CRP F12026 on

"Advanced moderators for intense cold neutron beams in materials research"

SUMMARY

The proposed CRP aims at providing a platform for collaborative research among research reactors of various sizes and accelerator-driven neutron sources from TC eligible and developed countries to increase the cold neutron fluxes available at existing neutron sources. Cold neutrons are ideal tools to study almost all forms of condensed matter through neutron scattering and at the same time they are preferred in neutron imaging or Prompt-Gamma Neutron Activation Analysis (PGNAA). As such, they have attracted the interest of many research groups all over the world and the need for intense cold neutron beams is continuously increasing. To date, the major drawback in the application of cold neutrons is the very low efficiency in their production via different types of moderators. The need for higher cold neutron fluxes has led to various improvements in moderator shapes and designs. Still, however, a breakthrough in enhancing cold neutron fluxes is still pending and the solution to the problem requires new ideas regarding brand new moderator materials.

Making progress in this field will require coordinated research among several institutions, with activities ranging from the development of new simulation tools and associated data libraries to the experimental characterization of the scattering from nano-structured materials and the experimental investigation of candidate designs and materials in test moderators. We anticipate a CRP that includes experts on simulating neutron facilities with modern neutron transport codes from some of the world’s premier neutron sources, researchers at research reactors in developing countries who need experience with such codes, and researchers at facilities capable of testing new moderator designs experimentally. A key element in the program is identifying and characterizing the scattering properties of candidate materials, and assessing the influence of processing parameters on those properties. This materials survey task is one that is well suited to smaller research reactor or accelerator facilities in developing countries.

Background Situation Analysis

For more than 50 years research reactors and spallation neutron sources have been used for fundamental and applied research in the areas of material science, earth science and nuclear physics. The basic technique employed hereby is neutron scattering. To date, a host of innovative applications based on neutron scattering have tremendously improved our life standards. We mention here a few examples:

- Rechargeable batteries; Many of us rely today on tools like cell-phones or iPads. None of these gadgets would be user friendly without rechargeable batteries. The scientific base for this was laid decades ago, by studying magnetism in materials using neutrons.
- Hydrogen storage materials; Their design depends, among others, on the so-called Kubas interaction, which, roughly speaking, allows materials to storage at the molecular level as many as possible hydrogen atoms. This interaction, would have never been discovered without neutron scattering.

- Neutron radiography is the only non-destructive technique that can be used in Archaeology to image low Z materials inside high Z objects, e.g. wood inside metal. Neutron radiography is also used to study fuel cells.
- Small angle neutron scattering is heavily used by the detergent industry to study the formation of micelles in surfactants in solution, which helps them to improve their products.

Neutron scattering's success depends, among others, on the so-called spatial resolution, which appears to be the best when "cold", i.e. slow, neutrons are employed. Cold neutrons resulting from the slowing-down of thermal and fast neutrons have an energy from approximately 0.1 to 10 meV; the corresponding wavelengths are between 3 and 30 Angstroms. As such, cold neutrons are ideal tools to study almost all forms of condensed matter as their wavelengths match to the atomic spacing in solids and liquids and their kinetic energies are comparable to those of the thermal motions of atoms within the materials under investigation. Because of these features, cold neutron beams have attracted the interest of many research groups all over the world and the need for intense cold neutron beams is continuously increasing.

To date, the major drawback in the application of cold neutrons is the very low efficiency in the production of slow neutron beams. In fact, only a tiny fraction of the neutrons delivered by a research reactor or a spallation source directed to and exiting from the material ("moderator") that slows-down the fast neutrons will travel along the desired direction leading to the sample under investigation. Roughly speaking, when we deal with unguided neutron beams, i.e. when neutrons are emitted from the "face" of a moderator to all directions in space, then, only one in ten million neutrons reaches the sample positioned at 10 m away from the moderator face. In practice, only 10 to 100 neutrons, out of, typically, millions emitted from the moderator face actually contribute to a successful experiment. The need for higher cold neutron fluxes has led to various improvements in moderator shapes and designs, such as the so-called "grooved" moderators which proved to increase cold neutron fluxes up to a factor of 3. Additional solutions have also been proposed, such as the "convoluted" moderator in which layers of conventional moderating material is interleaved with single crystals of silicon. Bigger gains in cold neutron beam intensities have also been demonstrated using instrumentation based on neutron guides which act like light-pipes channelling neutrons down the instrument. Still, however, the performance of these guides is limited due to the relatively small angular acceptance and the susceptibility of the guide design to radiation damage (which limits how close to the moderator the guide may be positioned). In any case, a breakthrough in enhancing cold neutron fluxes is still pending and the solution to the problem requires new ideas regarding brand new moderator materials.

