Sagittal X-ray beam deviation at asymmetric inclined diffractors

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A new approach to focusing X-ray optics based on asymmetric inclined (or rotated inclined) diffraction has been experimentally studied. Using a linear longitudinal W-groove cut into the surface of an asymmetric silicon (111) diffractor perpendicularly to the line of intersection of its surface and crystallographic (111) planes, the out-of-diffraction-plane (or sagittal) deviation of the X-ray diffracted beam has been measured for three angles of asymmetry and constant angle of inclination on BM5 at the ESRF for a wavelength of 0.1 nm. It has been demonstrated that in the grazing-emergence case the sagittal deviation increases with increasing asymmetry angle. A discrepancy with the theoretical value for the largest asymmetry angle and inhomogeneities in the contrast of the diffraction spot have been discussed.

Keywords: X-ray optics; Si(111) W-grooved crystals; inclined diffraction; out-of-diffraction-plane beams; sagittal focusing.

1. Introduction

As shown by Hrdý & Pacherová (1993) and Hrdý (1998), an X-ray beam diffracted at a crystal with inclined surface (inclined diffraction) is slightly deviated in the direction perpendicular to the plane of diffraction. The first observation of this effect was reported by Hrdý *et al.* (1998). In their work the radiation was diffracted on the toothed surface of a crystal. The teeth created an array of longitudinal grooves with inclined walls in the surface of the crystal. Owing to the deviation of X-ray beams diffracted at these walls, a splitting of the diffraction spots on the tops of the teeth was observed. The size of the splitting was compared with theory and a reasonable agreement was found. Hrdý (1998) suggested utilizing this effect for sagittal focusing of synchrotron radiation. Successful demonstration of this focusing was reported by Hrdý & Siddons (1999). Recently, the measurement of the sagittal (out-of-diffraction-plane) deviation δ of the Bragg-diffracted X-ray beam at a symmetrically cut Si(111) single crystal with W-shape longitudinal groove was performed on beamline BM5 at the ESRF for the wavelength λ = 0.1 nm (Artemiev *et al.*, 2000). With $\delta = 0$ the walls of the W-groove should produce homogeneous diffraction spots, while in the real case of $\delta \neq 0$ a splitting at the central part of the picture of the groove (owing to the diffraction on the sharp edge region) occurs. From the measured splitting a good coincidence between the experimental ($\delta = 1.096 \times 10^{-4}$) and the theoretical ($\delta = 1.07 \times 10^{-4}$) values was obtained considering some blur introduced by the finite value of the range of the total reflection (Artemiev *et al.*, 2000).

Korytár *et al.* (2000, 2001) used a three-dimensional concept of the dynamical theory of X-ray diffraction to calculate the out-of-diffraction-plane components (sagittal beam deviations) of the X-ray beams diffracted at asymmetrical inclined diffractors (with general orientation of the surface with respect to the diffracting planes: partly inclined, partly asymmetrical). According to Korytár *et al.* (2001), the out-of-diffraction-plane component x'_{kh} of the wavevector of the X-ray beam diffracted at an asymmetric inclined diffractor can be expressed in the form

$$x'_{kh} = \frac{\left\{-R_{h1} + \left[R_{h1}^2 + (1+\tan^2\beta)\left(R_{h2}^2 - R_{h1}^2\right)\right]^{1/2}\right\}\tan\beta}{1+\tan^2\beta}, \qquad (1)$$

where β is the inclination angle and R_{h1} and R_{h2} can be expressed as

$$R_{h1} = -\left(k\gamma_h - \frac{1}{2}\frac{k|\varphi_0|}{\cos\Theta_{\rm B}}\sin\alpha\right) \qquad (2)$$

and

$$R_{h2} = R_{h1} - \frac{k|\varphi_0|}{2\gamma_h}, \qquad (3)$$

where $\Theta_{\rm B}$ is the Bragg angle, α is the angle of asymmetry, directional cosine $\gamma_h = -|\gamma_h| = \sin(\Theta_{\rm B} - \alpha)$ in the grazing-emergence Bragg case, $\varphi_0 = -(e^2/mc^2)(\lambda^2/\pi)F(0)/V$, where e^2/mc^2 is the classical radius of an electron and is equal to 2.817×10^{-15} m, $F(0)$ is the structure factor, $\lambda = 1/k$ is the wavelength of the X-ray beams and V is the volume of the elementary structure cell. From these expressions it may be seen that, in comparison with the symmetrical inclined case, a much higher δ of the diffracted beam can be obtained for a grazing-emergence asymmetric inclined diffractor. Similar equations hold for the out-of-diffraction-plane component of the incident beam, which is much less than that for the diffracted beam in the grazing-emergence case. Table 1 illustrates that the higher the angle of asymmetry α the higher the sagittal deviation $\delta \simeq \lambda x'_{kh}$ for a given tilt angle β (Fig. 1).

