

## ***Report on the inquiry into the scientific case for and technical feasibility of intense very cold neutron beams***

On April 27 and 28, 2016 neutron science experts met at Oak Ridge National Laboratory to consider opportunities intense very cold neutron beams at the Second Target Station (STS) offer the neutron scattering community. Loosely defined, very cold neutrons span the wavelength range of  $\lambda \sim 10$  to  $100 \text{ \AA}$ . The workshop consisted of a series of short talks during the morning of the first day. Then, the participants divided into two groups. One group—the source group—considered a variety of technical advances and challenges in developing moderators optimized to produce very cold neutrons. The second group—the applications group—considered emerging technologies that yield improved performance scaling at least by  $\lambda$ , or better  $\lambda^2$ . This group evaluated implications on existing instrumentation and opportunities to perform radically different (transformative) experiments. At the conclusion of the workshop notes were compared and recommendations formulated. F. Mezei closed the discussions with the succinct observation: “*The neutron scattering case for very cold neutrons is beyond convincing.*”

A list of participants, agenda and shared documents is found at <https://conference.sns.gov/event/18/overview>.

### **History of Very Cold Neutrons (Carpenter)**

J. Carpenter briefly summarized results of two prior VCN workshops—ones in 2005 (ANL) and 2012 (ORNL). The previous workshops identified interesting materials for 2-4 K moderators, challenge of nuclear heating (neutron and  $\gamma$ -ray), and an impressive list of science (many still germane today) problems that could be studied with an intense source of very cold neutrons and more efficient/practical lens technologies.

### **Overview of novel instrumentation for the STS workshop (Herwig)**

Earlier in the week (April 25-26), a workshop was held at ORNL to discuss ideas for novel instrumentation that could impact the initial suite of instruments built at the SNS second target station provided sufficient R&D is carried out in the near term. In order to link the ideas discussed to emerging scientific themes, participants at the workshop were asked to consider neutron applications to the five overarching scientific challenges identified in a recent report by the Basic Energy Sciences Advisory Committee, entitled *Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science*. These themes are:

- Hierarchical Structures and Materials Beyond Equilibrium
- Heterogeneity, Interfaces and Disorder
- Coherence
- Revolutions in Models, Algorithms, Data Management and Computing
- Transformations in Imaging Across Multiple Length Scales

Some members of the STS workshop also participated in the VCN workshop. Some topics were common to both workshops. Members of the VCN workshop who had not participated in the STS workshop provided additional perspective.

Two important conclusions of the STS workshop that impacted discussions at the VCN workshop were:

- *There are opportunities for gains from moderator optimization.* The current STS suite of moderators was optimized to provide maximum brightness below 5 meV. If the optimization were performed maximizing *intensity below 0.8 meV*, then a significantly different system might be obtained.
- There is a need to develop detailed metrics for moderator performance for all planned instruments.

These conclusions emboldened the VCN participants to consider opportunities for neutron science using not just cold neutrons (as presently planned for the STS), but for very cold neutrons.

### Present state-of-the-art calculations for a VCN source (Gallmeier)

F. Gallmeier presented calculations of source intensity, brightness and pulse shapes for a selection of scattering kernels used to represent neutron moderation processes. The model was made for a source that was displaced from the target in order to mitigate heat load, pre-moderated by H<sub>2</sub>O and surrounded by a Be

