limit. It has been observed [13] that introducing a re-entrant hole or cavity into the liquid volume may enhance the cold neutron flux in the direction of the cold beams and our initial simulations concur. The CNS brightness was estimated from a neutron current (f1-type) tally in a direction along the cold neutron guide axis connecting the CNS center and through a perpendicular rectangular area representing the cold neutron guide entrance. Because the brightness at this position depends on the polar angle with respect to the guide axis,  $\theta$ , a specific angular tally bin, described by  $\mu_1 - \mu_2 = \cos\theta_1 - \cos\theta_2 = 0.99875 \rightarrow 1$  (about  $2.9^\circ \rightarrow 0^\circ$  with respect to the guide axis), was chosen, corresponding to a typical range for which cold neutrons can

be transmitted by the guide. To obtain the brightness in units of  $\text{cm}^{-2}\text{s}^{-1}\text{MeV}^{-1}\text{sr}^{-1}$ , the tally was normalized by multiplying by the number of fission neutrons produced per second at 20 MW ( $=1.525 \times 10^{18} \text{ s}^{-1}$ ) and dividing by the area of the tally (in this case  $6 \text{ cm} \times 15 \text{ cm} = 90 \text{ cm}^2$ ) and by  $\Delta\Omega = 2\pi\Delta\mu$  (in this case  $2\pi \times [1 - 0.99875]$ ). In this way, the current tally representing the bin  $0.99875 \rightarrow 1$  is obtained directly in units of  $\text{cm}^{-2}\text{s}^{-1}\text{MeV}^{-1}\text{sr}^{-1}$ . Conversion to  $\text{cm}^{-2}\text{s}^{-1}\text{\AA}^{-1}\text{sr}^{-1}$  is via the Jacobian  $2\sqrt{2m_n E_n^3}/h$ , where  $m_n$  is the neutron mass,  $E_n$  is the neutron energy, and  $h$  is Planck's constant.

Results for the proposed NNS model CNS brightness are compared with the existing NBSR (LH<sub>2</sub>) and future planned (LD<sub>2</sub>) CNSs in Figure 2.

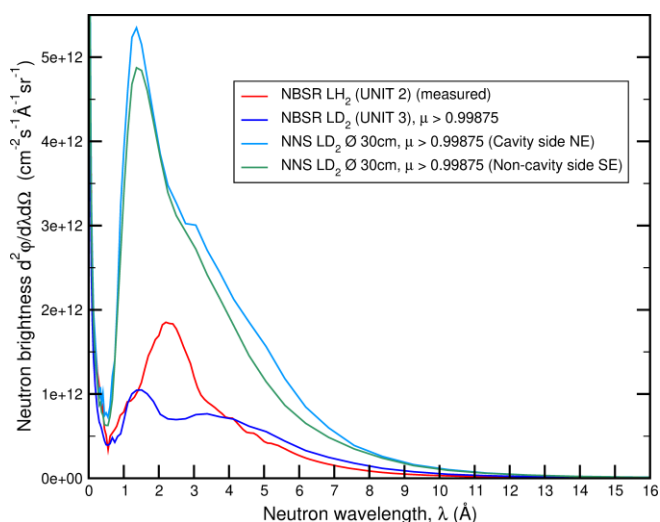


FIGURE 2. MCNP simulations of the CNS brightness for the model shown in Figure 1. The results are compared with similar simulations for the existing (Unit 2 LH<sub>2</sub>) NBSR CNS (red curve) and the future ungraded Unit 3 LD<sub>2</sub> CNS (dark blue curve). The light blue and green curves show the difference between the cavity and non-cavity side brightness for the NNS model.

The dimensions, exact locations, and configuration of the CNSs will be further optimized following the pre-conceptual design phase within the constraints of being able to remove the nuclear heat load from the cryogenic circuit and maintain the LD<sub>2</sub> in a sub-cooled liquid phase. The estimated nuclear component of the heat load for the CNSs shown in Figure 1 is about 4.5 kW per unit.

## THERMAL NEUTRON BEAMS

The thermal beams are represented schematically in Figure 1 as provided by the tubes not pointing towards the CNSs. Figure 3 compares MCNP simulations of the thermal neutron brightness emitted through these tubes with a typical thermal beam tube at the NBSR (BT3) at equivalent (20 MW) reactor power. The brightness in units of  $\text{cm}^{-2}\text{s}^{-1}\text{MeV}^{-1}\text{sr}^{-1}$

was obtained in a similar manner to that described for the cold neutrons above. The results indicate that the NNS should have at least a factor 2 thermal neutron brightness gain with respect to the NBSR, associated with the higher peak thermal flux view. Further optimization of the size, thimble tip position, and inclination of the tubes will be performed which may yield additional gains.

