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Neutron forward diffraction by single crystal prisms

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Abstract. We have derived analytic expressions for the deflection as well as transmitted fraction of monochromatic neutrons forward diffracted by a single crystal prism. In the vicinity of a Bragg reflection, the neutron deflection deviates sharply from that for an amorphous prism, exhibiting three orders of magnitude greater sensitivity to the incidence angle. We have measured the variation of neutron deflection and transmission across a Bragg reflection, for several single crystal prisms. The results agree well with theory.

Keywords. Single crystal prism; neutron diffraction; neutron deflection.

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1. Introduction

Prisms of most materials produce neutron deflections in the arcsecond regime [1,2]. In a single crystal prism, for neutron incidence close to a Bragg reflection, coherently coupled incident and diffracted wave components propagate together, separating only on exiting the prism into forward diffracted and diffracted beams, respectively [3–5]. As the Bragg reflection is approached from either side, the deflection of the forward diffracted beam changes monotonically from its off-reflection (amorphous-prism) value, reaching an extremum at either end of the total reflectivity domain. We present here calculated and measured variations of the deflection and intensity fraction of neutrons forward diffracted by single crystals.

2. Theory

We consider neutron incidence on a single crystal prism at $\theta = \theta_{\rm B} + LR/k_0$ outside the total reflectivity domain, viz. $|y| > 1$, in an asymmetric Bragg configuration (figure 1) with a wave vector **RO** of magnitude k_0 in vacuum. Here $y = (\theta - \theta_{\rm c})/w$ symbolizes the reduced incidence angle, $\theta_{\rm c}$ and w representing the centre and the half-width, respectively of the domain of total reflectivity [4]. $\theta_{\rm B}$ and $\theta_{\rm S}$ denote the Bragg angle and the angle between the front face and the diffracting planes

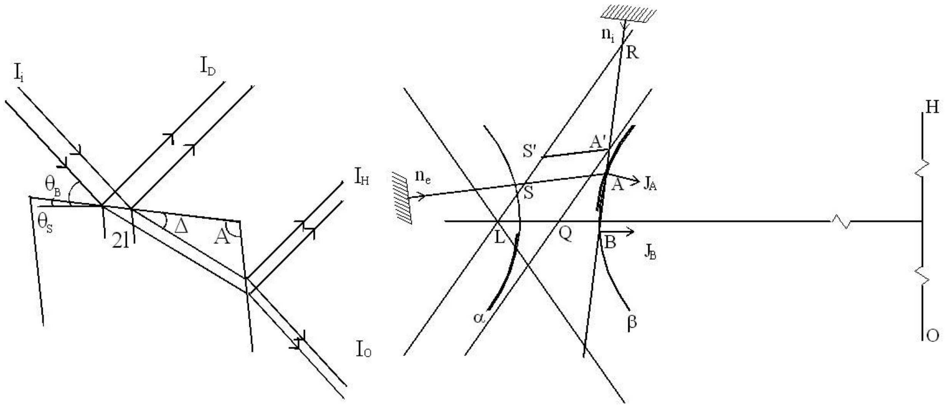

Figure 1. Bragg diffraction of a neutron beam from a thick single crystal in real and reciprocal spaces.

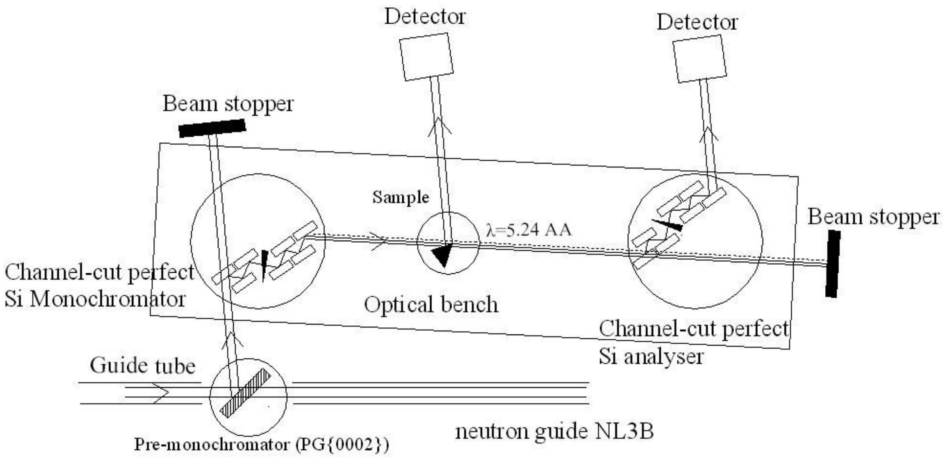

Figure 2. Experimental lay-out for the determination of $\delta_{\rm cr}$and I_0.

