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Evaluation of USANS move from SNS BL-1A to HFIR Cold Guide Hall

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1.1 Approvals

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Technical Concurrence				
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Author 3				

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0	Initial Release

2. INTRODUCTION

This document evaluates the feasibility, potential advantages, and drawbacks of relocating the USANS instrument from its current location at Spallation Neutron Source (SNS) BL-1A to the High Flux Isotope Reactor (HFIR) Cold Guide Hall, NB-2 location. This move is envisioned to be carried out after completion of the HFIR beryllium reflector replacement (HBRR), cold source outage, and neutron guide rebuild.

3. SCIENCE CASE AND GENERAL CONSIDERATIONS

The move of the USANS instrument from SNS to HFIR is considered primarily for the expected benefit of greatly increased neutron flux and therefore shorter measurement times and increased sample throughput. Measurement quality benefits of this move include higher time-integrated neutron flux, lower neutron and gamma radiation background, and USANS operations unimpeded by the operations of the BL-1B NOMAD instrument, which currently involves unpredictable, sometimes frequent and lengthy closures of the shared main neutron shutter. This would offer relief for the USANS oversubscription problem. More predictable and reduced measurement times might also allow time-resolved measurements and in-situ studies of systems reacting over a period of hours. This capability would, for instance, enable kinetics studies of aging, and more generally phase transitions, of colloidal solutions. The currently used crystals will work equally well at HFIR.

A more generously spaced sample area will permit use of bulky sample environments that currently don't fit. The increased footprint of the USANS instrument in the HFIR Cold Guide Hall will enable implementation of a robotic sample changer similar to those already used at other beam lines. The robot would, in combination with the higher neutron flux, allow for more efficient measurements. The robot or a larger sample table would also physically decouple the sample environment from the instrument, which is advantageous for vibrating sample environments (rheometers, cryostats, vacuum pumps) that may disturb the alignment of the crystals. A larger sample environment area allows operation of furnaces and magnets, which currently don't work because of space constraints and radiant heat disturbing the instrument alignment.

Drawbacks of the move include the significant and inevitable productivity losses from disassembly, move, and rebuild of the instrument, i.e., there would be no USANS at ORNL for at least 1 year, and possibly up to 2 years. With the potential closure of ILL Grenoble in 2033 and the uncertain status of NIST NCNR, there would possibly be no USANS available in North America or Europe during the move.

The USANS instrument inherently separates coherent from incoherent scattering contributions because it is double-monochromator instrument. This important characteristic is source-independent and will be preserved if the instrument is relocated to HFIR.

3.1 Multiple Scattering

A commonly encountered USANS problem is the diminishment of signal quality at ultra-small angles by multiple scattering, which then necessitates sample thinning, reducing count rates and prolonging measurement times. Multiple scattering is more pronounced for longer wavelengths. Relocation of the USANS to the HFIR guide hall and its operation at the primary wavelength of 3.6 A only may make it harder to identify and eliminate multiple scattering for some samples. This will in turn require thinner samples, with sample thicknesses approaching the size of structural features interrogated (tens of microns). Use of choppers or an alternative pre-monochromator might alleviate these problems when needed. Preparation of very thin samples is prone to introducing artefacts that cannot be corrected.

Installation of a pseudo-random or Fourier chopper would allow for the discrimination of multiple harmonics, restoring that unique capability currently available for the SNS USANS. Alternatively, wavelength filters could also be used to discriminate between different harmonics. It is important to note that this becomes important only at the smallest angles where the measurement time is the fastest or statistics are the strongest so the use of a chopper or filter would have the least impact on overall measurement time.

4. TECHNICAL DETAILS AND FOOTPRINT OF THE INSTRUMENT

The USANS currently located at BL-1A of the First Target Station (FTS) at SNS utilizes a copper pre-monochromator that provides 3.6 Angstrom wavelength neutrons to the instrument. Time-of-Flight is used to distinguish between the primary and higher-order reflections that scatter from the monochromator into the flight tube to the sample position.

A guide, proposed to support the Crystal Alignment Station, Polarization Test Station, and ultimately a Neutron Spin Echo Instrument, will be installed during the HFIR Beryllium Reflector Replacement Maintenance Activity, and is referred in conceptual design documents as “NB-2”. This guide will sit west of the HB-4 beam tube centerline and be accessible from the west side of the guide hall at distances beyond the sample position proposed for the Imagine-X Dynamic Neutron Polarization (DNP) instrument. This is seen in the concept layout provided in Figure 2, highlighted in green.