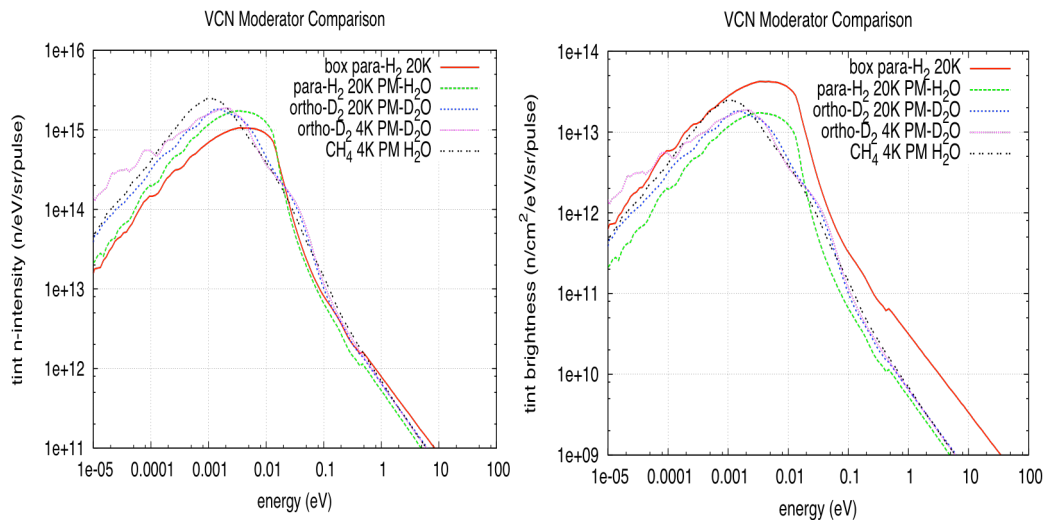


Figure 1 Total integrated intensity (left) and brightness (right) calculated for a small selection of kernels presently available.

reflector. Gallmeier considered para-liquid H<sub>2</sub>, ortho-liquid and solid D<sub>2</sub>, solid CH<sub>4</sub>, water ice, solid Be and solid Ne (these are the only kernels for cold moderators presently available). Displacement of the moderator from the optimal position for a

coupled liquid H<sub>2</sub> moderator of the same size (5 cm by 5 cm) (the baseline STS case) reduced the brightness by a factor of ~3. Gallmeier optimized moderator size, pre-moderator thickness to maximize the integral brightness ( $E < 3.2\text{meV}$ ,  $\lambda > 5 \text{ \AA}$ ). The intensities of the VCN options integrated over the entire face of a 10 cm by 10 cm moderator were only about twice the baseline case, while the brightness of the VCN options suffered (see Figure 1). Notably, most calculations exhibited little moderation of the spectra to temperatures consistent with 4 K.

### **Nuclear physics community interest in 8.9 Å neutrons (Brousard)**

A VCN moderator at the Second Target Station would enable the next generation of fundamental neutron physics experiments and the exploration of some of the most important science questions of our day. For example, one of the required ingredients for the baryon asymmetry in the universe, a process that violates both Charge and Parity (CP) symmetries, has not yet been found at a large enough scale to account for the abundance of matter. The current effort to search for a nonzero electric dipole moment in the neutron (nEDM), which necessarily violates CP, is expected to be statistics-limited at the First Target Station. The full parameter space of CP violation which could explain the observed imbalance could be explored with increased flux of 8.9 Å neutrons from a VCN moderator. Furthermore, a slightly modified version of the nEDM storage cell would itself be a world-class high-density source of ultracold neutrons (UCN), making possible a broad program of fundamental studies using UCN including precise tests of the electroweak interaction through measurements of the neutron decay lifetime and decay correlations. In addition, sensitive studies of gravity at the micron scale could be studied using UCN bound in gravitational quantum states. These experiments and others would address further questions on whether our understanding of the Standard Model of particles and interactions is complete.

### **Imaging with very cold neutron beams (Tremis)**

Very long wavelength neutrons (10-20 Å) bring new imaging applications that were previously not practical owing to lack of high intensity VCN beams. Quantification of hydrogen will be more accurate in thinner samples and can be pushed to much lower values than currently possible. Even water vapor at moderate pressures may become possible for imaging with sub-100 μm resolution.

