

Neutron Instrument Simulation

Ray tracing is becoming more and more an essential tool to project new instruments as well as in the upgrade of the existing ones. Considering the potential development of neutron activities related to the European neutron source, the OGG is devoting part of its resources to the creation of expertise in instruments ray tracing. With this aim a collaboration among the OGG, the Neutron Optics Groups of ILL and the Scientific Software Group of ESRF has started. The OGG is also partner of the European project SCANS devoted to this topic.

Simulation of the upgrade of the backscattering spectrometer IN13 at ILL (C. Mondelli)

IN13 is a spectrometer particularly suited for the study of the local dynamics of soft matter, such as polymers and biological systems, as it covers a large momentum transfer range ($0.3 < Q(\text{\AA}^{-1}) < 5.5$) with an energy resolution of few μeV . In the present configuration the performance of the instrument is overall limited by the low incident flux, so a progressive upgrade of IN13 is planned in order to improve the incident flux and the instrument versatility. In this way, different possibilities other than the present standard configuration will be available in order to allow the user to define the best compromise between flux, energy resolution and Q-range for each experiment.

The first step of this project consists of simulating the instrument and the different modifications envisaged in order to verify our ideas and to determine which are the most promising modifications and the possible degradation of certain characteristics of the instrument such as the energy resolution (see Fig.1). Thus we have performed Monte Carlo simulations (using the McStas package) of the primary spectrometer. The results show that we can obtain on IN13, in particular conditions (using supermirrors guides, small samples out of the backscattering), a gain in neutron flux up to a factor of 12.

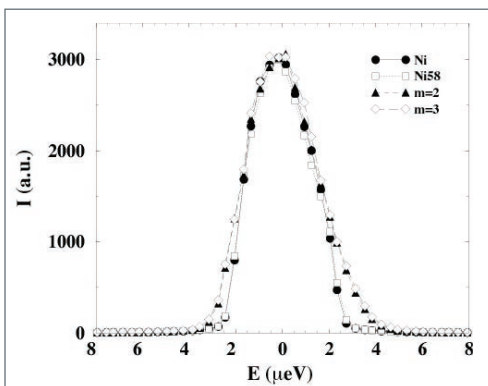


Fig.1 Effect of the change of the neutron guide reflectivity proposed in the ILL project of replacement of the guides (the curves are normalized at the maximum). The results show that the FWHM of the energy distribution of the neutrons arriving at the sample position does not change significantly with the use of supermirror guides in place of the present guides coated with Ni.

Modeling non-perfect crystals (L. Alianelli)

The crystal monochromator is often the heart of a neutron instrument. We are developing simulation tools for calculating the diffraction properties of non-perfect crystals. The aims are: 1) to compare the calculations results to the performance of real crystals, measured both with neutrons and x-rays; 2) to predict which is the effect of different kinds of deformation (mosaic, bent or d-spacing gradient) on the properties of the reflected beam.

New methods are being developed at the ILL and elsewhere for the production of bent perfect and bent mosaic crystals: an example of calculated, simulated and measured rocking curves is given in Fig. 2. This work is carried out in close collaboration with M. Sanchez del Rio of the ESRF and with the Service for Neutron Optics of the ILL.

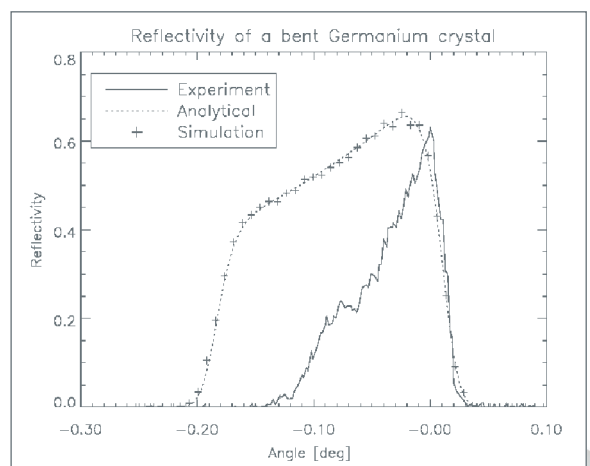


Fig. 2 Neutron reflectivity of a Ge crystal, $\langle 331 \rangle$ reflection at 27meV in Bragg symmetric geometry. The crystal is cylindrically bent with a radius of curvature $R = 5\text{ m}$. The crystal used for the experiment is obtained by assembling 10 wafers. The wafers are glued and plastically deformed in the hot press of the Monochromator Laboratory of the ILL. The simulation is done by using the Monte Carlo method.