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A method for detailed simulations of neutron diffraction from imperfect crystals

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Abstract

An upgraded version of the McStas Monochromator-curved module is presented. The new component, called Monochromator-reflect, is based on the use of input files for interpolating the neutron reflection and transmission probabilities according to the theoretical reflectivity of the crystal. These probabilities depend on the energy and angle at the crystal surface and also on the crystal mosaicity, geometry, material scattering cross-section, attenuation coefficient, and Bragg planes. We present details of the algorithm and definitions which are essential for a correct use of the module and show the improvements that it offers.

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1. Introduction

McStas [1] is a widely used tool for the simulation and design of neutron instruments. It exploits a large component library, a part of which results from users' original contributions or upgrade of existing modules. A crucial part of the instrument simulation is, in many cases, the exact computation of the monochromator or analyser crystal reflectivity, which defines the monochromated intensity and the resolution in reciprocal space. In this work we present a new crystal component, called Monochromator-reflect [2]. It is based on Monochromator-curved [3], with an improved treatment of the reflectivity, and allowing a detailed description of crystals with mosaicity of the Bragg planes and spatial variation of the d-spacing. The focusing slab geometry, which is well described in Monochromator-curved, has not been modified. None of the two versions is appropriate for simulating elastically bent perfect crystals. Neither imperfect crystals in asymmetric

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or transmission geometry are included. We carry out a benchmarking of the component by comparison with the Monochromator-curved component.

2. Computation method and examples

Monochromator-curved is a ray-tracing module, i.e. a code in which the Monte Carlo method is used to choose the fate of a ray impinging on the crystal. The crystal has no thickness, hence the beam penetration and secondary extinction are not simulated. There are two input parameters required for describing the crystal reflectivity: peak reflectivity $R0$ and mosaicity *mosaic*. These are used to build a probability distribution of the reflected rays versus the grazing angle. In Monochromator-curved, the input parameter *mosaic* is the full-width at half-maximum (FWHM) of the reflectivity profile. The same parameter *mosaic* is used for sampling the additional divergence of the outgoing beam. Hence, in the original Monochromator-curved code, there is not a clear distinction of the difference between the two different concepts of mosaicity and FWHM of the reflectivity profile. In the new component, we use a more suitable definition of mosaicity: η is the intrinsic mosaicity, i.e. the FWHM of the angular distribution of the small perfect crystallites in the mosaic crystal. The theory [4] shows that the FWHM and peak value of the reflectivity profile are functions of the crystal intrinsic mosaicity η, but depend also on other parameters, like thickness, scattering and attenuation factors. It is important, therefore, when simulating a mosaic crystal, to use weight distributions (or reflectivities) that have the correct dependence on energy and angle. This is not possible when using Monochromator-curved. Concerning the angular