of the crystal, respectively. Boundary conditions at the front face of the prism select a unique tie point A on the dispersion surface and at the exit face, dictate the emergent wave vector **SO** for the forward diffracted beam. The deflection, $-RS/k_0$, effected by the crystal prism is hence given by

$$\delta_{\rm cr} = \delta_{\rm am}\left\{1 + \frac{F_{\rm H}}{F_0}\sqrt{\frac{\sin(\theta_{\rm B}-\theta_{\rm S})}{\sin(\theta_{\rm B}+\theta_{\rm S})}}\,y\left(1-\sqrt{1-y^{-2}}\right)\right\}. \tag{1}$$

Here F_0 and $F_{\rm H}$ signify the crystal structure factors for the O and H directions, respectively and

$$\delta_{\rm am} = -RS'/k_0 = (n-1)\{\cot(\theta_{\rm B}-\theta_{\rm S}) - \cot(A+\theta_{\rm B}-\theta_{\rm S})\}, \tag{2}$$

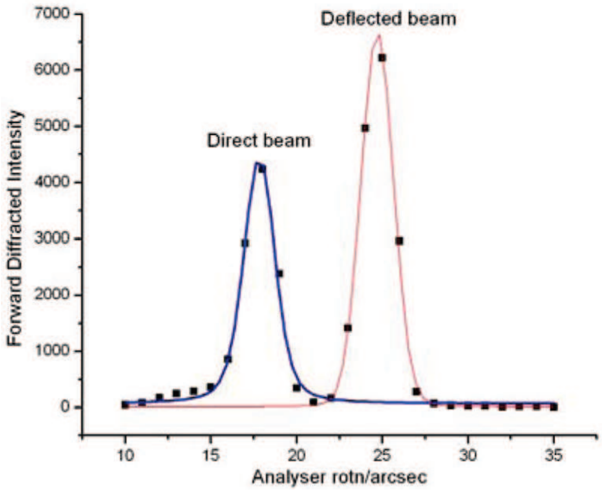

Figure 3. Voigt function fits (curves) to the direct and deflected beam scans (points).

is the amorphous prism deflection. $\delta_{\rm cr}$ varies with θ in the arcsec/arcsec range just outside the total reflection domain ($|y| \gtrsim 1$), in contrast to the arcsec/deg variation of $\delta_{\rm am}$, implying three orders of magnitude increase in sensitivity to the angle of incidence. As the Bragg reflection is approached from the low angle side, the magnitude of $\delta_{\rm cr}$ decreases from $|\delta_{\rm am}|$, reaching a minimum at $y = -1$. The deflection may even change sign for an appropriate choice of asymmetry. On approaching the Bragg reflection from the higher angle side, the magnitude of the deflection increases symmetrically by the same amount, attaining a corresponding maximum at the other extreme, viz. $y = 1$, of total reflectivity (see upper curves in figure 4). If the angle A between the front and side faces lies between $\theta_{\rm B} + \theta_{\rm S}$ and $\pi - (\theta_{\rm B} - \theta_{\rm S})$, a fraction

$$I_0 = \frac{\sin\Delta \sin(A + \theta_{\rm B} - \theta_{\rm S})}{\sin(A + \Delta)\sin(\theta_{\rm B} - \theta_{\rm S})} \tag{3}$$

of incident intensity gets forward diffracted through the prism [5].

3. Experiment

Over three decades ago, due to the nonavailability of arcsec wide neutron beams, Shull [6] could only map $I_{\rm H}(\theta)$ variation by scanning a narrow slit across the diffracted beam from a crystal prism. The advent of a 5.24 Å neutron beam with an angular FWHM ∼2 arcsec [7] at the V12b double crystal spectrometer (figure 2) of Hahn-Meitner-Institut in Berlin facilitated our experiment. Only a part of the neutron beam illuminated a silicon crystal prism, the remaining beam reaching the analyser directly to serve as a reference for the prism deflection measurement. One symmetric {1 1 1} prism of apex angle A equal to 56.7° and two asymmetric

