Refraction in general asymmetric X-ray Bragg diffraction

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When the surface of a single-crystal monochromator is not parallel to the diffracting crystallographic planes, the diffracted beam is generally deviated from the plane of diffraction and the angle between the diffracted beam and the diffracting planes is different from the angle between the incident beam and the diffracting planes. The angular diffraction regions for the incident and diffracted beams are also different. This is the manifestation of the refraction occurring during Bragg diffraction. Very simple formulae are presented which describe this situation in a general case (*e.g.* for a rotated-inclined X-ray monochromator). These formulae allow sagittally focusing monochromators for synchrotron radiation to be easily designed, based on X-ray diffraction–refraction phenomena. Some important properties of such types of monochromators are deduced.

Keywords: X-ray diffraction; focusing X-ray monochromators; X-ray optics.

1. Introduction

From a geometrical point of view, Bragg-case X-ray diffraction on a symmetrically cut crystal behaves like reflections on a mirror. The angle between the incident beam and the surface of the crystal equals the angle between the diffracted beam and the surface of the crystal. This is no longer valid if the surface of the crystal is not parallel to the diffracting crystallographic planes. Here we can have two extreme cases. First, the impinging X-ray beam, the normal to the diffracting planes and the normal to the surface are in one plane. This is the well known asymmetric Bragg-case diffraction. Second, starting from the asymmetric case, the surface is rotated around the normal to the diffracting planes by 90°. Then the plane containing the impinging beam and the normal to the diffracting planes is perpendicular to the plane determined by the normals to the diffracting planes and to the surface. This situation is often called inclined diffraction. If the angle of rotation is different from 90°, we have a mixture of the asymmetric and the inclined cases, and here this situation will be called general asymmetric or rotated-inclined diffraction. (This is an analogy of a general asymmetric or rotated-inclined monochromator which is based on this kind of diffraction.)

In asymmetric Bragg-case diffraction, not only the angle between the incident beam and the surface differs from the angle between the diffracted beam and the surface, but also the angle between the incident beam (more precisely the centre of the diffraction region) and the diffracting crystallographic planes ($\theta_B + \Delta\theta_0$) differs from the angle between the diffracted beam and the diffracting planes ($\theta_B + \Delta\theta_h$). The angular width ω_0 of the diffraction region of the incident beam for a certain wavelength λ and the width ω_h of the diffraction region of the reflected (diffracted) beam are also different. This is a consequence of the dynamical theory of diffraction on perfect crystals and the situation is described well by, for example, Matsushita & Hashizume (1983). The following simple relations are stated for the asymmetric diffraction between the widths and positions of the centres of the diffraction regions (crystal functions):

$$\begin{aligned}
\omega_0 &= \omega_s b^{-1/2},\\
\omega_s &= \left[2r_e\lambda^2 P\left|F_{hr}\right|\exp(-M)\right]/\pi V\sin 2\theta_B,\\
\Delta\theta_0 &= (1/2)(1+1/b)\Delta\theta_s,\\
\Delta\theta_s &= r_e\lambda^2 F_{0r}/\pi V\sin 2\theta_B,\\
\omega_h &= \omega_s b^{1/2},\\
\Delta\theta_h &= (1/2)(1+b)\Delta\theta_s,\\
\theta_0 &= \theta_B + \Delta\theta_0,\\
\theta_h &= \theta_B + \Delta\theta_h,\\
b &= \sin(\theta_B-\alpha)/\sin(\theta_B+\alpha).
\end{aligned} \tag{1}$$

Here, V is the unit-cell volume, $r_e = e^2/mc^2$, F_{hr} is the real part of the structure factor F_h (h stands for Müller indices hkl), P is the polarization factor, and $\exp(-M)$ is the temperature factor. The index s stands for symmetrical diffraction. The angle α is the angle between the diffracting planes and the surface and is taken as positive for grazing incidence. The typical values of $\Delta\theta$ and ω are from fractions to tens of angular seconds. For the cross sections CS_0 and CS_h of the incident and reflected beams, it holds that

$$CS_h = CS_0/b, \tag{2}$$

and, together with (1),

$$\omega_h CS_h = \omega_0 CS_0. \tag{3}$$

From the above it is seen that in the case of the asymmetric Bragg-case diffraction the angle between the incident beam (the centre of the diffraction region) and the diffracting planes is different from the angle between the diffracted beam (again the centre of the diffraction region) and the diffraction planes, and their (meridional) difference $\delta_{m,asym}$ is given by (Hrdý & Hrdá, 2000)

$$\delta_{m,asym} = \Delta\theta_0 - \Delta\theta_h = 2\Delta\theta_s\tan\theta_B\tan\alpha/\left(\tan^2\theta_B - \tan^2\alpha\right), \tag{4}$$

or simply

$$\delta_{m,asym} = (1/2)(1/b - b)\Delta\theta_s. \tag{5}$$

The deviation from the mirror-like behaviour, δ_{asym}, was used for the proposal of the meridional focusing of diffracted synchrotron radiation on the crystal with a transversal groove on its surface (Hrdý & Hrdá, 2000).