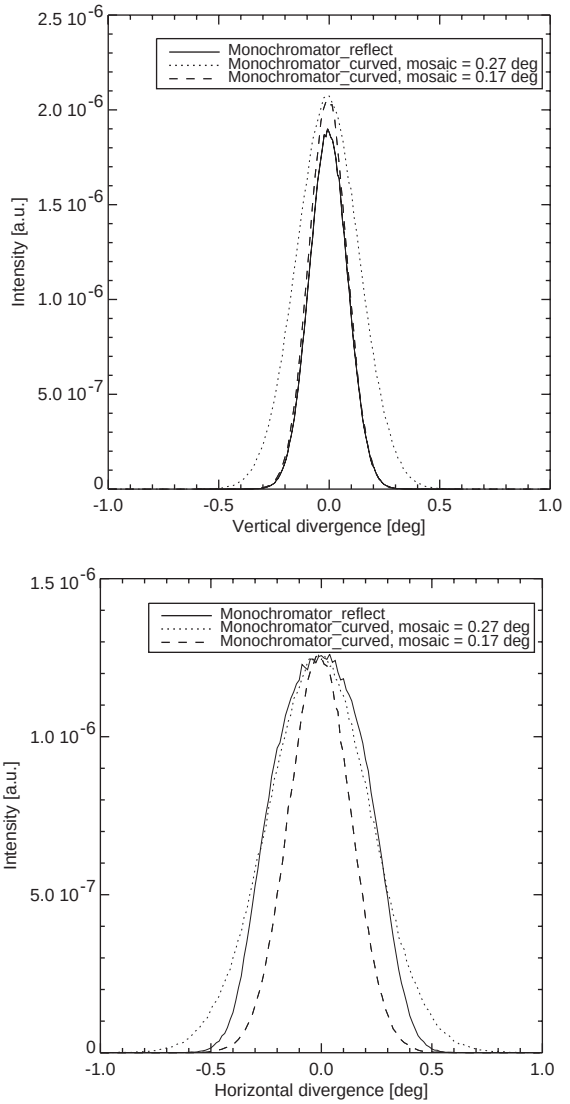

Fig. 1. Divergence profiles after reflection by a mosaic crystal Cu 220 with $\theta_{\mathrm{Bragg}} = 37.5^\circ$, $\eta = 10' \sim 0.17^\circ$, simulated with Monochromator-reflect (solid lines) and Monochromator-curved (dotted and dashed lines). The incident beam is highly collimated and non monochromatic. TOP: Monochromator-reflect gives a vertical divergence distribution with FWHM equal to $0.20^\circ = 2\eta \sin\theta$. The profile calculated with Monochromator-curved has FWHM of 0.33°. This result is due to the ambiguous definition of mosaicity in Monochromator-curved, i.e. FWHM of the reflectivity curve, rather than intrinsic mosaicity. The dashed curve, obtained by using *mosaic* $= \eta$ as input parameter for Monochromator-curved, provides the correct outgoing vertical divergence. BOTTOM: the FWHMs of the horizontal divergence distributions agree well, except that the Monochromator-curved simulated data have a Gaussian shape (the fit is not shown), which in general does not correspond to reality. The horizontal resolution, in fact, is determined by the shape of reflectivity. The use of *mosaic* $= \eta$ with Monochromator-curved (dashed line) gives a smaller divergence.

behaviour, we recall that the reflectivity does not necessarily follow a Gaussian profile, as assumed in Monochromator-curved, even when the mosaic distribution is a Gaussian. In Monochromator-reflect we use input files for the reflectivity, that are created by a program [5] that provides the analytical solutions of the Darwin equations [6], with the possibility to correct for primary extinction. The reflectivity profiles include secondary extinction and have the correct theoretical dependence on all the crystal parameters: material cross-section and attenuation coefficient, Bragg planes, Debye-Waller factor, mosaicity and grazing angle θ. As stated above, a correct definition of mosaicity is important, not only because it determines the reflectivity, but also because it produces an additional angular spread of the beam.

In the ideal case of a perfectly collimated incident beam, the divergence of the reflected beam in the plane perpendicular to the scattering, is equal to $2\eta \sin\theta$. This result can be explained by geometrical arguments and has been confirmed by detailed simulations using the Monte Carlo method applied to the beam interaction with the microscopic crystallites forming a mosaic crystal [7]. This is clearly seen in Fig. 1, where a mosaic copper 220 is set to reflect a collimated and non monochromatic neutron beam with $\lambda_{\text{average}} = 1.6$ Å. The mosaic distribution is a Gaussian with $\eta = 10' \sim 0.17^\circ$. The simulation performed with Monochromator-reflect shows that the average vertical divergence (top) of the beam increases to $0.20^\circ = 2\eta \sin\theta$, whereas Monochromator-curved gives 0.33°. In both cases, the profiles are Gaussians. The horizontal divergence depends on the shape of reflectivity versus energy and angle. The Monochromator-curved data (Fig. 1, bottom) have a Gaussian behaviour which does not correspond to reality. It is seen that, even for the simple case of an isotropic mosaic crystal, Monochromator-curved cannot exactly reproduce the horizontal and vertical beam divergence at the same time.

For the case of anisotropic mosaic crystals, the description in Monochromator-curved is even more unrealistic. In these crystals, in fact, the peak reflectivity and the FWHM depend on the azimuth, i.e. the ϕ rotation of the crystal around the diffraction vector. The input files used in Monochromator-reflect contain reflectivity in the horizontal and vertical planes and hence give more realistic results. The upgraded McStas module allows also the simulation of crystals with a variation of the d-spacing. The REF.pro [5] code can provide input files with the correct deformed crystal reflectivities. For this, it uses an algorithm developed in the framework of the layer-coupling model [8], allowing a solution of the Darwin equations in layered media.

3. Conclusions

The use of Monochromator-reflect allows better simulations of imperfect crystals with McStas. When used together with the REF.pro program, gradient and mosaic (isotropic and anisotropic) crystals can be accurately modeled. This description includes, by definition, secondary extinction. Primary extinction can also be simulated, if appropriate correction factors are used. The penetration of neutrons in the bulk crystal, and the consequent spread of the beam at the exit surface due to secondary extinction, is not simulated because of the infinitely thin crystal approximation. Hence, a further improvement of the code, with thickness included, is envisaged. Moreover, other geometrical details will be added, allowing the simulation of asymmetric reflections, including Laue (or transmission) geometry, that are often used in neutron instruments.

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