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X-ray Inclined Lens

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As defined here, the term 'inclined lens' means a longitudinal parabolic groove fabricated into a crystal monochromator. If properly designed, it should provide the horizontal (sagittal) focusing of an X-ray beam. The focusing is based on the sagittal deviation of the beam diffracted on the wall of the groove. This effect follows from the dynamical theory of inclined diffraction. The focusing efficiency is limited compared with other methods. On the other hand, the simplicity is the main advantage of this device. The exact shape of the groove is calculated and several methods of keeping the vertical dimension of the beam small are proposed.

Keywords: X-ray lenses; inclined diffraction; inclined monochromators; sagittal focusing.

1. Introduction

Inclined diffraction is diffraction on a crystal whose surface is not parallel to the diffracting crystallographic planes and where the plane containing the normals to the surface and to the diffracting crystallographic planes are perpendicular to the diffraction plane, *i.e.* the plane containing the incident beam and the normal to the diffracting planes. Inclined diffraction may be created from conventional asymmetric diffraction by rotating the crystal about the normal to the diffracting planes by 90°; the diffraction is still symmetric. An X-ray monochromator based on inclined diffraction is called an inclined monochromator (Hrdý, 1992; Khounsary, 1992).

The theory of inclined diffraction was developed by Macrander *et al.* (1992) and Hrdý & Pacherová (1993). It was shown by Hrdý & Pacherová (1993) that an X-ray beam diffracted from an inclined crystal is deviated from the diffraction plane by a small angle, δ, in the direction away from the surface (Fig. 1). This deviation increases when the angle of inclination increases. From this it follows that a longitudinal groove fabricated in a symmetrically diffracting crystal (the walls of the groove represent an inclined diffraction and thus must not be perpendicular to the diffracting planes), when properly designed, should concentrate the beam onto the plane of symmetry of the groove. Recently we have observed this effect (Hrdý *et al.*, 1998) on the toothed monochromator (Hrdý & Pacherová, 1993) at the GILDA CRG beamline at the ESRF. The toothed crystal consisted of simple V-shaped grooves. Each wall of such a groove deviated the diffracted beams sagittally by some constant angle towards the plane of symmetry of the groove. For the groove to behave like a lens, it is necessary that the angular deviation increases with increasing distance from the centre of the groove. This implies that the slope of the wall must increase with increasing distance from the centre of the groove. However, as will be shown later, due to the diffraction from the groove, the vertical dimension of the diffracted beam increases. Such a grooved crystal may obviously be used to concentrate narrow (*e.g.* undulator) beams sagittally. As the focal length changes with wavelength and cannot be tuned as in the case of a sagittally bent crystal, several different and parallel grooves fabricated into one crystal may cover the desired range of wavelengths. Compared with the Bragg–Fresnel optics or a refractive lens (Elleaume, 1997), there are at least two disadvantages. First, the focusing is one-dimensional. Moreover, for short wavelengths the groove is deep and it may be necessary to compensate for the increase of the vertical dimension of the diffracted beam. Second, the horizontal dimension of the focus has its minimal value (it can never be a point), which is connected to the finite width of the single-crystal diffraction pattern. This means that the focusing efficiency

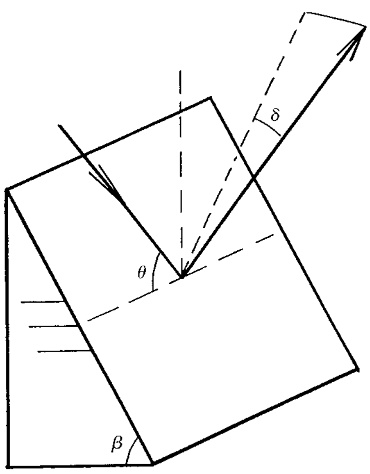

Figure 1
Schematic diagram of the inclined diffraction.