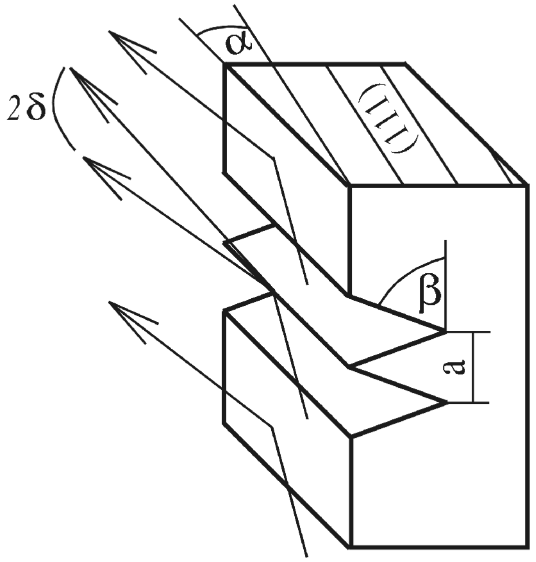

Figure 1
W-groove prepared in an asymmetric Si(111) sample to form an asymmetric inclined diffractor. α and β are the angle of asymmetry and the tilt or inclination angle, respectively. The distance between the bottoms of the two V-grooves forming the W-groove is a = 0.8 mm. The incident and diffracted beams are also depicted. The beam diffracted at the central ridge of the W-groove is split (the splitting angle being twice the sagittal deviation δ) by the inclined surfaces of the crystal.

Table 1
The angle of asymmetry α, corresponding sagittal deviation δ, and the central splitting of the diffraction spot $2\Delta x$ corresponding to 2δ, as calculated for a Si(111) diffractor for a wavelength λ = 0.1 nm, Bragg angle Θ_B = 9.175°, and tilt angle β = 70°.

α (°)	δ (μrad)	$2\Delta x$ (mm) at 0.97 m	$2\Delta x$ (mm) at 1.7 m
0.0	54	0.10	0.18
4.0	96	0.19	0.33
7.0	230	0.45	0.78
8.5	680	1.32	2.31
9.0	1800	3.49	6.12

The purpose of this work was to verify the theoretical results outlined and to check the possibility of preparing X-ray sagittally focusing elements with decreased focusing distance.

2. Experiment

A series of Si(111) asymmetric diffractors with α = 0, 4 and 8.5° have been prepared with an accuracy of better than 0.1°, and W-shape longitudinal grooves giving inclination angles $\beta = \pm 70°$ have been cut into the surface of the diffractors perpendicularly to the line intersection of (111) and the crystal surface planes (Fig. 1). A thorough chemical polish etch was applied to remove surface damage and residual strains. The same method as utilized by Artemiev *et al.* (2000) has been used for the measurements of sagittal deviations δ of the Bragg diffracted beams. The experiment was performed on BM5 at the ESRF for the wavelength λ = 0.1 nm which gives a Bragg angle Θ_B = 9.175°. The experimental arrangement is presented in Fig. 2 and shows that the dispersive $(m,-m,-m)$ setting of a channel-cut Si(111) monochromator and a sample crystal has been used, with the sample crystal being an asymmetric inclined diffractor in grazing emergence. The presence of the channel-cut monochromator did not influence the effect we were looking for but it reduced the power delivered to the sample and also the parasitic reflections which would otherwise be present. The crystals were oriented in such a way that the plane of diffraction was horizontal in order to utilize the smaller vertical dimension of the X-ray source. X-ray topographs were recorded by means of a CCD camera with 50 μm or 15 μm resolution.

3. Results and discussion

Fig. 3 shows the (111) X-ray topographs of the area of the W-groove, registered by the CCD camera with 50 μm resolution giving a larger field of view. The crystal-to-camera distance is 1.7 m. The shape of the groove is clearly discernible in the case of α = 0° (*a*) and α = 4° (*b*), but we had to increase the incident beam size both horizontally and vertically to understand more clearly the diffraction spot in the case of α = 8.5° (*c*). The central splitting and the two side half-splittings are obscured by the beams, strongly sagittally deviated by non-central side walls of the groove in the latter case. To decrease this effect we narrowed the slit vertically to shield off the beams diffracted from the outer walls of the groove (*d*). The central splitting and also the trace of the third harmonics (two narrow lines in the central gap) are clearly seen. Central splittings corresponding to theoretical sagittal deviations are depicted by horizontal lines. While the correspondence between experimental and theoretical values is satisfactory for α = 0° and α = 4°, the experimental value for α = 8.5° is about half of the theoretical value.