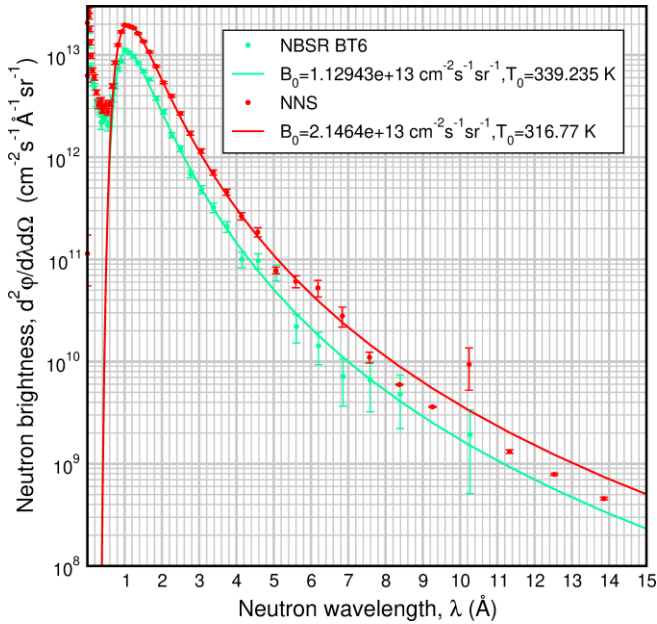


FIGURE 3: MCNP simulations of the thermal beam brightness for the model shown in Figure 1. The solid lines are fitted Maxwellian functions.

## COLD AND THERMAL NEUTRON GUIDES

The facility layout with a large number of neutron scattering instruments requires the cold neutron instruments to be placed quite far from the core. This is advantageous as they are then in areas of lower background radiation, however, the natural beam divergence dictates that the beam flux would reduce as  $1/\text{distance}^2$ . This problem is mitigated by using neutron guides in which neutrons may be totally reflected to preserve the beam intensity many meters from the core. Neutron guides are usually in the form of rectangular tubes with specially-prepared, very highly polished surfaces (tenths of nanometer roughness and tenths of mrad waviness). The polished surfaces are coated with thin films, most commonly of nickel or graded multi-layers of nickel and titanium (supermirrors). The total reflection angle is proportional to the neutron wavelength and small - about  $1^\circ/\text{nm}$  for Ni, but may be extended using supermirrors by a factor  $m$  which is often used to label them. Supermirrors up to  $m=4$  are now routinely available and supermirrors having  $m$  up to 8 have also been manufactured [14]. Because the reflection angles of the perpendicular surfaces of the guide are proportional to  $\lambda$ , a perfectly reflecting, long neutron

guide, where most of the emerging neutrons have undergone reflection, would tend to have a transmission proportional to  $\lambda^2$ , so neutron guides naturally filter out unwanted fast neutrons. We intend to use neutron guides to view both CNSs. Like the thermal beam tube arrangement, the cold neutron tubes and guides are orientated such that they cannot transmit neutrons or gamma-rays directly from the fuel region. The current model envisages a total of 16 cold neutron guides oriented approximately perpendicular to the thermal beams (Figure 1), which could accommodate a large suite of cold neutron instruments on end-guide and side positions. Furthermore, by curving the neutron guide axes such that a direct line of sight through the guide between the instrument and the source is excluded, the residual component of fast and epithermal neutron and gamma-ray contamination is largely eliminated from the emerging beam. The curvature not only improves the background filtration of the beam but also allows easier separation and accessibility of larger footprint instruments without the need to displace them further from the source. Using a higher or lower  $m$  supermirror on the outer radius (concave surface) of a curved guide adjusts the suppression of the shorter wavelengths transmitted by the guide in order to tune the transmitted bandwidth to instrumental needs.

As for cold neutrons, thermal neutron guides may be used in some instances, however, the smaller total reflection angles of the shorter wavelength thermal neutrons usually require higher  $m$  supermirror coatings. Thermal neutron guides may be used to facilitate thermal neutron instrument placement further from the core to allow an increased number of experimental stations. This is usually favorable when the gain of reflected neutrons of the desired wavelength from the guide outweighs the loss of solid angle of direct neutron paths from the introduction of the guide itself. It will also require careful customization of the beam tube cross-section and the void path that this introduces into the reflector, but initial studies indicate that  $m=4$  thermal neutron guides may be advantageous for instruments more than about 8 m from the biological shield face.

One important technical aspect to consider for all neutron guides is the nuclear heating of their upstream portions and the ability to remove sufficient heat. This determines the closest approach of the guide front ends to the source. Untreated Ni-Ti supermirrors usually require maximum temperatures below 120 C to avoid inter-diffusion of the metallic layers and degradation of their performance, but reactive sputtering can increase this threshold to about 260 C [15]. They must also be kept in an inert environment, e.g. a vacuum or helium atmosphere. The latter may aid in-pile guide heat removal by convection and nowadays we tend to use thermally-conductive and robust aluminum substrate guides closest to the core. The cold neutron guides shown in Figure 1 start 1.5 m from the CNS centers.