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is limited. On the other hand, the inclined lens is very simple. The subject of this paper is the determination of the exact shape of the groove (lens), the estimation of the efficiency of focusing, and the discussion of the possibilities of keeping the vertical dimension of the beam unchanged or at least reasonably small.

2. The shape of the groove

The method of determining the deviation δ of the diffracted beam from the diffraction plane was explained by Hrdý & Pacherová (1993) and will be used (with small modifications) in this paper. However, because of certain simplifications used by Hrdý & Pacherová (1993), the theory developed below is not valid for very high inclination angles β (*i.e.* for the angles between the diffracting planes and the surface of the crystal near 90°). The simplifications consist of replacing the incident and reflection spheres in reciprocal space by planes and replacing the dispersion surface by a hyperbolic cylinder. The situation in the reciprocal space is seen in Fig. 2, taken from Hrdý & Pacherová (1993), and in Fig. 3 (Batterman & Cole, 1964). The deviation δ is given by

$$\delta = 2\underline{LQ}\tan(90-\theta)\tan\beta/k. \qquad (1)$$

The distance $\underline{LQ}$ between points L and Q shown in Fig. 3 is

$$\underline{LQ} = [k^2 - (1/2d)^2]^{1/2} - [k'^2 - (1/2d)^2]^{1/2}, \qquad (2)$$

where

$$k' = k(1 - \Gamma F_0/2), \qquad (3)$$

$$\Gamma = r_e\lambda^2/\pi V, \qquad (4)$$

r_e is the classical electron radius, V is the volume of the unit cell, F_0 is the structure factor for 'zero' reflection, k is the vacuum value of the wavevector (= $1/\lambda$), θ is the Bragg angle and d is the net plane spacing for (hkl) reflection.

It is easy to show that

$$\tan(90-\theta) = 1/\tan\theta = 2d[k^2 - (1/2d)^2]^{1/2}. \qquad (5)$$

Substituting (3) into (2), neglecting $(\Gamma F_0/2)^2$, and using the Taylor formula, it holds that

$$\underline{LQ} = k^2\Gamma F_0/2[k^2 - (1/2d)^2]^{1/2}. \qquad (6)$$

Finally, by substituting (6), (5) and (4) into (1), we obtain

$$d = K\tan\beta, \qquad (7)$$

where

$$K = (2r_eF_0/\pi V)d\lambda. \qquad (8)$$

For silicon, $K = 1.256 \times 10^{-3}d[\mathrm{nm}]\lambda[\mathrm{nm}]$. The value of δ is small. For example, for diffraction on (333) planes, $\beta = 69°$ and $\lambda = 0.0775$ nm, *i.e.* for the case described by Hrdý *et al.* (1998), the obtained value of δ is 2.65×10^{-5}. The corresponding deviation of the beam at a distance of 10 m is 0.265 mm. This value may already be important for thin beams from an undulator. For (111) diffraction and λ = 0.155 nm, the deviation δ is 1.6×10^{-4}. The deviation δ may be easily measured from the splitting of the beam diffracted from the top of a triangular tooth (Hrdý *et al.*, 1998).

It has been shown by Hrdý & Pacherová (1993) that the deviation δ increases when passing through the angular range of a diffraction curve (region of total reflection) creating a small divergence in the direction perpendicular to the diffraction plane. This means that a synchrotron radiation beam which is vertically divergent and which has zero horizontal divergence will have, after deviation by an angle δ, a horizontal (sagittal) divergence given by

$$w = \delta D/\underline{LQ}, \qquad (9)$$

where

$$D = k\Gamma F_{333}\sec\theta, \qquad (10)$$

is the diameter of the hyperbola (Batterman & Cole, 1964). The horizontal divergence (9) is determined as the difference of the deviations corresponding to points Q_1 and Q_2 (Fig. 2). D is the distance between these points.