The increase of absorption of VCN beams compared to cold or thermal beams has several advantages. (1) Detector technology pushing the limits of spatial and time capabilities are much easier to realize with VCN beams than cold or thermal neutron beams. The detection efficiency for most devices, including neutron counting detectors with microchannel plates, will be substantially improved at longer wavelengths, because the larger absorption cross section for the elements used for primary neutron interaction (<sup>10</sup>B, <sup>6</sup>Li, Gd, <sup>3</sup>He, *etc.*) will lead to a substantially higher probability of neutron detection, up to 100 % efficiency values for wavelengths approaching 20 Å. (2) Time resolution can also be improved as thinner absorbing layers will be required and both charge and light

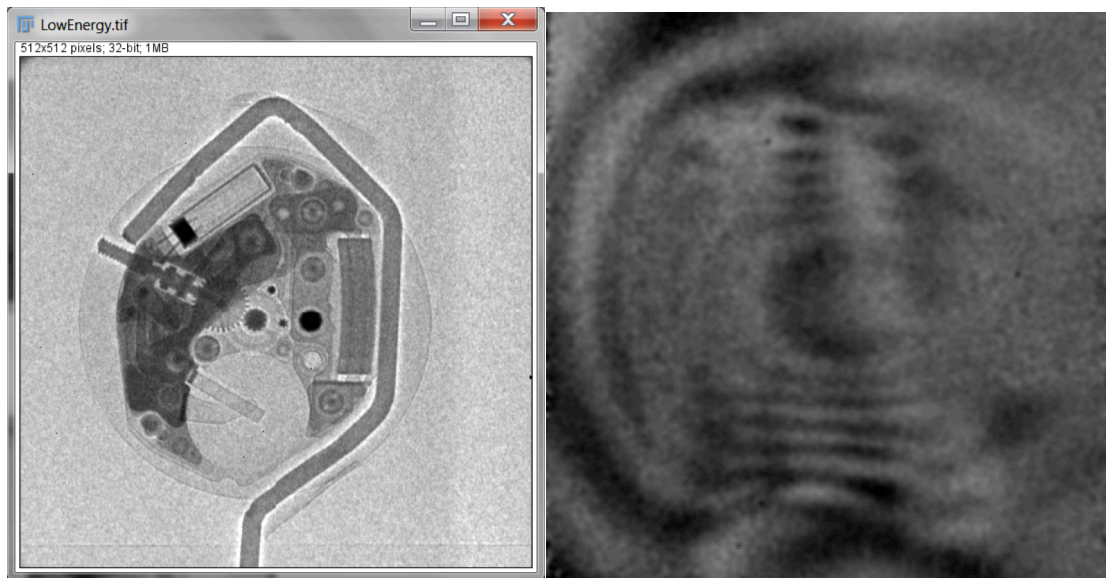


Figure 2 Refraction effects visible with cold neutrons in (left) objects or (right) magnetic fields provide additional imaging contrast and resolution thermal neutrons beams. Such effects will be even more pronounced with VCNs.

spreading will be reduced. (3) Spatial resolution will also be improved in some detection technologies due to smaller attenuation length within the detector active volume (by reducing the active volume necessary for example to detect a 20 Å neutron), and the ability to manufacture (perhaps with additive manufacturing techniques) highly efficient neutron beam collimators. (4) Image contrast particularly rising from hydrogen in soft matter and biological systems, *e.g.*, thin films and membranes, is more easily achieved with VCN beams than with thermal or cold beams.

### Summary of Source group brainstorming

The calculations of Gallmeier of admittedly a small number of scattering kernels are not yet promising—little increase of integrated intensity was achieved for pulse widths that were significantly, though likely tolerably, broadened. (Partially because of lack of thermalization of the spectrum to low temperatures, and partially because the geometric removal of the moderator from the target reduced the exposure of the moderator to the neutron production zone.) This realization motivated the question: How much of an increase of intensity is needed to catalyze interest in using very long wavelength neutrons? The consensus opinion was a 10x increase of intensity in the range integrated over the range of wavelength from 10 to 40 Å would be extremely interesting. *A 10x increase of VCNs resulting from a moderator optimized to produce VCNs at a 1MW/20 Hz STS would yield more VCNs than would be provided at the 5MW/14 Hz ESS, which has no moderator optimized to produce VCNs.*

The workshop discussed the surprising (to some) result that spectra from 4 K moderators did not have a peak in the spectrum corresponding to 4 K. In the case of H<sub>2</sub> and D<sub>2</sub>, the spectra were little moderated from 20 K. Attendees discussed the

observation that continued cooling of moderator materials does not result in unlimited reduction in spectral temperature; most thermalizing materials (*e.g.*, polyethylene, water, ethane, methane) reach a physical temperature for which further reductions in temperature does not change the spectral temperature. The temperature at which this saturation occurs varies with material. We hypothesize that this effect arises from a lack of low energy inelastic modes, which could facilitate further neutron energy loss and thermal equilibration.