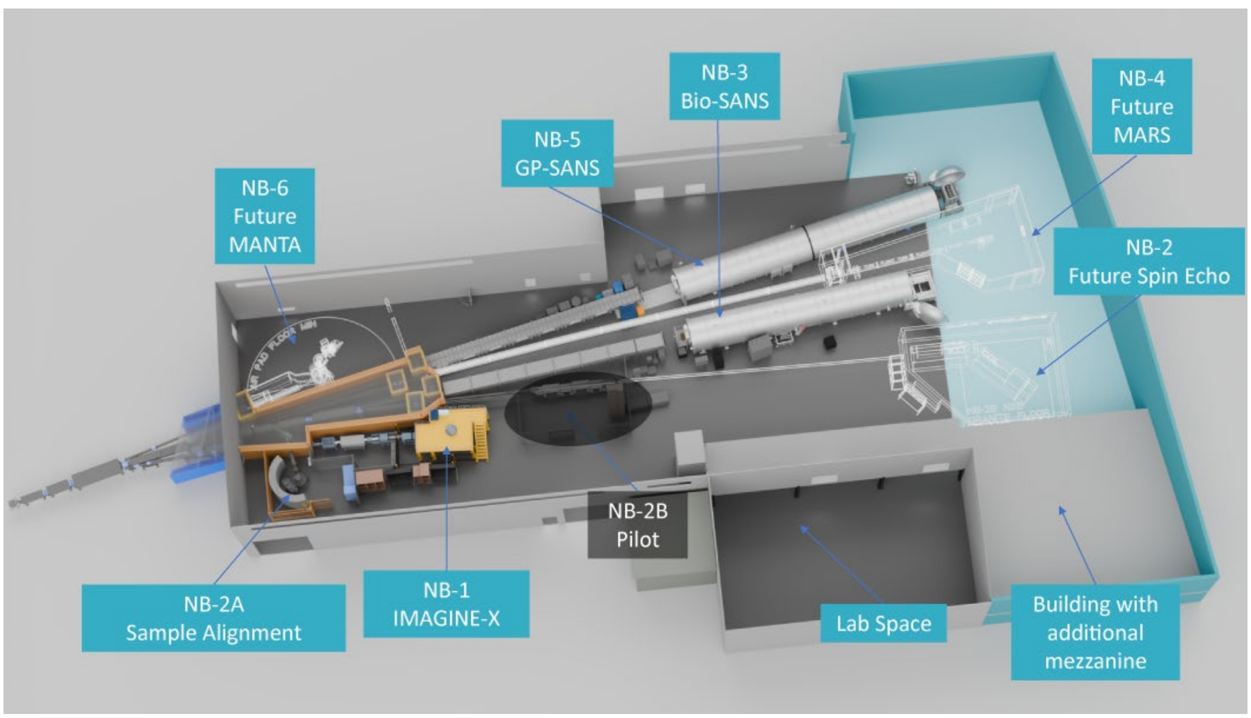

Figure 1: Layout of the HFIR Cold Guide Hall after the upgrade. The location reserved for USANS is NB-2B Pilot.

That said, the NB-2 guide will be capable of providing 3.6 Angstrom neutron brightness at the proposed polarization test station position (NB-2B Pilot) of about 2.48×10^{12} neutrons/(cm^2-steradian-Angstrom-second). The FTS Cryogenic Poisoned and Decoupled Moderator would provide 3.6 Angstrom average brightness of 1.0×10^{11} neutrons/(cm^2-steradian-Angstrom-second) at 2 MW operating power. The layout

of the existing instrument at FTS BL-1A downstream of the copper monochromator can be placed in the proposed HBRR guide hall for fit estimation in the NB-2B Pilot position, shown in Figure 2.
One notes that the existing instrument is quite compact and the only limiting factor is the current distance from the pre-monochromator (noted as "A" in Figure 2) to the nominal sample position (noted as "B"). This distance can be shortened to accommodate the anticipated floor plan with little to no impact on the anticipated performance of the instrument. The biggest challenge with the addition of this kind of instrumentation is the requirement that any instrument sharing the NB-2 beamline that may utilize variable wavelength operations will need to have its wavelength-defining components located downstream of the pre-monochromator position.

