Title

Enhance Cold Neutron Beam Production for Materials Research and Applications via Advanced Moderators

Background Situation Analysis

For over 50 years research reactors have supported developments in neutron beam research, new materials, and component integrity testing, and are expected to continue to do so in the coming decades. Many of the benefits from research reactors have to be brought into today’s technical, economic, and social realities. The demands on neutron research are increasing and new coordinated research interfacing different branches of science will be necessary. New techniques, besides using research reactors, require access to spallation neutron sources, where peak neutron intensity is increased by two orders of magnitude with high-energy sources.

Neutron scattering encompasses all scientific techniques whereby the deflection of neutron radiation is used as a scientific probe. Neutrons readily interact with atomic nuclei and magnetic fields from unpaired electrons, making a useful probe of both structure and magnetic order. For many good reasons, moderated neutrons provide an ideal tool for the study of almost all forms of condensed matter. Initially, they are readily produced at a nuclear research reactor or a spallation source. However in such processes neutrons are produced with much higher energies than are needed. Therefore moderators must be used to slow the neutrons down and therefore produce wavelengths that are comparable to the atomic spacing in solids and liquids, and kinetic energies that are comparable to those of dynamic processes in materials.

Moderated neutron beams are produced by a slowing-down and thermalization process, which suffers from very low efficiency. Indeed, only few neutrons which enter the moderator will appear in the useful neutron beam direction. The most inefficient step in this process occurs when neutrons are emitted from the face of the neutron moderator uniformly in all directions, and only the small fraction, that happen to be going along the neutron beamline, make it to the sample position. Following a 1/r2 approach, it is simple to show that, for unguided beams, only one in ten million neutrons makes it to a sample position at 10 m from the moderator face. When the probability of interacting with the sample, probability of being analyzed properly (polarizers, crystals, etc.), and the probability of detection are factored in, it is easy to conclude that only 10-10 neutrons, or less, emitted from the moderator face actually contribute to a successful experiment. Some improvement is given by the “grooved” moderator concept, implemented at IPNS, ANL (USA), KENS, and ISIS-TS2 (UK) in which neutrons leaving the bright “groove” surfaces in the wrong direction are scattered back into the moderator from the “fins” and get another chance to be usefully directed. However, even grooved moderators provide only a modest increase in the useful neutrons reaching the sample position. Clearly there is ample room for improvement.

Nuclear Component and Proposed Work

Neutrons are produced by various means, from isotropic sources, generators, accelerators, research reactors and spallation sources. Scientists and other users of neutron beam are requesting more intense flux of neutron in specific wavelength, where their application will lead to improved knowledge and understanding of investigated materials. High energy neutrons, produced at research reactors or spallation sources, need to be moderated to reach the desired energy. Cold neutron production requires better understanding of neutron cross sections for old and new moderator materials. Simulations and combination of various modeling of reactions are mandatory to enhance the new moderators. Experiment at small scale facilities (small spallation source, or low flux research reactor) will bring the full understanding of moderator material behaviour in some controlled environment.

At several facilities research is underway to develop moderators which focus neutrons beams in a preferred direction as opposed to emitting neutrons isotropically. One key is thought to be the use of materials and geometries which may scatter neutrons anisotropically as a function of neutron wavelength. For example, recently the use of diamond nanoparticles reflectors for cold, very cold and ultracold neutrons revealed very promising results at the ILL (France), where significant increase of the neutron brightness was observed for wavelengths above 7 Å reaching a factor of 5 at 20 Å. Other similar studies are on-going at SNS (USA), JPARC (Japan), ISIS (UK), and elsewhere. It may be possible to use these materials on the moderator itself, or outside of the moderator, essentially extending the moderator along the direction of the extracted neutron beam.

Identifying and testing these anisotropically scattering materials is a critical step in the process. Small scale accelerator facilities at Sapporo (Japan), Bariloche (Argentina) and LENS (USA) are collaboratively developing new moderator experiments and simulations to improve available cold neutron fluxes. These facilities will be critical to the development of advanced moderators, including those with anisotropically scattering materials/geometries. The results need to be shared with larger spallation neutron sources and research reactors.

The experimental investigations need to be complemented by an adequate development of the theoretical/computational capabilities. Simulations of neutron transport within the target-moderator-reflector system of a spallation neutron source is traditionally carried out by means of particle transport codes such as MCNPX and PHITS. The simulation of the proposed directional enhanced neutron moderator systems cannot be performed using the current versions of these particle transport codes, as they do not describe the coherent neutron scattering underlying the scattering anisotropy of the moderator systems. It is therefore necessary to develop new computational tools that incorporate the physics of coherent scattering. One notable example of something that needs to be implemented in the current MCNPX framework is small angle scattering, which is vital for looking at these systems. The coupling of particle transport codes to raytracing codes such as McStas would allow ultimately the complete simulation of these complex systems, from the moderation to the neutron beam extraction.

The high energy neutrons are initially slowed-down by iterative Compton scattering to reach thermal energies below 100 meV. Additional cooling is obtained by neutron energy transfer into material internal modes, especially in low temperature materials (hydrogen, deuterium, methane, light and heavy water, mesitylene, ...). Accurate modeling of these processes require to improve the existing MCNPX/PHITS S(a,b) scattering kernel data base (dynamic structure factor) for moderator materials (liquids and powders). New or improved dynamic structure factor data will then need to be measured and simulated by means of molecular dynamic techniques. Additionally, super-mirror reflection, single crystal and small angle scattering kernels will have to be implemented in MCNPX/PHITS, possibly benefiting from low energy neutron propagation codes such as McStas, which provide advanced neutron scattering sample kernels for coherent, incoherent, elastic, and inelastic processes in the low neutron energy range.

CRP Overall Objective

Enhancement of cold neutron beam flux for applications in material research

Specific Research Objectives

1. Identify high albedo materials e.g. exploiting mesoscale scattering
2. Identify innovative geometries that enhance anisotropic neutron moderation
3. Improve accuracy of thermal-to-low temperature moderator material cross section data bases
4. Implement anisotropic scattering models within neutrons transport codes
5. Define optimal combination of materials, reflector and geometries
6. Perform experiments demonstrating gains in cold neutron brightness using the identified materials

Expected Research Outputs

1. Document materials with high albedo to be considered for experiments
2. Complete and document at least three experiments campaigns using high albedo materials
3. Implement improved scattering kernel for small angle and single crystal scattering in neutron transport codes
4. Document advanced moderator simulation models and compare to experiments

CRP Expected Research Outcomes

1. Identified new moderator materials and geometries which will enhance the production of cold neutron at research reactor and spallation sources by at least 50% for 10 Å neutron production.
2. Developed ability to model low temperature mesoscale physics in existing neutron transport codes.
3. Gained knowledge in moderator material data bases

List of potential participating countries

Argentina, Australia, Austria, Belarus, Brazil, Canada, China, Czech Republic, Denmark, European Union, France, Germany, Hong Kong - China, Hungary, Indonesia, Italy, Japan, Korea - Republic of, Malaysia, Netherlands, Poland, Romania, Russian Federation, South Africa, Spain, Sweden, Switzerland, United Kingdom, United States of America, Vietnam.