In the case of inclined diffraction the situation is different and was probably first studied by Hrdý & Pacherová (1993), and later, with respect to possible application for focusing, in some of our preceding papers (Hrdý, 1998; Artemiev *et al.*, 2000). It was shown that the diffracted beam is sagittally deviated from the plane of diffraction (*i.e.* the plane determined by the impinging beam and the normal to the diffracting planes) by an angle $\delta_{s,incl}$ given by

$$\delta_{s,incl} = K\tan\beta, \tag{6}$$

where β is the angle between the surface and the diffracting planes (angle of inclination) and K for silicon crystals is given by

$$K = 1.256\times 10^{-3}\, d_{hkl}\ [\mathrm{nm}]\ \lambda\ [\mathrm{nm}]. \tag{7}$$

It has been shown both theoretically (Hrdý, 1998) and experimentally (Hrdý & Siddons, 1999) that, owing to the tangential dependence (6), an X-ray synchrotron radiation beam diffracted on a crystal with a longitudinal parabolic groove may be sagittally focused.

Korytár, Boháček & Ferrari (2000, 2001) suggested that a substantial increase of this sagittal deviation may be achieved if the asymmetric diffraction component is present, *i.e.* in the case of general asymmetric (or rotated-inclined) diffraction. They also performed a numerical calculation of this effect taking into account the exact shapes of surfaces in the reciprocal space. By diffraction on an asymmetrically cut crystal with a longitudinal W-shaped groove we have unambiguously proved that this effect exists (Korytár, Hrdý *et al.*, 2001).

In fact, the sagittal deviation of a beam in the case of rotated-inclined geometry was studied even earlier (Kashihara *et al.*, 1998; Yabashi *et al.*, 1999; Blasdell & Macrander, 1994). The results of these works (including the papers of Korytar), however, are in rather complicated form and do not allow the focusing properties to be studied directly.

In this paper a very simple formula for the sagittal deviation of the beam in the case of general asymmetric (or rotated-inclined) diffraction is derived which allows sagittally focusing monochromators based on this kind of diffraction to be studied and designed easily. Some important properties of these monochromators are also deduced.

2. Derivation of the formula for sagittal deviation of an X-ray beam for general asymmetric diffraction

Let us consider as a starting position an asymmetrical Bragg-case diffraction. The situation in the reciprocal space for this kind of diffraction (Batterman & Cole, 1964) is shown in Fig. 1. P and P' are the starting points of the wave vectors for the incident and the diffracted wave vectors for the symmetrical diffraction. Sp_O and Sp_H are spheres of radius $1/\lambda$ centred on the reciprocal space points O and H. $LP = LP' = \Delta\theta_s(1/\lambda)$. For asymmetric diffraction the starting points for the incident and diffracted wave vectors are P_1 and P_2, respectively. Obviously, $LP_1 = \Delta\theta_0(1/\lambda)$ and $LP_2 = \Delta\theta_h(1/\lambda)$. The distance $P_1P_2 = AP_2/\cos\alpha$ and $AP_2 = LP_1\cos\theta_B + LP_2\cos\theta_B$. From this and from (1) it follows that

$$P_1P_2 = 2\Delta\theta_s\cos\theta_B(1/\lambda)(2 + b + 1/b)/4\cos\alpha. \qquad (8)$$

So far we have been working in a plane. To take into account the rotated-inclined diffraction it is necessary to work in a three-dimensional space. With a reasonable approximation we can consider the spheres passing through the points L and Q as planes perpendicular to the plane of the drawing. Similarly, the dispersion surfaces are taken as hyperbolical cylinders perpendicular to the plane of the drawing. We have used the same approximation in deriving (6) and it proved to be good for β up to about 85°. Creating a groove in the surface of such an asymmetrically cut crystal means that the plane of the surface is rotated by some angle β about the axis o which is parallel to the surface (see Fig. 1). It also means that the normal P_1P_2 to the surface is rotated by the angle β and now it intersects the plane LP_2 (or Sp_H) at some point P_β which is above the point P_2 (above the plane of diagram); thus in Fig. 1 both points coincide. The distance $P_2P_\beta = P_1P_2\tan\beta$. This implies that the diffracted wavevector starts now at P_β and for the sagittal deviation of the diffracted beam it holds that

$$\delta_{s,r\text{-}i} = P_2P_\beta/(1/\lambda). \qquad (9)$$

In the inclined case ($\alpha = 0$) the sagittal deviation would obviously be

$$\delta_{s,incl} = PP'\tan\beta/(1/\lambda), \qquad (10)$$

where $PP' = 2\Delta\theta_s\cos\theta_B(1/\lambda)$. Now it is possible to write the final formula for the sagittal deviation of the diffracted beam in the rotated-inclined case,

$$\delta_{s,r\text{-}i} = \delta_{s,incl}(2 + b + 1/b)/4\cos\alpha. \qquad (11)$$

[We can create the rotated-inclined case differently. Starting from the asymmetric case, we can rotate the surface about the axis which is parallel not to the surface as considered above but to the diffracting planes by a certain angle β. Then we will obtain practically the same formula as (11); only $\cos\alpha$ will be missing.]