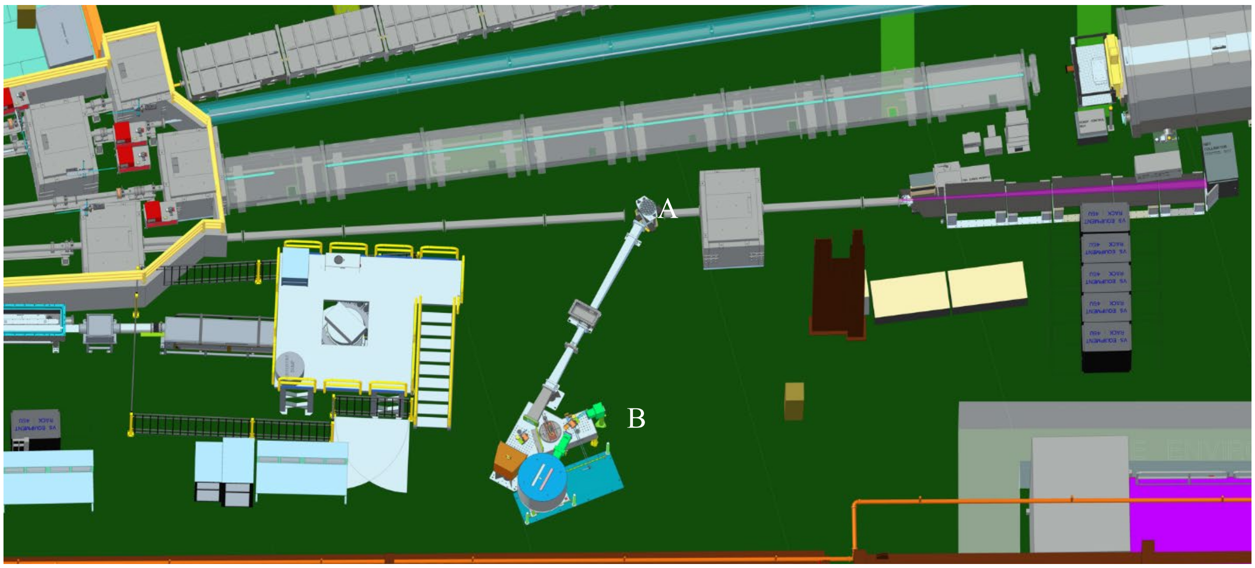

Figure 2: Zoom into the USANS location and layout in the HFIR Cold Guide Hall. This location offers significantly more space for the instrument than the current setting at SNS.

4.1 Estimation details of neutron flux gains at new HFIR location

In Figure 3, a flux spectrum taken from the proposed Neutron Spin Echo instrument at NB-2 is shown. The divergence utilized is 0.5 degrees in both vertical and horizontal directions. To translate the flux measured into brightness one applies a factor of $(0.5/180.0*\text{pi})^2$, or 7.615×10^{-5}. This results in the brightness estimate of 2.481×10^{12} neutrons/(cm^2-steradian-Angstrom-second) available at the exit of guide NB-2.

Figure 4 shows the average source brightness taken from the source data available in the FTS instrument development repository at code.sns.gov. The kinetic energy equivalent to 3.6 Angstrom wavelength is 0.0063 electron Volts (eV) for neutrons. We find the associated average brightness from the FTS Top-Upstream Cryogenic moderator to be $2.614\text{x}10^{13}$ neutrons/(cm^2-steradian-eV-second). Converting this to Angstroms we find the equivalent wavelength spectral brightness to be $1.00\text{x}10^{11}$ neutrons/(cm^2-steradian-Angstrom-second) by using the following conversions:

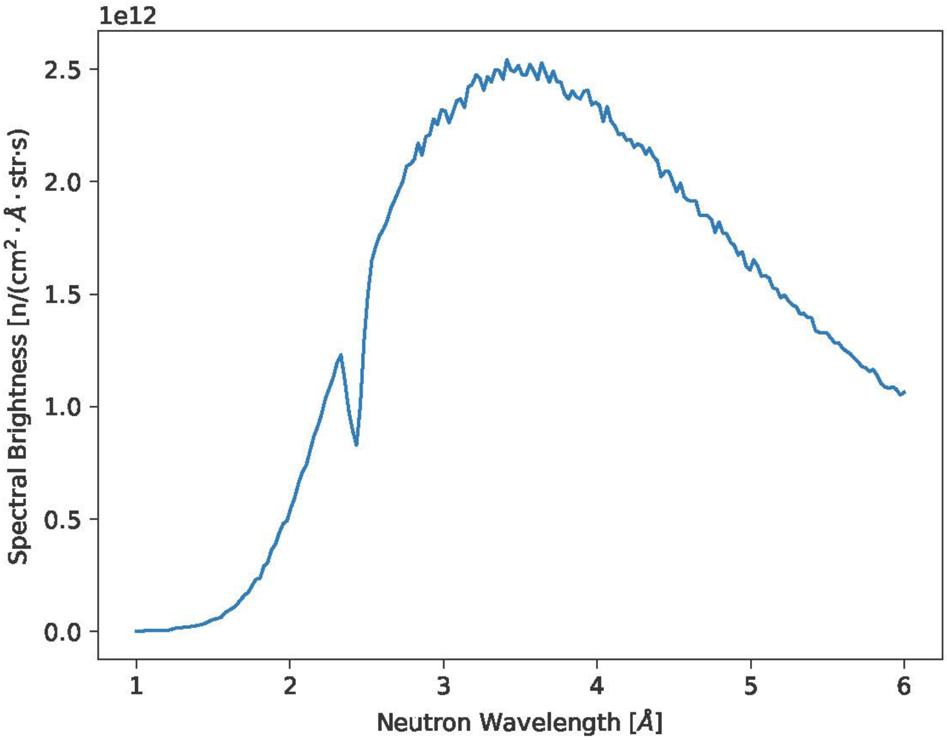

Figure 3: Source neutron brightness at HFIR's NB-2.

