Neutron Optics and Monte Carlo Simulation in NMI3

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Significant improvements in the performance of neutron instrumentation over the past decade have been enabled by the continuous development of innovative neutron optics and of Monte Carlo methods for modelling instrument performance. Two of the NMI3 Joint Research Activities (JRA) were therefore focussed on these areas.

Neutron optics

The Neutron Optics JRA was coordinated by Peter Böni from the Technische Universität München (TUM) with partners from PSI, LLB, CNR INFM (Perugia, Italy), Helmholtz Centre Berlin (HZB, previously HMI) and BNC. There were two main goals. The first was to develop and explore new focusing techniques based on either diffractive optics or the reflection of neutrons from surfaces coated with artificial multilayer structures (supermirrors). The second was to investigate specific possibilities for phase-space transformation.

We have developed two new small-angle neutron scattering (SANS) techniques which allow us to decrease the momentum transfer by one to two orders of magnitude while maintaining a high intensity, thus challenging the presently used U-SANS techniques based on perfect crystal optics. In the first technique, a multi-beam collimator has been developed, featuring 7 masks each with 51 pinholes. Test experiments, using a suspension of Latex spheres with a diameter of 225 nm, proved that the principle works, leading to the expected flux gains while maintaining the resolution. The second design, using multiplexing of highly collimated beams, makes measurements on objects with up to 50 microns diameter feasible. Each individual beam produces a SANS pattern in a different region of the area detector (Fig. 1), and these can then be summed to increase statistical accuracy. The tests were carried out at the beam line MIRA at FRM II, but other neutron scattering centres such as the ILL and PSI are now considering similar instruments, which are likely to play a significant role in the study of composite and hybrid materials, with direct connections to industrial materials.

A honeycomb collimator (^{10}Be coating on Al:Mg alloy) has been developed and installed on the BRISP spectrometer at ILL. A similar device will be installed on the new FSANS instrument at BNC. A new Fresnel zone plate with a diameter of 1 mm was designed at INFM and tested on the Morpheus beam line at PSI. The resolution of the device is 400 nm with an efficiency of 30% in the first diffraction order at a wavelength of 4 Å, in excellent agreement between theory and experiment. A Monte Carlo simulation code was developed to include the effect of the finite transverse coherence of the neutron source. These results are quite promising for the future use of Fresnel zone plates as focusing devices in real instruments (e.g. multi beam applications).

The Q resolution for inelastic neutron scattering experiments can often be relaxed, so concepts have been developed for focusing devices that concentrate the neutron beam by reflection from supermirror-coated glass tubes that are elliptically curved or from solid state Si-lenses. A flux gain of approximately 25 has been measured using neutrons with a wavelength in the range 3 Å $<\lambda<$ 6 Å.

Doubly focusing elliptic guides have been developed for the transport of neutrons from a moderator to an instrument: first prototypes showed over 5 times higher flux compared to regular neutron guides. Such an elliptic guide, 90 m long, has already been installed on the HRPD diffractometer at ISIS (Fig. 2), giving a flux increase of between 5 and more than 100 compared to the original Nickel guide (over 20 years old). An elliptic guide has also been installed on the WISH instrument at ISIS TS2; it is expected that elliptic guides will soon become the standard for many instruments.

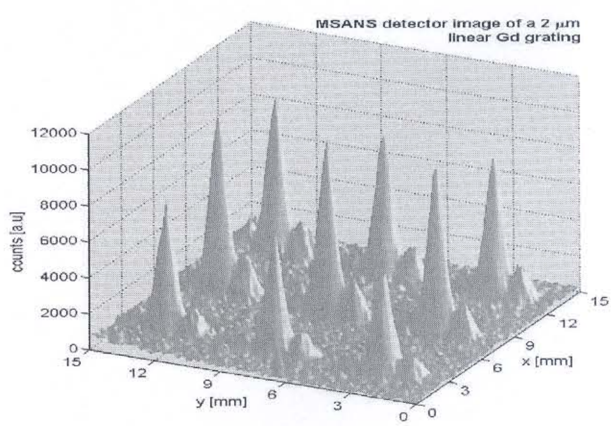

Figure 1. MSANS detector image of a 2 µm linear Gd grating. The first fringes from the grating diffraction pattern can clearly be seen on either side of the nine main peaks. (Picture courtesy of TUM).