## DISCUSSION

A detailed study of a proposed suite of cold and thermal neutron instruments has been undertaken and demonstrated. The feasibility of accommodating all 16 end-guide position instruments on high-performance neutron guides using today's neutron guide technology has been established. Furthermore, multiple side positions and branched guide end-positions can be added. Comparing the projected NNS experimental capacity with the NBSR could be discussed in terms of usable neutron currents at the combined experimental stations. However, such a comparison is difficult since neutron instruments use different bandwidths, beam sizes, and divergences, which in turn depend on the detailed neutron guide designs and number of additional side-positions created. Neither the instrument suite nor their customized guide designs, nor indeed the beam configurations are finalized, and final decisions on the instrument suite will likely involve further involvement of the neutron user community, as indicated in [1]. Therefore, a more useful metric is to compare the flux per steradian at the beam entrances within the usable beam divergence range. For the cold neutron beams this reduces to the product of the cold neutron ( $\lambda > 4$  nm) brightness within the cold neutron guide transmission range and the summed area of available guide entrances. For the NNS we envisage accommodating at least 16 cold neutron guides (compared with 12 at the NBSR). This comparison yields at least a factor 5 increase in potentially usable cold neutrons, assuming 6 cm  $\times$  15 cm cross-section guide entrances and a factor 6.4 increase if 6 cm  $\times$  20 cm guides are used, excluding the possibility of further optimizing the  $\lambda > 4$  nm CNS brightness. We also anticipate at least the indicated brightness gain factor of 2 for the thermal instruments. Further performance improvements are anticipated by more efficiently using the available neutrons via advanced neutron instrument designs (e.g. multiplexing monochromatic instruments) and advanced neutron optics including focusing techniques as well as future technological advances in neutron instrumentation.

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## REFERENCES

1. JEREMY C. COOK, HUBERT E. KING, CHARLES F. MAJKRZAK, DAGISTAN SAHIN, JOY S. SHEN, OSMAN S. CELIKTEN, DAVID DIAMOND, ROBERT E. WILLIAMS, and THOMAS H. NEWTON, "Proposed NIST Neutron Source User Facility", these proceedings.
2. F. J. WEBB, "Cold neutron sources," *J.Nucl.Energy. A/B*, **17**, no. 4, pp. 187–215, (1963).
3. I. BUTTERWORTH, P. A. EGELSTAFF, H. LONDON, AND F. J. WEBB, "The production of intense cold neutron beams," *Phil.Mag.*, **2**, no. 19, pp. 917–927, (1957).
4. P. AGERON, PH. DE BEAUCOURT, H. D. HARIG, A. LACAZE, AND M. LIVOLANT, "Experimental and theoretical study Cold Neutron Sources of Liquid Hydrogen and Liquid Deuterium," *Cryogenics*, **9**, no. 1, pp. 42–50, (1969).
5. W. GAUBATZ and K. GOBRECHT, "The FRM-II cold neutron source," *Physica B*, **276–278**, pp. 104–105, (2000).
6. S. J. KENNEDY, "Construction of the neutron beam facility at Australia's OPAL research reactor," *Physica B: Condensed Matter*, **385–386**, pp. 949–954, (2006).
7. A. MÁRQUEZ AND F.SÁNCHEZ, "Neutron Cold Source Optimization for RA-10 reactor" – Proceedings of the 16th meeting of the International Group On Research Reactors, November 2014, Bariloche, Argentina.
8. R. E. WILLIAMS, M. MIDDLETON, P. KOPETKA, J. M. ROWE, and P. C. BRAND, "A Liquid Deuterium Cold Neutron Source for the NIST Research Reactor – Conceptual Design," Proceedings of the 15th meeting of the International Group On Research Reactors 2013, Daejeon - South Korea.
9. C.J. WERNER, et al., "MCNP6.2 Release Notes", Los Alamos National Laboratory, report LA-UR-18-20808 (2018).
10. C.J. WERNER (editor), "MCNP Users Manual - Code Version 6.2", Los Alamos National Laboratory, report LA-UR-17-29981 (2017).
11. J. L. CONLIN, "Listing of Available ACE Data Tables," Los Alamos National Lab. (LANL), Los Alamos, NM (United States), LA-UR-17-20709, (2017). [Online]. Available: <https://permlink.lanl.gov/object/tr?what=info:lanl-repo/lareport/LA-UR-17-20709>.
12. F. ATCHISON *et al.*, "Ortho-para equilibrium in a liquid D<sub>2</sub> neutron moderator under irradiation," *Phys. Rev. B*, **68**, no. 9, p. 094114, (2003).
13. P. AGERON, "Cold neutron sources at ILL," *Nucl.Instrum.Methods A*, **284**, no. 1, pp. 197–199, (1989).
14. <https://www.swissneutronics.ch/products/neutron-supermirrors/>.
15. P. Böni, Private communication, 2006.