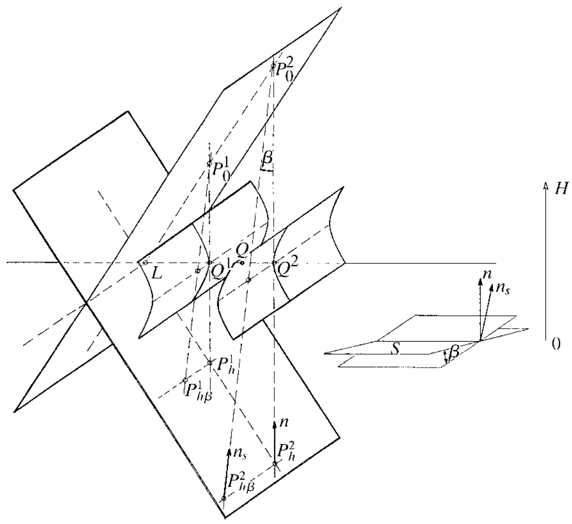

Figure 2
Part of a diffraction diagram in reciprocal space. The spheres of incidence and reflection are approximated by planes and the dispersion surfaces by hyperbolic cylinders. n and n_s are normals to the diffracting planes and surface, respectively.

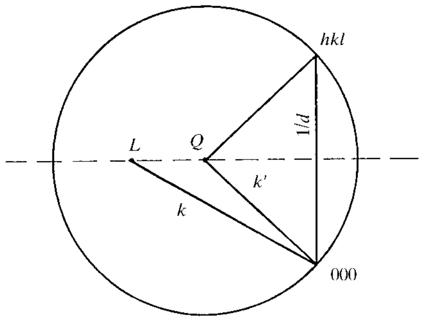

Figure 3
Ewald sphere in reciprocal space corrected for the average index of refraction. L, the Laue point, would be the centre in a vacuum; Q is the centre in the real crystal.

For the determination of the shape of the groove we will suppose that the distance of the monochromator from a point source is S and the focal length is f (Fig. 4). Let the shape of the groove be described by a function $y(x)$ (Fig. 5). For the groove to act as a lens, it is necessary that the beam impinging on the crystal at a distance x from the plane of the symmetry of the groove be deviated by an angle

$$\delta \simeq \tan\delta \simeq [x(S+f)/S]/f = xR/f. \qquad (11)$$

Equation (7) may be rewritten in the following way,

$$\tan\delta = K(\mathrm{d}y/\mathrm{d}x). \qquad (12)$$

Equations (11) and (12) give a differential equation with the solution

$$y = (R/2Kf)x^2 + \text{constant}. \qquad (13)$$

The meaning of the above result is that the parabolic groove focuses the radiation and thus acts as a horizontally (sagittally) focusing lens. For a parallel incident beam, $R = (S + f)/S$ may be taken as equal to unity. In fact, the incident beams corresponding to different values of x strike the crystal at different distances from the source and thus the diffracted beams intersect the plane of symmetry of the groove also at different distances from the crystal, which may cause a slight smearing of the focus. However, this effect is negligible as far as the length of the crystal is negligible compared with the focal length f. It should also be noted that the groove fabricated into the first crystal represents the inclined diffraction and thus is advantageous from the point of view of heating the crystal by the radiation because it increases the footprint area of the radiation on the crystal.

From (13) it also follows that a particular shape of inclined lens fabricated for a certain wavelength may also be used for other wavelengths, but then the focal length f will be different. If a short focal length is required, then the groove may be fabricated in the second crystal also or multiple diffraction from the groove may be utilized. Fig. 5 shows the shape of the groove for a silicon crystal, (111) diffraction, $\lambda = 0.15$ nm and $f = 10$ m ($R = 1$).

3. Properties of the focused beam

As was shown above, the radiation diffracted from the parabolic groove is sagittally focused but this is accompanied by an increase in the vertical size of the beam, as may be seen in Fig. 6. There are several possibilities of how to keep the vertical size small; this will be discussed in the following paragraph.