Figure 2. The new elliptic supermirror guide of the HRPD beam line at ISIS. The insert shows the flux increase relative to the original Nickel guide. (Picture courtesy of ISIS).

Several key technologies had to be improved for achieving the project goals:

- Highly efficient absorbing and reflecting coatings were developed using magnetron sputtering in order to define well-collimated beams and to provide highly efficient transport and focusing of neutron beams, respectively.
- Atomically smooth coatings exceeding 2000 layers had to be optimised.
- Laterally and vertically graded interfaces were produced for parabolic focusing and as higher order filters, respectively. These systematic studies have led to an improvement of the coatings with respect to both the critical angle of reflection and the reflectivity.
- Reliable high resolution etching techniques had to be provided for the production of Fresnel lenses.
- Detailed simulations were performed for the solid state Si-lens and a precise holding and bending system was developed.

Another task of the project was to design, construct and build a phase-space transformation (PST) device for the acceleration of ultra-cold neutrons (UCN) to produce a beam of monochromatic cold neutrons, taking advantage of the high phase-space density that can be achieved by new UCN sources. The working principle is to use the Doppler-effect from one or several rotating crystals (highly oriented pyrolytic graphite contained in aluminium cassettes) that match the Bragg condition for most of the UCN. This is mechanically a very challenging problem due to the high crystal velocity required.

An important new aspect was the improvement of the PST design from a simple rotor to a double-handlebar (two-axis) rotor. This was necessary in order to decrease the velocity gradient along the surface of the reflecting crystal(s), which is high for the single-rotor case and a radius less than 2 meters. The Bragg condition requires a constant velocity at each point of the crystal surface belonging to a single Bragg angle and *d*-spacing. The double-handlebar rotor, with a radius less than 0.7 meter, would move the crystal in such a way that the surface remains parallel all the time. The velocity vector of any point of the crystal surface evolves according to a circular motion with one single radius instead of a continuum of radius values. However, the double-rotor option can only be tested after 2009. A single axis system has therefore been used for a proof of principle experiment.

Experiments were carried out at the ILL PF2-UCN source in April and May of 2008 and gave good results in comparison to the predictions of Monte Carlo simulations. Further experiments will be performed after commissioning of the new super-thermal UCN source at PSI. This should give a gain in UCN density of approximately 30 compared to ILL. Further detailed simulations are in progress to work out the detailed specifications of the experimental device and the possibilities of further optimisation by using intercalated PG crystals or altering the PST parameters.

Monte Carlo simulations

The JRA for Monte Carlo Simulations of Neutron Scattering Instruments – MCNSI – was coordinated by Kim Lefmann from Risø/Copenhagen University with partners from NPL (Czech Republic), ISIS, Helmholtz Centre Berlin (formerly HMI), PSI, ILL, Jülich and CNR (Italy). The 'back-bone' of MCNSI is the development and support of the three software packages for neutron ray-tracing Monte Carlo (MC) simulation: McStas, VITESS, and RESTRAX. The main tasks were to introduce new capabilities, including updated documentation, to test the packages by inter-comparison and comparison with experiment, and to develop the concept of virtual experiments. Software has been developed for all common platforms, including Windows, Linux, and MacOS, using the newest tools available for e.g. visualization and graphical user interfaces.

The improvement of the packages has had a large impact on their reliability and accessibility. The testing scheme has rendered the three packages in MCNSI the most trusted packages worldwide, and all neutron instruments under development around the world have been simulated using (at least) one of the MCNSI packages. In addition, the high level of documentation has increased the user base to cover a large fraction of all instrument scientists. Both McStas and VITESS have more than 100 unique downloads for each new version. They have made a major contribution to the success of the Neutron Optics and Polarised Neutron Techniques JRA (see separate article), with many of the new capabilities being specifically tailored to the needs of the technical developments in those projects.

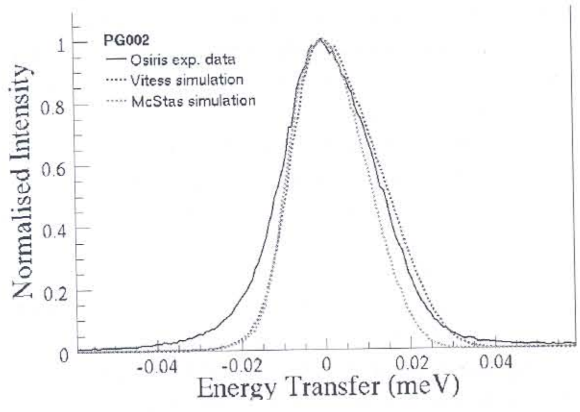

Figure 3. Comparison between McStas, VITESS and experiment for the resolution line shape on the OSIRIS instrument at ISIS (Picture courtesy of Peter Christiansen, University Lund).

