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Supplementary Material for *Optimum velocity of a phase space transformer for cold neutron backscattering spectroscopy*

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Here we provide supplementary material for the implementation of the numerical methods quoted in the paper.

1. Bragg reflection on a mosaic crystal

To mathematically describe the Bragg reflection of neutrons on a mosaic crystal, we consider a polychromatic and divergent neutron beam, denoted by a single random wavevector $\mathbf{k}$ impinging on a mosaic crystal with lattice spacing d. As first step, we assume an isotropically reflecting powder. Hence, an impinging neutron will find a crystallite in the powder with an orientation such that the condition for Bragg reflection is fulfilled. By assigning a probability for reflection according to the Sears equation (Sears, 1997a; Sears, 1997b) we can then readily reduce the powder to a mosaic crystal. For each neutron with wave vector $\mathbf{k}$ the reciprocal lattice vector $\mathbf{Q}$ of the crystallite is determined by the set of equations:

$$\begin{aligned} \mathbf{k}_f &= \mathbf{k} + \mathbf{Q} \\ ||\mathbf{k}_f|| &= ||\mathbf{k}|| \quad \text{and} \quad ||\mathbf{Q}|| = \frac{2\pi}{d}. \end{aligned} \tag{1}$$

Given $\mathbf{k}$ and d, and be $\mathbf{Q}_0$ a solution of the equations 1, the continuous set of all possible solutions is obtained by rotating $\mathbf{Q}_0$ about the incident wave vector $\mathbf{k}$ with an angle $\varphi \in [0, 2\pi]$,

$$\mathbf{Q}(\varphi) = \exp\left(\varphi \frac{\mathbf{k}}{||\mathbf{k}||} \wedge\right) \mathbf{Q}_0 \tag{2}$$

where $\exp\left(\varphi \frac{\mathbf{k}}{||\mathbf{k}||} \wedge\right)$ acts as a rotational operator and $\wedge$ denotes the vector cross product.

It remains to find an arbitrary solution $\mathbf{Q}_0$. It is possible to solve equation 1 in two dimensions and construct from this result the three-dimensional solution to equation 1. In the following all vectors are considered to be elements of the two-dimensional space. We expand $||\mathbf{k} + \mathbf{Q}||^2 = ||\mathbf{k}_f||^2$, and by introducing the angle θ between $\mathbf{Q}$ and $\mathbf{k}$ we obtain

$$\mathbf{k} \cdot \mathbf{Q} = Q\,k\,\cos(\theta) = -\frac{Q^2}{2}. \tag{3}$$

This relation enables us to generate $\mathbf{Q}$ by both scaling and rotating $\mathbf{k}$ about the point of origin by an angle θ:

$$\mathbf{Q} = \frac{Q}{k} \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix} \mathbf{k}. \tag{4}$$

Using equation 3 to express θ in terms of Q and k yields

$$\mathbf{Q} = -\frac{Q^2}{2\,k^2} \begin{pmatrix} 1 & -\sqrt{\frac{4\,k^2}{Q^2} - 1} \\ +\sqrt{\frac{4\,k^2}{Q^2} - 1} & 1 \end{pmatrix} \mathbf{k}. \tag{5}$$

For a physical solution we have to require that the matrix has no complex entries, which is fulfilled if

$$Q^2 \leq 4k^2 \Leftrightarrow Q \leq 2k \Leftrightarrow \lambda \leq 2\,d \tag{6}$$

which coincides with Bragg's law. Finally we construct a solution in the three-dimensional space by projecting the wavevector onto the inclined plane that is perpendicular to the XY-plane. To this end, we introduce an isomorphism, consisting of a polar transformation and the identity function:

$$\mathbf{k} \to \begin{pmatrix} \varphi \\ \mathbf{k}_2 \end{pmatrix} = \begin{pmatrix} \arg(k_x, k_y) \\ \sqrt{k_x^2 + k_y^2} \\ k_z \end{pmatrix} \tag{7}$$

and its corresponding inverse

$$\begin{pmatrix} \varphi \\ \mathbf{k}_2 \end{pmatrix} \to \mathbf{k} = \begin{pmatrix} k_{xy} \cos\varphi \\ k_{xy} \sin\varphi \\ k_z \end{pmatrix} \tag{8}$$

We transform the three-dimensional wavevector $\mathbf{k}$ using the coordinate transformations 7, obtaining both the two-dimensional wavevector $\mathbf{k}_2$ and the angle φ. For the given $\mathbf{k}_2$ we calculate the corresponding $\mathbf{Q}_2$ using equation 5. Transforming φ and $\mathbf{Q}_2$ back to the three-dimensional space by using equation 8 results after some algebraic manipulations in

$$\mathbf{Q} = -\frac{Q^2}{2k^2} \left\{ \mathbf{k} + \frac{1}{Q} \sqrt{\frac{4k^2 - Q^2}{k_x^2 + k_y^2}} \begin{pmatrix} k_x k_z \\ k_y k_z \\ -k_x^2 - k_y^2 \end{pmatrix} \right\}. \tag{9}$$

With this, we have one arbitrary solution $\mathbf{Q}_0$ to equation 1. The continuous set of all possible solutions is then generated by means of a rotation as described by equation 2. Among all possible $\mathbf{Q}$ we chose the one which is in the scattering plane orthogonal to the crystallite surface, which is precisely $\mathbf{Q}_0$ due to its construction. Finally, we obtain:

$$\mathbf{Q}(\mathbf{k}) = -\frac{Q^2}{2\,k^2} \left\{ 1 + c \begin{pmatrix} k_z & 0 & 0 \\ 0 & k_z & 0 \\ -k_x & -k_y & 0 \end{pmatrix} \right\} \mathbf{k} \tag{10}$$

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with

$$c = \sqrt{\left(\frac{4\,k^2}{Q^2} - 1\right) \,/\, \left(k_x^2 + k_y^2\right)}. \qquad (11)$$

2. Monte Carlo Algorithm

We employ a Monte Carlo simulation in order to estimate the distribution of wavevectors after the neutrons passed the PST. For this purpose, we generate first a set of random neutrons described by a wavevector $\mathbf{k}$, a position $\mathbf{r}$ and a weight p. The random wavevectors $\mathbf{k}$ are drawn from an appropriate distribution function such that they have the required divergence and polychromaticity. The weight p of all neutrons is initially set to unity and the total of all weights corresponds the the flux of the neutrons. After performing a raytracing by shifting the position $\mathbf{r}$ of the neutrons such that they hit the crystal surface, their wavevectors are transformed by

$$\begin{aligned} \mathbf{r}' &= \mathbf{r} \\ \mathbf{k}' &= \mathbf{k}' + \mathbf{Q}(\mathbf{k}' - \mathbf{K}) \\ p' &= R \cdot p \end{aligned} \qquad (12)$$

where $\mathbf{K}$ corresponds to the velocity of the crystal as defined in the paper and R is the Sears reflectivity (Sears, 1997a; Sears, 1997b) taking the mosaic structure of the crystal into account. The momentum transfer vector $\mathbf{Q}$ is calculated using equation 10.

References

Sears, V. (1997a). *Acta Crystallographica Section A*, **53**, 35–45.
Sears, V. (1997b). *Acta Crystallographica Section A*, **53**, 46–54.