For simplicity, let us suppose that the horizontal width of the impinging monochromatic radiation at the monochromator position is W and the horizontal distribution of the intensity in the impinging beam is constant. Then the beam diffracted from the bottom of the groove ($x = 0$) is not deviated and thus has zero horizontal divergence and creates a short vertical line at the focal plane (due to the finite width of the single-crystal diffraction pattern). The

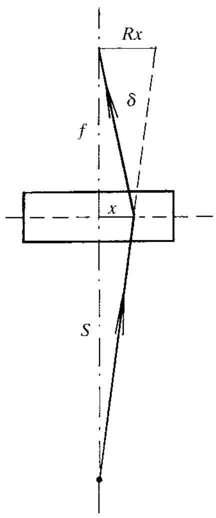

Figure 4
The geometry of an X-ray beam diffracted from the groove at a distance x from the plane of symmetry of the groove. S is the distance between the point source and the crystal, and f is the distance between the crystal and the focal plane.

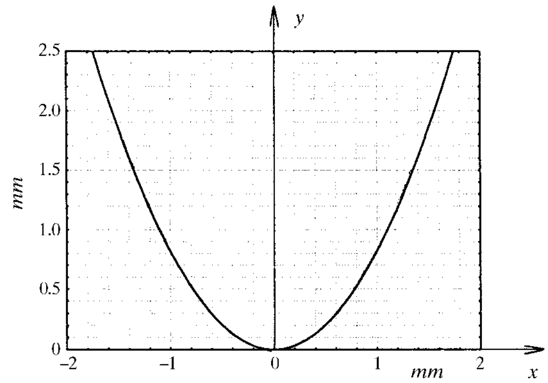

Figure 5
The shape of the groove is described by a function $y(x)$. For the groove to behave as a sagittal lens, it is necessary that $y(x)$ is a parabola. The parabola shown here is calculated for (111) diffraction on an Si crystal, $\lambda = 0.15$ nm, $f = 10$ m and $R = 1$.

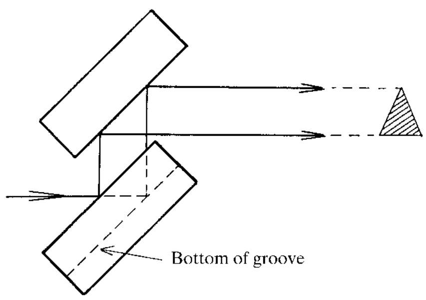

Figure 6
The diffraction on the groove increases the vertical dimension of the diffracted beam. The profile of the focused beam is roughly triangular.

side beam ($x = W/2$) is deviated according to (11) by an angle $\delta = WR/2f$ and, owing to its horizontal divergence (9), it creates a tilted line in the focal plane with horizontal projection $WDR/2\underline{LQ}$. Thus the image of the whole beam in the focal plane is similar to a triangle with a full width at half-maximum equal to $WDR/4\underline{LQ}$. This may be compared with the width of the beam at the focal plane without focusing, which would be WR. From this it follows that, after focusing, the beam is narrowed $4\underline{LQ}/D$ times and thus the peak intensity at the centre of the focus (when integrated in the vertical direction) is increased also by the same value. For λ = 0.0775 nm and (333) diffraction, the value of $4\underline{LQ}/D$ is 7.3, and for λ = 0.155 nm and (111) diffraction, $4\underline{LQ}/D = 4.44$. These values represent a rough estimation of the increase of the intensity at the centre of the focus, provided that the vertical size of the beam is not increased (see §4). The real values will be rather higher. An increase of the vertical dimension of the beam would lead to a decrease of the intensity at the centre of the focus (see §4). The above explanation demonstrates the limitation of the inclined lens.