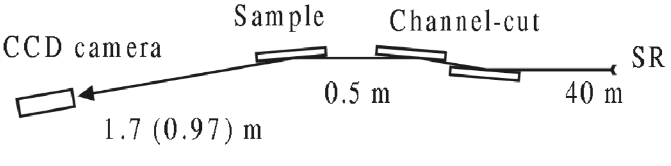

Figure 2
Experimental arrangement at BM5 at the ESRF for the measurement of the sagittal deviation at asymmetric inclined diffractors. As a sample an asymmetric inclined W-grooved Si(111) diffractor in grazing emergence, depicted in Fig. 1, has been used.

Fig. 4(*a*) shows in more detail the central splitting for α = 8.5° and for the decreased sample-to-CCD camera distance of 970 mm. Again, the horizontal lines represent theoretical splitting. Contrast variations across the diffraction spot can be attributed to surface unevenness in the W-groove. Narrowing of the vertical slit in Fig. 4(*b*) preserves rough contrast features around the central splitting of the diffraction spot taken using a 50 μm-resolution camera. Moreover, Fig. 4(*b*) clearly shows that some diffracted beams are sagittally deviated even more than theoretical values depicted by horizontal lines. These observations can be explained by the fact that at high asymmetry angles and high inclination angles the sagittal beams deviations are extremely sensitive to inaccuracies in α and β, as shown by the theoretical results presented by Korytár *et al.* (2001). These inaccuracies originate in surface waviness and irregularities induced by cutting the crystals (0.1° inaccuracy), which were not fully removed by a subsequent chemical polishing etch. In our opinion, the optical quality of the surfaces would be desirable to minimize surface unevenness. A lapping step is to be inserted between the cutting and chemical polishing steps in the technology of W-groove manufacturing. Bragg-angle and wavelength-setting inaccuracies represent further important causes of large changes in the splitting at α = 8.5°. The increase of the spread of the sagittal deviation is caused by the increase of the intrinsic rocking-curve half width and also by surface unevenness in the groove.

4. Conclusions

We have clearly demonstrated that, in accordance with the dynamical theory calculations, the sagittal (out-of-diffraction-plane) deviation of the X-ray beam Bragg diffracted at an asymmetrical inclined (or rotated inclined) diffractor increases with increasing asymmetry in grazing-emergence setting. In comparison with the symmetrical inclined case (α = 0°), a sagittal deviation larger by more than five times has been experimentally obtained for an angle of asymmetry α = 8.5°. This is very important if sagittal focusing of synchrotron radiation is to be based on this technique. In comparison with the symmetrical case, a parabolical groove fabricated into an asymmetric-cut crystal can provide a much shorter focusing distance and can allow the size of the beam to be focused to substantially increase. It is concluded that, even if full quantitative agreement with theory has not been achieved, it is possible to enlarge significantly the sagittal deviation δ on an inclined surface by introducing the asymmetry and thus to use this principle for sagittal focusing.

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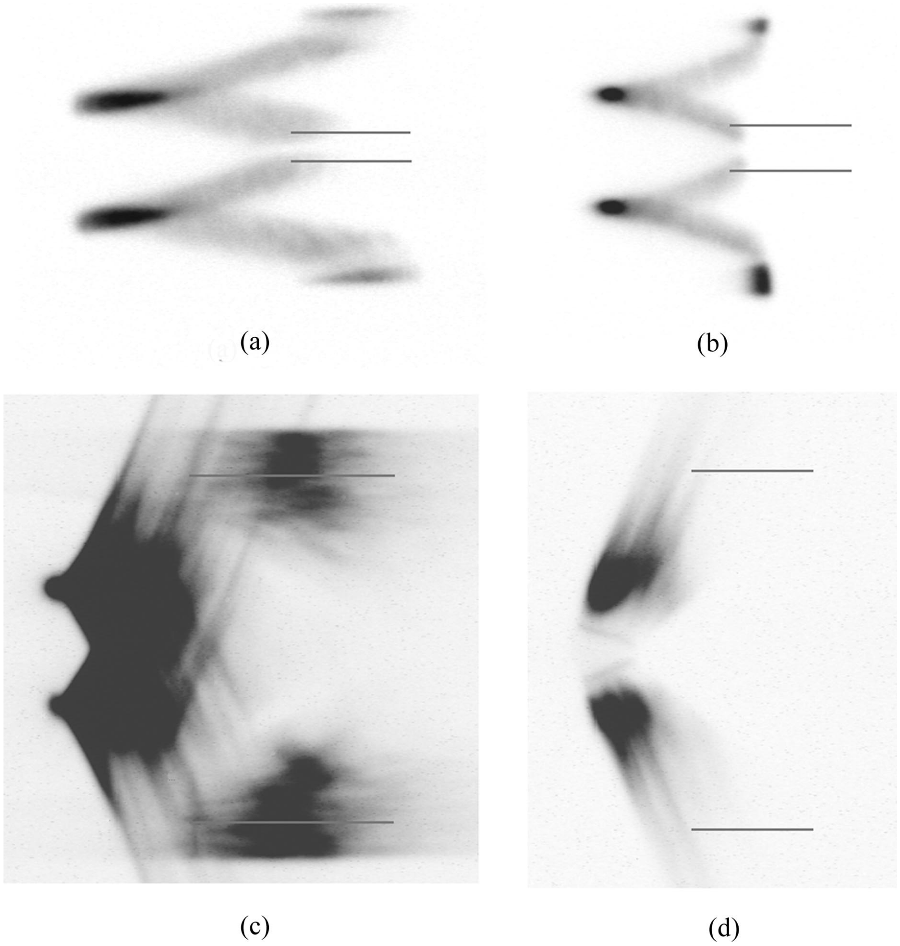

