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A novel Monte Carlo algorithm for simulating crystals with McStas

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Abstract

We developed an original Monte Carlo algorithm for the simulation of Bragg diffraction by mosaic, bent and gradient crystals. It has practical applications, as it can be used for simulating imperfect crystals (monochromators, analyzers and perhaps samples) in neutron ray-tracing packages, like McStas. The code we describe here provides a detailed description of the particle interaction with the microscopic homogeneous regions composing the crystal, therefore it can be used also for the calculation of quantities having a conceptual interest, as multiple scattering, or for the interpretation of experiments aiming at characterizing crystals, like diffraction topographs.

Keywords: Neutron monochromators and analyzers; Monte Carlo method; Bragg scattering; Mosaic; Bent and gradient crystals

1. Introduction

The technical and economical effort needed to build or renew a neutron instrument requires to have a precise and accurate idea of the effect of each optical element on the neutron beam. Moreover, the cost needed for increasing diffracted intensity of optical elements like crystals and multilayers, cannot be compared with that needed to increase the neutron source intensity. These are the principal reasons for the importance of modelling neutron optical elements. Modelling of a complete neutron instrument can be done in several stages: as a first step one can make a precalculation of the effect of the individual optical elements. For this the neutron optics package NOP [1] that we have developed can help. Ray-tracing and Monte Carlo are numerical methods used when a more detailed description is needed both for designing or up-grading neutron instruments and when calculating the experimental resolution. Almost all simulation codes [2–4] work using the sequential ray-tracing method. The source, i.e. the starting point for the simulation, is generated by random sampling the ray distribution in terms of energy position and angles. The other elements are modelled assuming that the neutron tracks are linear (or parabolic, if gravity is included) segments between one element and the next. At each instrument stage, the neutron trajectory is modified according to a macroscopic law governing the diffraction or transmission by this element. Finally, the description of some

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devices can be done by ab-initio modelling, using measured reflectivity or transmission profiles. Although this method has many advantages as high flexibility, it is limited by the fact that the measured properties of the optical device are not universally valid. For example, the crystal reflectivity profile measured at a given energy cannot be extrapolated to other energies because the extinction and absorption may be strongly dependent on energy. We present an original simulation tool for describing Bragg diffraction by crystals in a realistic way. The novelty of our method consists in the accurate microscopical description of the interaction of the "rays", representing the neutron beam, with the microscopic crystal regions. The difference with respect to other ray-tracing crystal modules is that our code calculates the full history of the rays and does not use any average or macroscopic law. Thus it is very realistic, allows an accurate control of all the calculation parameters and can be used for crystals having any kind of distortion, for example inhomogeneities of the mosaic structure, bending of the Bragg planes and variation of the d-spacing. Possible applications of the code are: estimating the different behaviour of mosaic, gradient and bent crystals, computing important quantities like multiple scattering, extinction lengths and the outgoing beam spatial and angular distribution. Moreover one can monitor the properties of the beam at any stage of the calculation, and compute images which can also be measured in an experiment, like diffraction topographs [5,6]. A full benchmarking of the algorithm against analytical models has been performed for some well-defined cases, with monochromatic and collimated incident beams. The codes described in this paper, called MOSAIC, BENT AND GRADIENT, originally written in $F77$, is now translated in C, in order to be interfaced to McStas [2], and can therefore be used for simulating neutron crystal monochromators and analyzers.

2. The algorithm

Let us consider the simulation of diffraction by a mosaic crystal as represented in Fig. 1. We

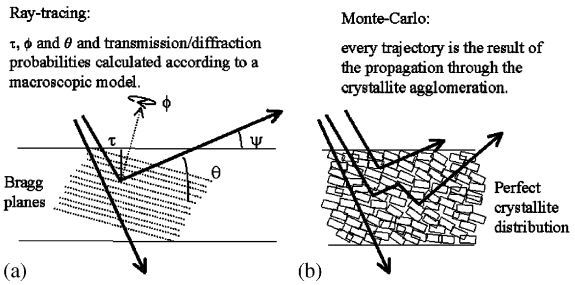

Fig. 1. Schematic representation of modelling diffraction by a mosaic crystal: ray-tracing (a) and Monte Carlo method proposed in this paper (b).