With non-thermalizing materials (*e.g.*, parahydrogen and beryllium) the dramatic decrease in the neutron scattering cross section below the cut-off energy (which in turn corresponds to a temperature somewhat above the physical temperature of the non-thermalizing material) implies that neutrons scattering to below this cutoff energy will immediately escape the system and not be further moderated, *i.e.*, the moderator is transparent to neutrons with an energy below the cut-off energy. This results in a significantly non-Maxwellian spectral distribution, which may in fact be advantageous in boosting the low-energy neutron intensity.

Our goals in exploring qualitatively different moderating materials intended to augment very cold neutron intensities can thus be divided into two approaches: First, identify materials with long-wavelength cut-offs in scattering cross section that, when cooled sufficiently, will produce non-thermalized spectra with favorable low-energy performance—the 4<sup>th</sup> moderator concept. Second, identify materials which maintain continued thermalization capabilities to very low temperatures (that is, materials for which physical temperature reductions to the 2-4 K range are tracked by spectral temperature reductions)—the 5<sup>th</sup> moderator concept.

#### *Develop a VCN concept for a 4<sup>th</sup> conventional moderator*

Optimize the position, environment and size of a coupled *l*-H<sub>2</sub> moderator to maximize the flux in the range of 10 to 40 Å. The need for sharp peaks and intensity below 8.9 Å could be sacrificed in order to achieve higher flux above 10 Å. For example, a moderator with a beryllium reflector-filter cannibalizes the spectrum for  $\lambda < 4$  Å in order to increase the spectrum above 4 Å. The strengths of this approach are the technological solution is low risk, and the availability of a large high intensity moderator (as opposed to the small bright moderator of the baseline) increases the flexibility of the STS to adapt to the changing landscape of science. The first approach achieves higher flux by shifting the *l*-H<sub>2</sub> spectra for  $\lambda > 10$  Å upwards along the vertical axes of Figure 1.

#### *Develop a concept for a 5<sup>th</sup> elevated moderator*

This approach involves identifying a better moderating material. The approach achieves a higher very cold neutron flux by shifting the peak of the spectrum towards lower energy (to produce a 4 K spectrum, *i.e.*, a shift left along the horizontal axis of Figure 1). A strategy to develop a VCN source (the 5<sup>th</sup> moderator)

consists of three steps. First identify materials with high density of states at low energies by data-mining the literature (K. Batkov demonstrated one method); followed by measurements of the DOS of likely candidates on the Vision spectrometer, and molecular dynamics calculations (such as those performed at NC-State) to develop scattering kernels. The kernels would be used in calculations similar to those described by Gallmeier. In order to minimize radiation heating of the moderator, the 5<sup>th</sup> moderator might need to be elevated above the planned upper *l*-H<sub>2</sub> moderator (or 4<sup>th</sup> moderator if present).

### **Summary of Applications group brainstorming**

The applications group considered the weighty question: “What are we trying to achieve by using very cold neutrons (rather than simply cold neutrons)?” The overwhelming view was access to very cold neutrons enables scientific research that is not possible or not practical to pursue presently or even in the future with cold moderators at the STS. Examples include: measurements of  $S(Q,\omega)$  tending towards smallish  $Q$ , very low energy excitations and imaging of micron-size (or less) structures. Disciplines of materials science most likely to benefit include materials that are complex due to a myriad of length scales, energy/time scales, and the emergent properties that arise from non-linear coupling between different length scales (*i.e.*, hierarchical structures). Hierarchical structures in hard and soft matter are increasingly a prominent focus of BES interest, especially with dramatic innovations in materials synthesis.