Figure 3
X-ray topographs of W-grooved diffractors taken with a CCD camera of resolution 50 μm and integration time τ. (*a*) $\alpha = 0^{\circ}$, $\tau = 0.01$ s; (*b*) $\alpha = 4^{\circ}$, $\tau = 0.04$ s; (*c*) $\alpha = 8.5^{\circ}$, $\tau = 2$ s, opened slits; (*d*) $\alpha = 8.5^{\circ}$, $\tau = 2$ s, slits set to limit the incident beam to the central inclined walls. The distance between the bottoms of the two V-grooves forming the W-groove is 0.8 mm. The sample-to-camera distance is 1700 mm. Horizontal lines represent theoretical values of central double splitting of the diffracted beam $2\Delta x$.

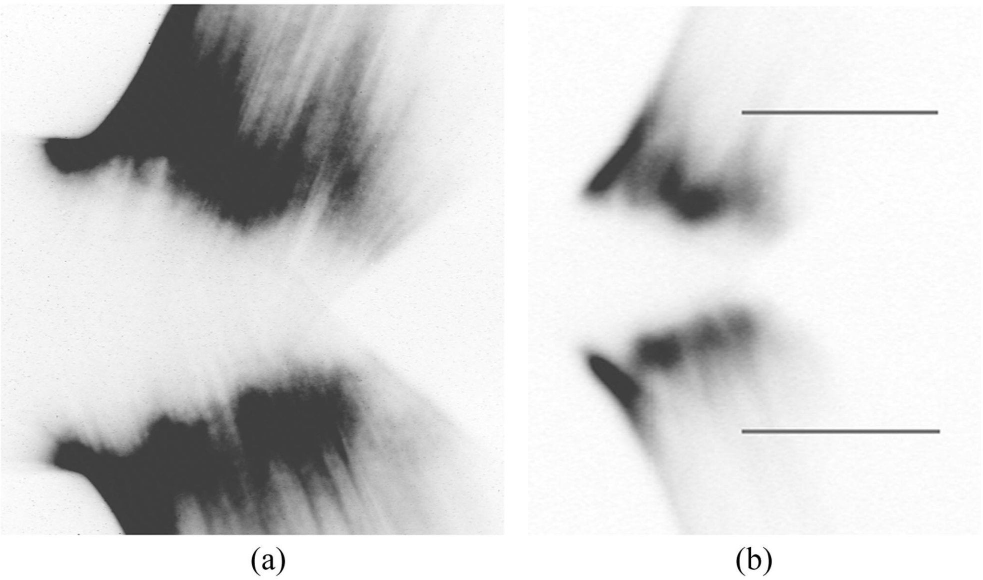

Figure 4
(*a*) The central splitting taken by a 15 μm-resolution CCD camera for $\alpha = 8.5^{\circ}$, $\tau = 2$ s, and for a decreased sample-to-CCD camera distance of 970 mm. The vertical slit was open in order to see the bottoms of the W-groove, which are 0.8 mm apart. Because of higher resolution the field of view is smaller and horizontal lines showing theoretical splitting are outside the image. (*b*) The vertical slit has been narrowed to take only the diffraction spot from the central inclined walls of the W-groove by a 50 μm-resolution CCD camera and $\tau = 0.4$ s. Horizontal lines again represent theoretical values of central double splitting of the diffracted beam $2\Delta x$.

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