4. Vertical dimension of the diffracted beam

It was pointed out in the previous paragraph that the diffraction from a single groove increases the vertical dimension of the diffracted beam, which partially deteriorates the effect of focusing in the horizontal direction. It may be shown that a horizontally divergent beam with a negligible vertical dimension will have, after diffraction from a crystal with a groove, the vertical dimension

$$h = 2g\cos\theta \qquad (14)$$

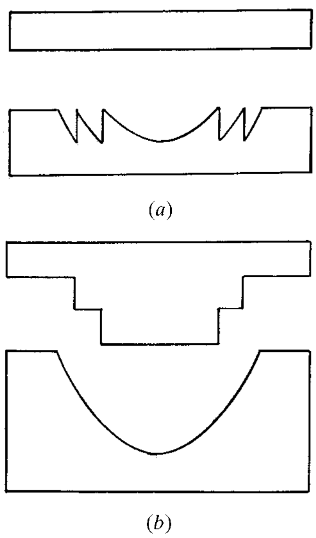

Figure 7
Schematic diagram of two possible methods of reducing the increase of the vertical dimension of the diffracted beam shown in Fig. 6.

at any distance from the crystal (g is the depth of the groove). This means that the vertical dimension of a real beam will be increased by h.

Let us suppose that the cross section of an undulator beam impinging on a grooved crystal is 1 mm × 1 mm. For λ = 0.155 nm and Si(111) diffraction, the shape of the parabola is shown in Fig. 5. It may be seen that the sufficient depth of the groove is 0.2 mm and, according to (14), the vertical dimension of the beam will be increased by h = 0.39 mm. Thus the vertical dimension of the beam at the focal plane will be (1 mm × R) + 0.39 mm, where the first term represents the vertical size of the beam without the groove. It may be seen that the increase of the vertical size of the beam is not substantial and thus the decrease of the intensity in the centre of the focal spot due to the smearing of the beam in the vertical direction is small.

For shorter wavelengths the depth of the groove increases and may substantially influence the intensity at the centre of the focus. A vertically focusing mirror may obviously be used to decrease the vertical dimension of the beam in the focal plane. Besides using a mirror, there are several other possibilities; some of them will be briefly discussed here.

Fig. 7(*a*) shows the modification of the groove profile (an approach known from visible optics) which may reduce the vertical size of the beam. Practical realization of such a lens is possible but obviously difficult. However, replacing the central segment of the groove by a cylindrical groove, and other parabolic segments by planes, would simplify the realization of the lens.

Another solution, which is presented in Fig. 7(*b*), consists of the reduction of the increased vertical dimension of the beam diffracted from the groove fabricated into the first crystal by making a step-like structure on the surface of the second crystal. This gives the same result as in the previous case and seems to be easier to make. The vertical size of the beam depends on the number of segments or steps. In both cases presented in Fig. 7, the vertical size of the beam is increased by $h/3$.

Probably the most elegant approach is shown in Fig. 8. It is based on a four-crystal dispersive $(-,+,+,-)$

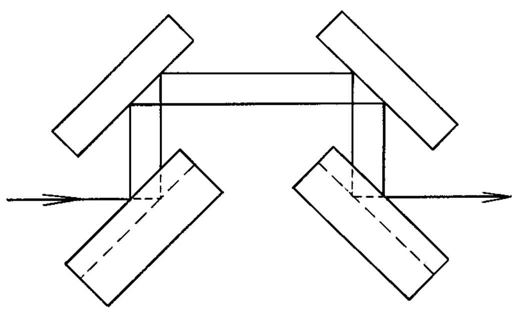

Figure 8
A four-crystal dispersive $(-,+,+,-)$ arrangement. The increase of the vertical dimension of the beam diffracted from the groove fabricated in the first or the second crystal is completely compensated by the groove fabricated in the third or the fourth crystal.

arrangement. In order for the height of the diffracted beam to remain unchanged, it is necessary that the groove is fabricated in one of the first pairs of crystals and in one of the second pairs of crystals or in all four crystals. This should be possible because δ is relatively small.

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