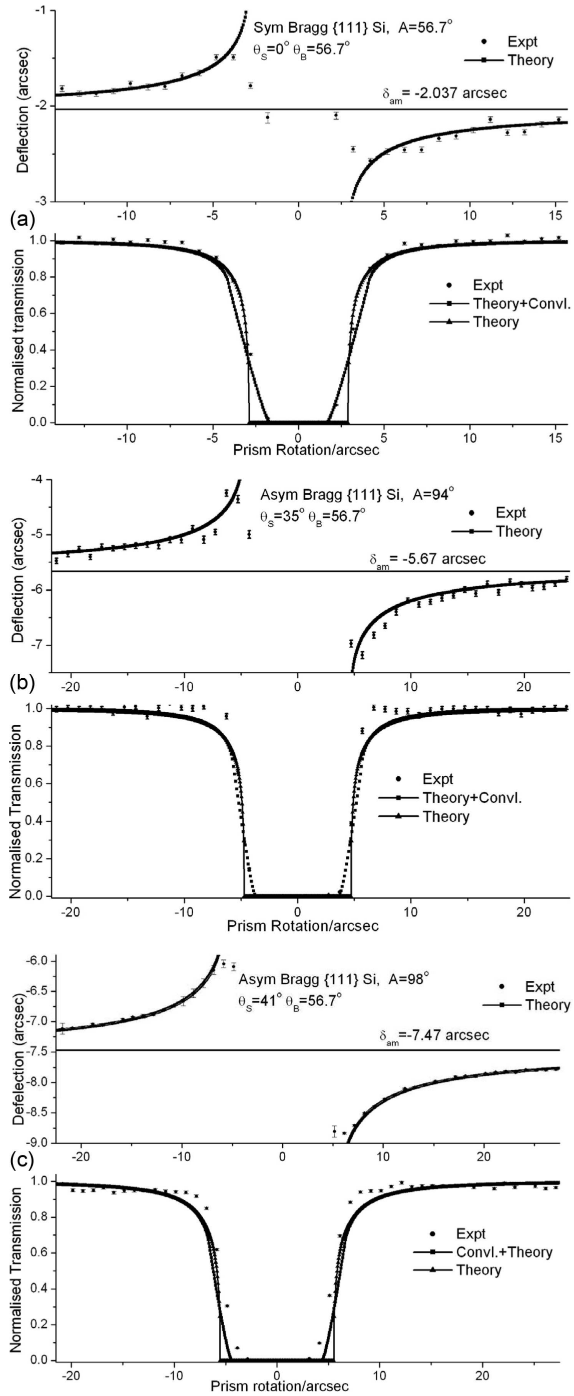

Figure 4. Deflection and transmitted intensity fraction of neutrons forward-diffracted by silicon crystal prisms: (**a**) symmetric {1 1 1} and asymmetric {1 1 1}: (**b**) $\theta_S = 35°$ and (**c**) $\theta_S = 41°$.

{1 1 1} prisms with asymmetry angles θ_S of 35° and 41° and apex angles of 94° and 98°, respectively were investigated. Another detector was used to locate and continuously monitor the Bragg reflection from the prism. The analyser rocking curves were recorded for several angles of incidence θ at the prism covering a span of about 40 arcsec centred at its total reflectivity domain. At each θ, least-squares Voigt function fits were made to the direct and deflected neutron peaks in the rocking curve. The shift from the direct peak of and the area under the deflected peak (figure 3) yielded δ_{cr} and I_0, respectively.

4. Results and discussion

Figure 4 depicts the experimental (points) and theoretical (curves) deflections δ_{cr} and transmitted neutron fractions I_0 by the three silicon crystal prisms mentioned above. The sharp I_0 curves (triangles) represent eq. (3), incorporating the appropriate Debye–Waller factor. Each smooth I_0 curve (squares) was obtained by convoluting the corresponding sharp curve with the incident 2 arcsec wide neutron angular profile, for comparison with the data. The neutron deflection and transmitted intensity fraction data [8–10] agree well with predictions (eqs (1) and (3)) of the two-beam, plane-wave dynamical diffraction theory outlined above. The observed δ_{cr} deviate from δ_{am} by upto 27% with sensitivities $|d\delta_{cr}/d\theta|$ up to 0.43 arcsec/arcsec.

5. Conclusions

We have presented the first calculations and experimental observation of the deflection and intensity fraction of neutrons forward-diffracted by a single crystal prism as a function of the angle of incidence θ. A crystal prism affords three orders of magnitude greater sensitivity of the deflection to θ than an amorphous prism. This observation has led to the design of a super-collimator monochromator [11] producing neutron beams I_H with sub-arcsec angular widths.

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