discuss here the two possible approaches for the case of a mosaic crystal because this is usually the optical element that requires a full physical description in a neutron instrument. The crystal is composed of an agglomeration of small perfect crystallites with their angular orientation following a distribution $W(\Theta, \Phi)$ not shown explicitly in the figure. The ray-tracing calculation of diffraction by this crystal uses a macroscopic approach [3,7,8] as schematically shown in Fig. 1a: (1) the particle penetration depth τ is sampled by a probability distribution depending on the secondary extinction and absorption depths; (2) the value of the angle θ formed by the Bragg planes and the emerging particle is sampled using the mosaic distribution $W(\Theta, \Phi)$ and considering that the Bragg's law must be satisfied; the emerging angle ψ is determined by θ and by the asymmetry angle between the Bragg planes and the crystal surface; (3) the azimuthal angle ϕ is also calculated by using $W(\Theta, \Phi)$, or a constant probability distribution if the mosaicity is isotropic, i.e. not dependent on Φ; (4) finally the probability or weight of the emerging particle being diffracted is sampled from analytical formulas depending on the absorption coefficient, strength of the reflection, Debye Waller factor, etc.

The novel Monte Carlo algorithm described in this paper, sketched in Fig. 1b, does not require any assumption on the macroscopic laws mentioned above. It provides numerical solutions of the Darwin's equations [9,10], that describe the transport of neutrons or X-rays in imperfect crystals. The input parameters are: crystal size, set of Bragg planes, mosaic distribution, bending

radius or d-spacing variation, size of the perfect domains and, if necessary, imperfections like inhomogeneities. A schematic representation of the code structure is shown in Fig. 2. A large number of particle's trajectories is simulated, inside a crystal of thickness d. The simulation of the each trajectory is done in steps. At each step the particle interacts with a crystallite as drawn in Fig. 3. The crystallite's orientation **N** is sampled by the distribution $W(\Theta,\Phi)$ thus giving the angle θ formed by the incident direction and the crystallite surface. The fundamental quantities governing the particle's fate are $R(\theta)$ and $T(\theta)$, that are respectively the probability of the particle being reflected or transmitted. These are calculated according to the dynamical theory of diffraction [11] and depend on the material, the Bragg planes, and the crystallite thickness t. The particle is followed until it intersects one of the crystal surfaces. The effect of absorption is included by assigning a weight or probability to the particle, which is calculated as $weight = e^{-path\times\mu}$, with *path* being the total path length and μ the absorption coefficient. This method of accounting for the effect of absorption is not an approximation: at the stage of the particle–crystallite interaction the absorption is present in $R(\theta)$ and $T(\theta)$. The final values of the particle coordinates (x, y, z), direction cosines (v_x, v_y, v_z), path length, and number of reflection events inside the crystal are written in a file. The case of an anisotropic mosaic distribution is handled, in the MOSAIC program, by using the

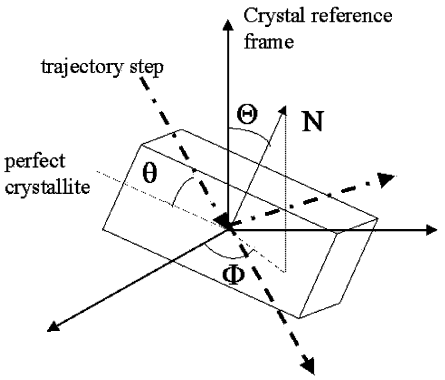

Fig. 3. Interaction between the particle and the crystallite. The probability associated to the two possible events (diffraction or transmission) are calculated according to the dynamical theory of diffraction. The Θ and Φ angles sampled, for each crystallite met by the particle, by the mosaic distribution $W(\Theta,\Phi)$.