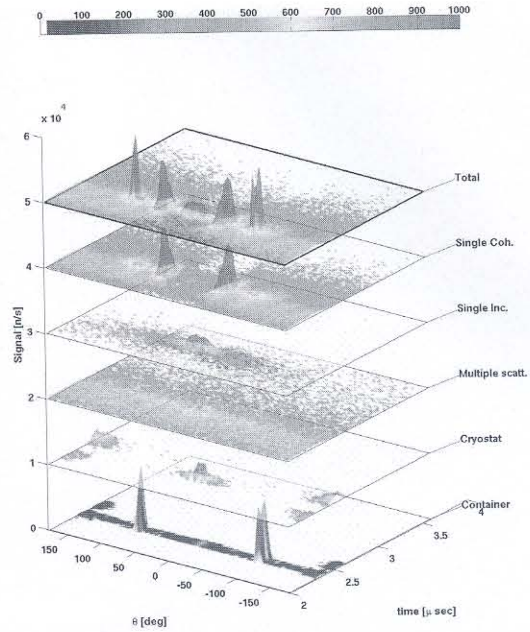

Figure 4. Virtual experimental data separating the scattering into contributions from sample, sample container, cryostat, and multiple scattering. This cannot be done for a real experiment and could have huge future benefits for experiment design and data analysis. (Picture courtesy of ILL).

The first major inter-comparison study was for the FOCUS spectrometer at the continuous spallation source SINQ (PSI). A very careful study compared the predicted flux along the length of the guide from McStas, VITESS, and RESTRAX with actual gold foil measurements. The second part of this work compared the measured flux and beam profile at the sample position using VITESS and McStas. The agreement was remarkably good, and the results agreed well with experiments apart from a 10% deviation in the absolute intensity.

The second major inter-comparison concerned the time-of-flight backscattering spectrometer OSIRIS at ISIS. Comparisons were made between VITESS, McStas and experiment. The agreement was very good and, despite the rather complex analyzer geometry, the experimental resolution function was reproduced to within 3–4% (Fig. 3). These simulations have raised a question as to the absolute flux of the real ISIS hydrogen moderator, which still needs to be settled.

The bottom line of the inter-comparisons is that the packages agree very well. Line shapes and resolutions are within 2–3% and absolute fluxes within 5%. Comparison with experiments is also good, resolutions being within 5% and intensities in general within 10–30%. Most of the latter discrepancy is attributed to uncertainties in the actual design of aged moderators and guides. Due to the quality of these results, MC simulations have become a widespread and trusted tool for designing neutron instrumentation.

The main future impact of MC instrument simulation clearly lies in the area of virtual experiments. The objective within MCNSI has been to develop tools for simulations of complete experiments, including scattering from model samples. This has been extremely successful and much more work has been performed than was originally planned.

One example is a simulation of the proposed upgrade of IN20 (ILL) to a flat-cone geometry. Here, a virtual experiment was performed using RESTRAX simulations, leading to the acceptance of the proposed upgrade. Another example is the virtual powder experiment performed for the proposed time-of-flight diffractometer EXED at HZB. It was shown that the performance was superior to existing instruments. The most remarkable examples have been performed by ILL, using the new capabilities in McStas for simulating sample environment and multiple scattering. For a virtual time-of-flight experiment using the IN6 spectrometer, the scattering data could be separated into contributions from sample, sample container, cryostat, and multiple scattering (see Figure 4). This approach could have a great impact on future data analysis schemes.

In a handful of years from now, virtual experiments will be used for a number of tasks closely related to the performance of actual experiments, e.g. instrument design, beamtime/proposal preparation, on-the-fly interaction with experiments, data analysis, teaching/training and outreach. A virtual experiment beamtime planner has already been installed at the powder diffractometer DMC at PSI. The first neutron course based on virtual experiments (related to PSI instruments) has been running at the University of Copenhagen since 2005 and in 2007 received the Niels Bohr Institute teaching award.

An article summarizing the use of virtual experiments written by all MCNSI members (and a few more co-authors) was recently accepted by the Journal of Neutron Research.