The experimental value of the sagittal deviation found by Korytár, Hrdý *et al.* (2001) was within the precision of the method, in good agreement with (11).

From the presented geometrical derivation and by using Fig. 1 it is obvious that the meridional component $\delta_{m,r\text{-}i}$ of the beam deviation in the rotated-inclined case equals $\delta_{m,asym}$ given by (4) and (5). Then from the above it follows that if the rotated-inclined diffraction is created in the above-described way, then, if the impinging beam spans its diffraction region ω_0, the diffracted beam is deviated in the meridional direction (from a mirror-like reflection) by an angle $\delta_{m,r\text{-}i}$ given by (5), and the meridional component of the diffracted beam span is the angular interval ω_h. At the same time the beam is sagittally deviated from the plane of diffraction by the angle $\delta_{s,r\text{-}i}$ given by (11), and the sagittal component $\omega_{s,r\text{-}i}$ of the diffracted beam span is given by (12).

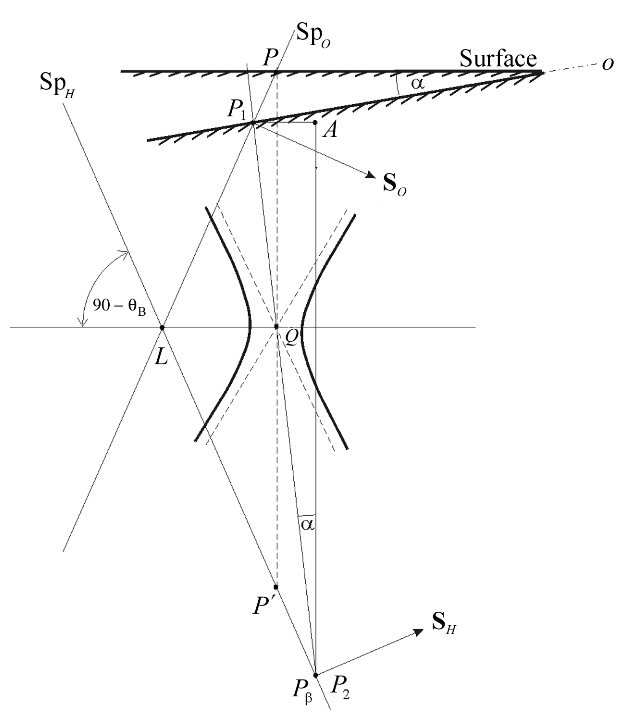

Figure 1
Schematic representation of the situation in reciprocal space for asymmetric Bragg-case diffraction. After the rotation of P_1P_2 about the axis o parallel with a surface by an angle β, this line will intersect the sphere Sp_H at a point P_β which will be the starting point of the diffracted wave vectors for general asymmetric Bragg-case diffraction. P_β is above the plane of the drawing and its projection onto this plane coincides with P_2.

3. Conclusions

From (6) and (11) it is seen that $\delta_{r\text{-}i}$ is proportional to $\tan\beta$ and that also for the rotated-inclined (or general asymmetric) case the sagittal focusing of diffracted radiation can be achieved by a longitudinal parabolic groove. $\delta_{r\text{-}i}$ has its minimal value for $b = 1$ (symmetrical case). The increase of the sagittal deviation occurs for both $b < 1$ and $b > 1$, *i.e.* for the grazing-incidence case and grazing-emergence case, and is independent of the sign of α. To design the shape of the focusing parabolic groove the procedure is the same as that described by Hrdý (1998) and Hrdý & Siddons (1999), though it is necessary to replace K with $K(2 + b + 1/b)/4\cos\alpha$. We have designed a sagittally focusing monochromator based on the above theory and have performed an experiment at the ESRF (Artemiev *et al.*, 2001). The focusing properties observed were in agreement with our expectation.

So far the treatment has only been concentrated on the central beams. As in the pure inclined case (see, for example, Artemiev *et al.*, 2000), when the incident beam spans the diffracting region ω_0 then the diffracted beam spans a certain angle, here $\omega_{\text{r-i}}$. From the geometry shown in Fig. 1 and from (1), it follows that

$$\omega_{\text{s,r-i}}/\delta_{\text{s,r-i}} = \omega_0/\Delta\theta_0 = \omega_h/\Delta\theta_h. \qquad (12)$$

From (1) it follows that (12) has its maximum value for $b = 1$. For $|\alpha|$ approaching $\theta_{\rm B}$, the left-hand side of (12) approaches zero. This means that the sagittal focusing for the rotated-inclined case is sharper than for the pure inclined case.

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