Diffractive refractive optics: the possibility of sagittal focusing in Laue-case diffraction

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The sagittal deviation of a Laue-diffracted X-ray beam caused by the inclination of an exit crystal surface with respect to an entrance crystal surface has been studied both theoretically and experimentally. The use of this effect for sagittal focusing of X-ray synchrotron radiation diffracted by a Laue crystal is suggested. The focusing is based on the refraction effect due to the parabolic profile of an exit or/and entrance surface. The crystal is not bent. In order to achieve a reasonable focusing distance, the crystal should be cut asymmetrically. The experiment was performed at beamline BM5 at the ESRF.

Keywords: asymmetric Laue diffraction; sagittal focusing; focusing Laue-crystal X-ray monochromator.

1. Introduction

It has been shown that in Bragg-case diffraction the sagittal focusing of a diffracted X-ray beam may be achieved when the crystal surface is shaped such that it forms a longitudinal parabolic groove (Hrdý, 1998, 2001; Hrdý & Siddons, 1999; Artemiev *et al.*, 2001). This effect occurs because in inclined (not asymmetrical) diffraction the diffracted beam is slightly deviated from the plane of diffraction. This deviation, δ, can be easily explained in terms of the configuration of the wave vectors in reciprocal space when taking into account boundary conditions. A summary of theoretical and experimental work on this subject is given by Hrdý *et al.* (2001). A similar approach can also be applied to Laue-case diffraction. By profiling, for example, the exit surface (or the entrance surface, or both) of a Laue crystal, it should be possible to focus the diffracted radiation meridionally or sagittaly, depending on how the surface is shaped. In fact, the meridional deviation of the beam diffracted from a Laue crystal whose exit surface is inclined to the incident surface was first observed by Kohra *et al.* (1965). To utilize this effect for meridional focusing it is necessary also to take into account polychromatic focusing and diffractional focusing (Afanasev & Kohn, 1977), which will not be treated here. On the other hand, the sagittal deviation of the diffracted beam in Laue-case diffraction has, to our knowledge, been studied neither theoretically nor experimentally and will be discussed in this paper. The discussion is based only on geometrical theory, *i.e.* on the influence of the crystal boundary on the directions of the wave vectors. Obviously, a detailed theory that describes the diffracted intensity is needed. The purpose of this paper is only to demonstrate the new effect.

2. Theory

The situation in the reciprocal space for symmetrical Laue-case diffraction is shown in Fig. 1. Let the incident wavevector be determined by the point L on the Ewald sphere. Then the normal to the entrance surface passing through L intersects the dispersion surface at the point P (the center of the diffraction region), which determines the wave vectors generated inside the crystal. The points on Ewald spheres that determine the exit diffracted and refracted wave vectors are determined as an intersection of the normal to the exit surface, passing through P, with the Ewald spheres. In this case, the normal intersects the Ewald spheres again at the point L.

Let us now rotate the exit surface about the vertical axis (see Fig. 1) by an angle β. The normal to the exit surface, passing through P, intersects the Ewald spheres at M, which lies out of the diffraction plane ($ML = LP\tan\beta$). The sagittal deviation, δ, of the exit diffracted and refracted beams is

$$\delta = LP\tan\beta/k, \tag{1}$$

where $k = 1/\lambda$ is the absolute value of the vacuum wavevector, and

$$LP = \left[r_e\lambda/(2\pi V\cos\theta_B)\right]\left[F_{0r} - \rho|F_{hr}|\exp(-M)\right], \tag{2}$$

where r_e is the classical electron radius, V is the volume of the unit cell, θ_B is the Bragg angle, ρ is the polarization factor, and F_{0r} and F_{hr} are the real parts of the structure factors of the corresponding reflections (see, for example, Batterman & Cole, 1964). We assumed here that in the vicinity of the Laue point the Ewald spheres may be replaced by planes.

This deviation is rather small (of the order of microradians for $\lambda = 0.1$ nm and $\beta = 45°$). As in Bragg-case diffraction, however, δ may be substantially increased by using asymmetric Laue diffraction (see Fig. 2). Here the normal to the exit surface, passing through P, intersects the Ewald spheres at the points N and R. The point N determines the outside-diffracted vector [$NP = LP\cos\theta/\cos(\theta + \alpha)$, where θ is the Bragg angle and α is the deviation of the entrance surface from that in the Laue symmetrical case]. The point R determines the outside refracted (forward diffracted) wave vector.