J. Katsaras spoke of the keen interest biologists have in the structure and properties of *living* cells. Biologists already have excellent probes of cells at micron+ length scales but lack probes to shorter length scales (primarily because living cells lack x-ray or neutron contrast). However, with the invention of techniques to selectively deuterate (and feed) living cells, scientists can pre-program contrast into living cells so they can be probed using scattering or imaging techniques from nm to micron+ length scales. Very cold neutrons provide an important means to obtain information that biologists lack and to provide information at larger length scales biologists have from other means (thus providing much needed overlap between techniques). The importance of opportunities to study living cells with VCN beams is difficult to overstate.

Instrumentation techniques believed to benefit most by very cold neutrons include: small angle neutron scattering, spin echo spectroscopy, indirect geometry inelastic neutron scattering and imaging. In addition spatial coherence (*e.g.*, speckle, interferometry and neutron microscopy) and spin coherence (Larmor precession) are more easily achieved with very cold neutron beams than cold (or thermal) neutron beams, primarily because the index of refraction varies as  $\lambda^2$ , which is important to the effectiveness of lens technologies (of all kinds, reflective, refractive, magnetic, gravity, *etc.*). Solid state neutron detection technology is another example of a technology that is well suited to very cold neutrons—possibly enabling 3D

neutron detection where the third dimension represents energy. Unquestionably the ease of implementation of new technologies and availability of intense very cold neutron beams will enable imaging of micron or sub-micron correlation length scale to be more readily achieved than for the case of cold or thermal neutron beams. Thus, we imagine in a decade the opportunity to create significant overlap in neutron science between scattering and imaging domains in the length and energy/time scales. *The possibility to perform sub-micron imaging or rudimentary neutron microscopy represents a transformative change in the way we do neutron scattering today.* Namely, measurements of phase space moves the community away from model fitting of intensities in which arguably a great deal of information is lost.

## Recommendations

The workshop participants believe the community has an opportunity to carve out a best-of-class capability to facilitate studies of hierarchical structures in hard and soft matter that exploit very cold neutron beams. We envisage a moderator of very cold neutron beams that produces a 10x increase of intensity in the range of 10 to 40 Å compared to the coupled *l*-H<sub>2</sub> moderators planned for the STS. Such a capability would be unique in the world for the foreseeable future. The workshop recommends the following:

1. Neutron science end-users should specify the beam characteristics, intensity, brightness, pulse width, over a wavelength range to be optimized, *i.e.*, quantify what catalyzes success.
2. Target/moderator concepts should be developed for the 4<sup>th</sup> and 5<sup>th</sup> moderators described previously.
3. STS design should allow provisions to install a 4<sup>th</sup> conventional large high intensity optimized to produce very cold neutrons.
4. STS design should allow provisions to install a 5<sup>th</sup> elevated moderator and beam ports for an elevated moderator.
5. Allocate resources to get work done. Resources should include input from a diverse group of people including, instrumentation experts, nuclear physicists (*viz.* choice of moderating materials) and engage ESS and JPARC.

The workshop developed a one-year work plan for next steps to be reported at a workshop (tbd) next year.

1. Why does a 6 K methane moderator provide a beam with spectral temperature similar to that of a 20 K methane moderator (of 30 K).
2. What moderating materials options are available to produce VCNs? And, what are the density of states measurements from candidate materials using Vision?
3. Study the dependence of the spectral temperature with physical temperature for many materials to understand what materials enable lower-temperature spectra and what density of states characteristics enable that behavior.

4. What is the best-case conventional (4<sup>th</sup>) moderator solution (*e.g.*, involving high-albedo reflector concepts and closely coupled guide concepts) to achieve high intensity from 10 to 40 Å?
5. The figure of merit reported for different techniques in the 2005 report needs to be better defined and articulated. Include realistic treatment of absorption.
6. Calculate the performance of a high resolution spin echo spectrometer and a VCN-SANS instrument. Develop solutions for 1 MW at 20 Hz and 0.5 MW at 10 Hz sources. And, if time and resources permit, simulate a 100 neV backscattering spectrometer.
7. Evaluate the possibilities to achieve coherence sufficient for speckle, holography and etalon interferometry.
8. Demonstrate proof of principle imaging using VCN.
9. Identify compelling cases for transformative science enabled by VCN. Articulate strengths of VCN at the STS vs. HFIR.