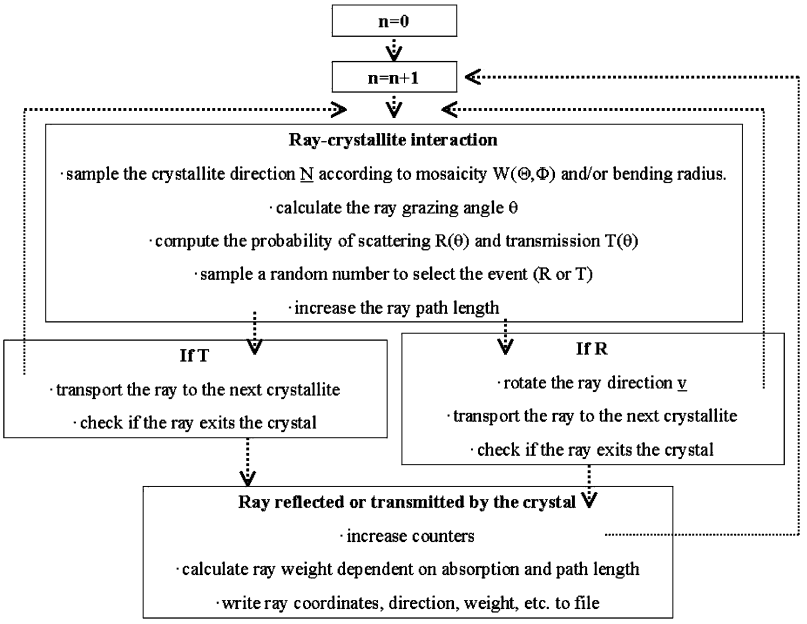

Fig. 2. Structure of Mosaic, Bent and Gradient crystal modules.

following probability distribution for the polar and azimuthal angles:

$$W(\Theta,\Phi) = \mathrm{e}^{-4\log 2\,\Theta^2[\sin^2\Phi/\eta_s^2+\cos^2\Phi/\eta_p^2]}, \quad (1)$$

where η_s and η_p are the FWHMs in the scattering plane and perpendicular to it, respectively.

By definition, this method allows us to know the complete history of each particle: how many scattering events it has undergone (and also at what spatial coordinates), the maximum depth it has reached in the crystal slab, and the total path length. These important quantities are related to multiple scattering and secondary extinction.

The BENT code used for simulating the diffraction properties of mosaic crystals in which there is a variation of the Bragg planes orientation along one direction is similar to the MOSAIC code for the undistorted mosaic crystal. It has simply been modified in the part concerning the surface and Bragg plane orientations. If we suppose that the crystal is cylindrically (and elastically) bent to a radius R, then the deviation of the Bragg planes from the orientation they have in the undistorted crystal, [12,13]:

$$\varepsilon_{\mathrm{Bent}} = \frac{|z|}{R}\,(\cot\theta - \nu\tan\theta_{\mathrm{Bragg}}), \quad (2)$$

where θ is the ray grazing angle, ν the Poisson's ratio and $|z|$ the depth below the incidence crystal surface. The first term on the right side of Eq. (2) is geometrical and the second accounts for the fact that, if the crystal density stays constant, then there is a linear variation of the d-spacing.

In the case of gradient crystals Eq. (2) is replaced by an expression accounting for the deformation due to the d-spacing variation $d_{hkl}(z)$:

$$\varepsilon_{\mathrm{Gradient}} = -\frac{d_{hkl}(z) - d_{hkl}(0)}{d_{hkl}(z)}\tan\theta_{\mathrm{Bragg}}. \quad (3)$$

This program can also be used for simulating bent or gradient crystals without any mosaicity: in this case the ray trajectory is no longer determined by interactions with the crystallite agglomeration as described above. The fundamental steps of the trajectory take place between one perfect lamella and the next. The lamella thickness is an input parameter for the simulation, it is a function of R, ν or Δd_{hkl} (deformation), Bragg angle and Darwin width, and is calculated as in the frame of the lamellar model [14]. The fundamental assumption is that each lamella is homogeneous, that it diffracts as a small perfect crystal according to the dynamical theory, with the Bragg angles following Eqs. (2) or (3).

3. Conclusions

The simulation scheme that we propose can provide important parameters, like the number of scattering events or real path length inside the crystal, which cannot be determined analytically or by other numerical means. Knowledge of these quantities is important especially, when computation of the crystal efficiency as a monochromator for high resolution instruments is needed. They can be used also for X-ray diffraction, provided that correct input parameters describing the dynamical diffraction by the small perfect crystallites, are used. This algorithm uses the crystallite size as an input parameter, therefore it describes correctly primary extinction.

The limits of applicability of the method we have presented are found in those cases where the description of the beam amplitude, rather than the intensity, is needed. In other words, when we talk of simulated trajectories or simulated particles we deal with something which resembles energy transport (intensity) in the crystal, rather than waves (amplitudes). Therefore these simulations cannot be used to calculate interference effects, such as appear in perfect crystals or crystals having a very small mosaicity, which is of the order of the perfect crystal Darwin width [11].

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