$$E[eV] = \frac{0.081805}{\lambda^2}$$

Spectral Brightness is $\partial B/\partial\lambda = \partial B/\partial E \cdot \partial E/\partial\lambda$, and thus the conversion factor at 3.6 Angstroms of $3.51\text{x}10^{-3}$ to determine a comparable available brightness estimate. Therefore, the brightness of the USANS beam at HFIR is about 24 times higher compared to that at SNS at 3.6 Angstroms.

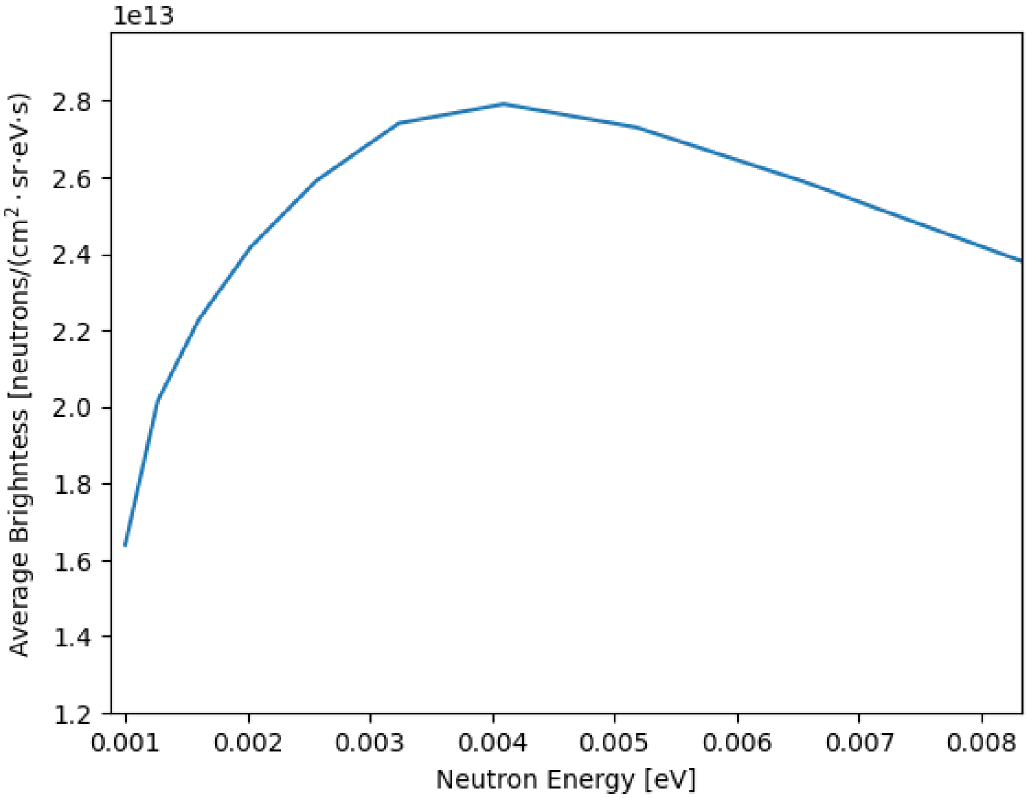

Figure 4: Average Source Brightness at SNS FTS.

5. SUMMARY

Relocation of the BL-1A USANS instrument to the future HFIR cold guide NB-2 beamline provides an opportunity to greatly increase the capabilities and productivity of the instrument through the ~25 times greater source flux and increased flexibility and access to the sample area. Benefits would include faster, broader-range, and better statistical quality measurements with bulkier and more complicated sample environments, allowing greater automation of experiments and possibly opening the door to in-situ studies on slowly evolving systems. The move would also remove the present operational conflicts arising from sharing a beamline and components with the BL-1B beamline.

Retaining the present capability to perform USANS measurements at extreme low Q would require additional analysis and expense. Measurements presently significantly benefitting from this capability account for ~10% of the current portfolio of experiments, and while the changes required to use the higher harmonics would reduce the flux gains, the gains wound still be substantial.

The most significant negative consequence to such a move would be the inevitable gap in North American USANS capability occurring during the relocation and recommission of North America’s only USANS instrument, especially at a time when there are few similar instruments available in the world.

6. REFERENCES

1. Frost, M. (2023, March 30). NScD Neutron Instrument Development / SNS / sourceTerms · GitLab [Software Repository]. GitLab. https://code.ornl.gov/nscd-neutron-instrument-development/fts/sourceTerms