By rotating the exit surface about the intersection line of the plane of diffraction and the surface by an angle β, the intersection point of

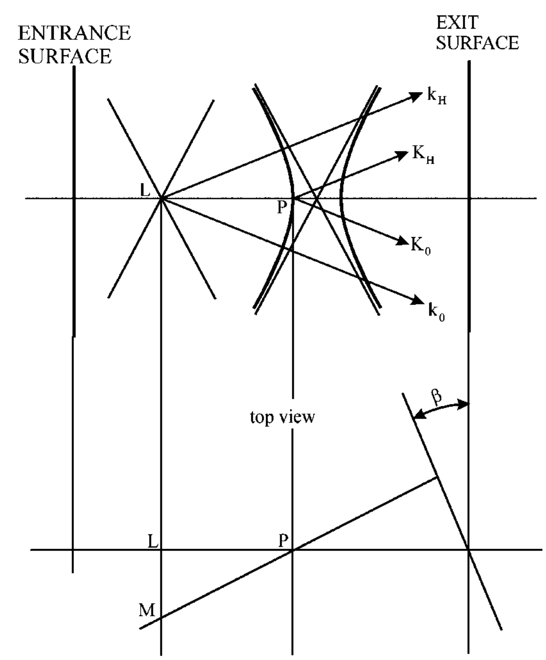

Figure 1
The situation in the reciprocal space for Laue symmetrical diffraction. The sagittal deviation of the diffracted beam is achieved by rotating the exit surface by the angle β.

the normal and the Ewald sphere moves from point N to point M in a direction perpendicular to the plane of diffraction ($NM = NP\tan\beta$). The sagittal deviation, δ, is then

$$\delta = LP\,[\cos\theta\,/\,\cos(\theta+\alpha)]\tan\beta/k. \qquad (3)$$

Clearly, for $\theta + \alpha$ close to 90° the sagittal deviation, δ, could be of practical interest. For example, for Si(111), λ = 0.1 nm, β = 45° and α = 79.3°, the expected value of δ is about 6×10^{-5}. For β = 60°, the expected value of δ is 1×10^{-4}. These values decrease with decreasing λ provided that we keep $\theta + \alpha$ constant. The possible realization of such a focusing element is shown in Fig. 3. To double the deviation, δ, the curved profile should be given to both faces of the Laue plate.

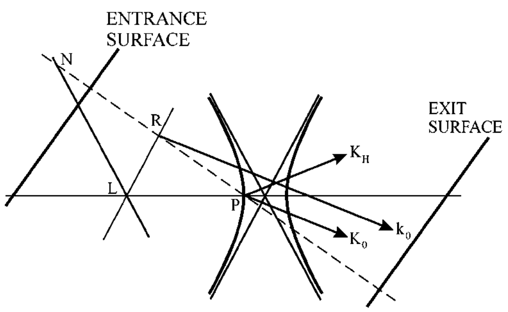

Figure 2
The reciprocal space diagram for Laue asymmetrical diffraction. As in Fig. 1, the sagittal deviation of the diffracted beam is achieved by the rotation of the exit surface by an angle β.

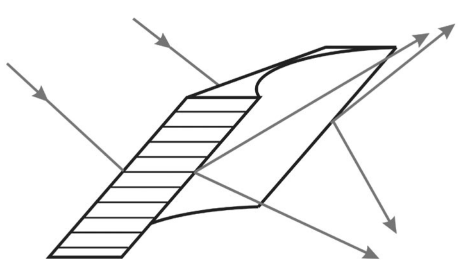

Figure 3
A sagittaly focusing Laue asymmetric crystal.

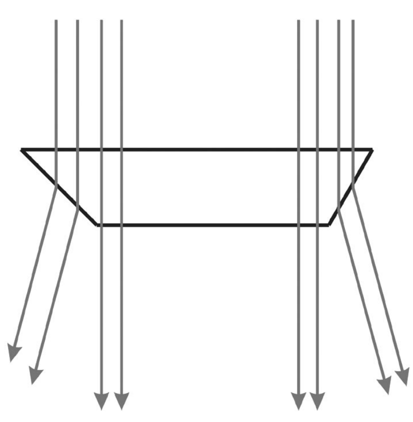

Figure 4
A schematic picture showing the splitting of the Laue diffracted beam on the wedge.

3. Experiment

To verify (3) we have performed a simple experiment. We prepared an asymmetrically cut Si single-crystal plate of thickness 1 mm (the other dimensions are 50 × 50 mm). The angle between the entrance surface and the (111) diffracting planes was 10.7°, which corresponds to α = 79.3°. We machined wedges on both sides of the crystal, such that the diffracted radiation should split in the sagittal direction, as shown in Fig. 4. The angles of the two wedges were 45 and 60° (we only used the 60° one). The experiment was performed at the ESRF BM5 beamline. The crystal was placed after the main monochromator, which was set to λ = 0.1 nm and detuned to suppress partially the higher harmonics. The diffracted beam formed an angle of 1.5° with the exit surface of the crystal, and the angle between the impinging beam and the entrance surface was 19.9°. The size of the beam was 0.1 mm (vertically) by 3 mm (horizontally). The vertical divergence of the beam was about 5 μrad. The image of the diffracted radiation was detected at a distance of 40 cm from the crystal by a CCD camera. The wavelength of 0.1 nm is large enough to see the effect, but because of the high absorption we could only see the beam diffracted from the edge of the crystal, where the thickness of the crystal was sufficiently small. On the other hand, we could see the image of the third harmonic in the whole region of the crystal, but the expected splitting for this harmonic is smaller. Fig. 5 shows the image of the third (and higher) harmonics, and in the lower part we also see the overexposed image of the first harmonic. The vertical direction corresponds to the sagittal direction (*i.e.* perpendicular to the plane of diffraction). The place where the image changes direction corresponds to the 120° edge of the crystal. Here we could see a 'crack', which is obviously the sagittal splitting for the higher harmonics. The size of this crack is within one pixel, which represents about 10 μm. Fig. 6 shows the same image as Fig. 5 but with a much shorter exposure time. The region out of the wedge is practically not seen, but at the lower part we see two spots; the upper spot is the image of the edge of the crystal seen by the higher harmonics, and the lower spot is the image of the edge seen by the first harmonic. The first-harmonic spot is displaced with respect to the higher-harmonic spot, both horizontally and vertically (meridionally and sagittally). The vertical displacement determines the sagittal splitting that we were looking for. The problem is that the comparison of the positions of the spots belonging to different harmonics is not straightforward, and thus we could make only a rough evaluation of the result. In any case, the vertical displacement is at least four pixels in the right direction, which supports the above theory.