As of today, an intense research effort to develop moderators which focus neutron beams in a preferred direction is underway at several facilities. As an example, we mention here the recent idea to use high-albedo materials enabling multiple scattering at the mesoscopic scale, thus acting as the aforementioned neutron guides, however with much larger angular acceptance for long wavelength neutrons and much higher radiation resistance. In this context, the recent use of diamond nanoparticles at the ILL research reactor (France) proved as a very promising solution: a significant increase of the neutron brightness was observed for wavelengths above 7 Angstroms and an enhancement factor of at least 5 was achieved at 20 Angstroms.

Given these technological challenges, a consultant meeting entitled "Directionally focused moderators for enhanced neutron beam intensities to support materials research and applications" was held at the IAEA Headquarters in December 2010. It was followed by a technical meeting on "Advanced moderators to enhance cold neutron beam production for materials research and applications" that took place in November 2011 in Japan. In the first event, 34 international experts from 18 member states have participated, whereas in the second meeting 32 international experts from 14 member states contributed with scientific ideas and recommendations on how to address the problem of enhanced cold neutron fluxes. Based on the scientific outcome of these meetings and the corresponding recommendations, a new CRP coined "Advanced Moderators for Intense Neutron Beams in Materials Research" is herewith proposed. The present CRP aims at facilitating coordinated research among several institutions including research reactors of various sizes as well as accelerator driven neutron sources with the primary goal to develop and test the next generation of cold moderator / cold neutron extraction via anisotropic scattering materials. Within the CRP, collaborative work is expected to be implemented via two major actions: 1) simulations and computing and 2) benchmarking and demonstration experiments.

<u>Action 1</u> is of key importance to achieve the goal of the CRP, as it will contribute decisively to the conceptual design of advanced moderators. It will furthermore improve existing computational tools, associated data libraries, and simulate experiments. A tentative list of tasks may include

- Identification of the materials for moderator and reflector, and claddings capable of increasing the currently available cold neutron fluxes. Candidate materials are hydrogen, nanoparticles, mesitylene and others.
- Evaluation of codes capabilities for the selected materials; code improvements; generation of data libraries; codes combination; study of materials and geometry.
- Determination of (non-existing) scattering cross sections for the selected materials: New scattering kernels will be determined (if required) either by measurement or simulation with theoretical codes.
- Simulation of the proposed experiments to be performed within action 2.

<u>Action 2</u> will focus on the characterization of new moderators and validation of new setups. There are some initial ideas to start with, such as the construction of an optical device, much like the beginning of a ballistic neutron guide, or by using the moderator material as a high-albedo (for long wavelengths) reflector, driving neutrons of long wavelength leaving the moderator in some direction other than a beam line back into the moderator for a "second chance," or even redirecting such neutrons into the extracted beam directly. In any case, realization of action 2 would require experimental study of the component materials (the nanoparticle diamond) and of conceptual mock-ups.

The CRP has raised strong interest among modern large-scale facilities as well as smaller or medium scale research installations from developing countries, including CNEA-Bariloche (Argentina), ANSTO (Australia), CSNS (China), ILL (France), Budapest RR (Hungary), BARC (India), BATAN (Indonesia), J-PARC and Hokkaido University (Japan), KAERI (Korea), MNA/Selangor (Malaysia), Dubna and St. Petersburg (Russian Federation), NESCA (South Africa), ESS (Sweden), PSI (Switzerland), SNS/Oak Ridge, LANL and LENS-Indiana (USA). It is worth noting that, given the letters of interest and the contributions presented during the consultant and technical meeting, the distribution of tasks among the interested labs in the final composition of the CRP is expected to be well balanced, i.e. smaller labs will contribute not only with simulations and computing; instead they will play a key role in moderator prototyping and in the characterization of new moderators and validation of new setups via benchmarking experiments at their facilities (as they can offer more access time compared to the overloaded larger-scale infrastructures), as well as in common demonstration campaigns at large scale infrastructures.

Nuclear Component

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 already proven and new moderator materials. Simulations and combination of various modelling of reactions are mandatory to enhance the new moderators. Experiments at small scale facilities (small spallation source, or low flux research reactor) will bring the full understanding of moderator material behaviour in some controlled and well defined environment.

CRP Overall Objectives

Advancing intense cold neutron beams for materials research.

Specific Research Objectives

1. Increase the efficiency in the production of cold neutron fluxes at existing and planned cold neutron facilities by developing new moderators
2. Improve modern neutron transport codes and data libraries by implementing anisotropic mesoscale neutron scattering for new moderators

Outcomes

1. New moderator materials enhancing the production of cold neutrons identified and tested
2. Enhanced cold neutron beam production with developed moderators and associated improvements in materials research demonstrated
3. Advanced neutron transport codes and associated data libraries validated

Outputs

1. Identify up to five materials on the basis of their albedo, shape and composition as candidates for the development of advanced cold neutron moderators
2. Determine scattering cross sections via measurements (if non-existing) for the selected materials
3. Improve scattering kernel and treatment in (small angle scattering) neutron transport codes
4. Perform and analyze measurements of at least three experimental campaigns to characterize the candidate materials for cold neutron production
5. Simulate experiments and validate improved transport codes, including associated data libraries