4. Discussion

Hrdý (1998) showed that the tangential dependence of δ on β requires, in the case of Bragg diffraction, a longitudinal groove of parabolic shape in order to generate the sagittal focusing. Analogically, in the Laue case, the tangential dependence of δ in (3) suggests that the correct shape of the groove (Fig. 3) should also be parabolic (like in the Bragg case). The expression $LP[\cos\theta/\cos(\theta+\alpha)]/k$ here plays the role of K' in the Bragg case (Hrdý, 2001) and can be substituted into the equation of a parabola. Note that in the Laue asymmetrical case, and in the situation shown in Figs. 2 and 3, the sagittal deviation of the diffracted beam is larger than the sagittal deviation of the forward-diffracted (refracted) beam because $PN > PR$.

The drawback of this method is that, although the groove squeezes the diffracted beam in the sagittal direction, at the same time the groove increases the size of the diffracted beam in the perpendicular

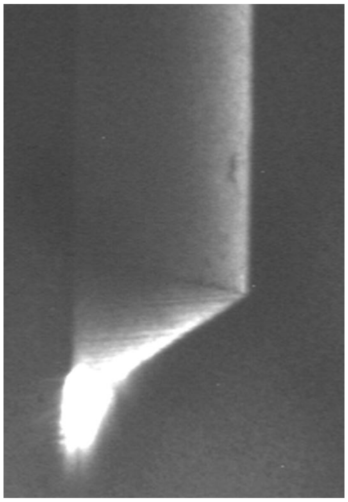

Figure 5
An image of the higher harmonics diffracted from the Laue crystal, with the wedge produced in the lateral part of the crystal. The almost horizontal 'crack' indicates the sagittal splitting of the beam. In the lower part of the picture the overexposed image of the first harmonic is seen.

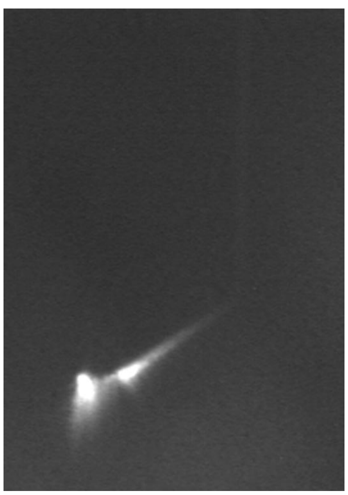

Figure 6
The same image as in Fig. 5 but with a shorter exposure time. The upper spot is the edge of the crystal (the tip of the wedge) seen by the higher harmonics and the lower spot is the image of the edge seen by the first harmonic.

direction. (The same problem arises in the Bragg case when only one grooved crystal is used.) Nevertheless, this effect will be hidden in the increased beam size caused by the Bormann triangle in the lateral thick part of the crystal. If the size of the impinging beam (measured in the plane of diffraction) is comparable to or higher than the depth of the groove, this effect is not too important. In the opposite case, however, the increased size of the diffracted beam must be compensated for in another way. One possibility is to create the profile of the crystal as shown schematically in Fig. 7. This solution also reduces the absorption in the lateral parts of the crystal.

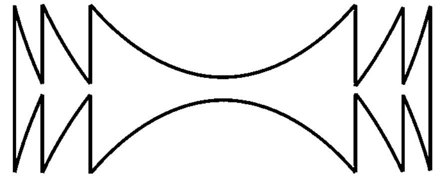

Figure 7
A possible profile of the Laue crystal to reduce the aberration and the absorption in the thick lateral part of the crystal.

Obviously, this kind of focusing monochromator works at one wavelength and in its close neighborhood. The dependence of the focusing distance on the Bragg angle does not show the almost flat region where the focusing distance is practically constant, as it is in the Bragg case.

The meridional bending of this type of crystal to achieve a meridional magnification other than 1:1 may be difficult.

Recently, Zhong *et al.* (2001*a*,*b*) showed that in the case of Laue asymmetrical diffraction the sagittal focusing of diffracted radiation might be achieved by sagittal bending of a crystal. This requires, however, a precise bending mechanism, and focusing at a long distance might be difficult. Like in the Bragg case, focusing may be achieved more easily with the use of the above-described refraction effect in the Laue asymmetrical case, but the estimation of the gain in intensity needs a more detailed analysis for a particular experimental arrangement.

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