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Meridional focusing of X-rays diffracted onto a single crystal with a transversal groove (Bragg-diffraction asymmetric lens)

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It is shown that a properly designed transversal groove machined into the surface of a single-crystal monochromator may concentrate (focus) the diffracted radiation meridionally. From this result and from previous papers on the Bragg-diffraction inclined lens it follows that a properly designed depression fabricated into the surface of a single-crystal monochromator should provide two-dimensional focusing of a diffracted synchrotron radiation beam.

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

1. Introduction

Recently it was shown (Hrdý, 1998) that a longitudinal parabolic groove fabricated into the surface of a single-crystal X-ray monochromator should concentrate a diffracted synchrotron radiation beam in the sagittal direction. In a subsequent paper (Hrdý & Siddons, 1999) the sagittal focusing of 15 keV synchrotron radiation at a distance of ~5 m was successfully demonstrated at the NSLS. It was shown that the refraction effect at Bragg-inclined diffraction is responsible for the sagittal focusing. Here it is shown theoretically that it is also possible to concentrate synchrotron radiation meridionally by diffraction on a properly designed transversal groove. It is concluded that two-dimensional focusing should be generated by diffraction of X-ray synchrotron radiation on a crystal with a properly designed depression in a diffraction surface.

2. Diffraction on a transversal groove

It is well known that in asymmetric Bragg diffraction the angle of incidence is different from the reflection angle, as shown in Fig. 1. According to Matsushita & Hashizume (1983) the following relations hold for monochromatic radiation,

$$\Delta\theta_0 = 0.5(1 + 1/b)\Delta\theta_s, \tag{1}$$

$$\Delta\theta_h = 0.5(1 + b)\Delta\theta_s, \tag{2}$$

$$\omega_0 = \omega_s / b^{1/2}, \tag{3}$$

$$\omega_h = \omega_s b^{1/2}, \tag{4}$$

$$b = \sin(\theta_B - \alpha)/\sin(\theta_B + \alpha), \tag{5}$$

where $\Delta\theta_s$ is the deviation of the center of the Darwin–Prins curve from the Bragg angle θ_B for a symmetrical diffraction ($\alpha = 0$) and ω_s is the width of the Darwin–Prins curve for a symmetrical diffraction. The angle ω_0 is an angular region in which an asymmetrically cut crystal accepts monochromatic radiation which is diffracted into an angular region ω_h. [For Si(111) and $\lambda = 0.15$ nm these values are $\Delta\theta_s = 3.04 \times 10^{-5}$ and $\omega_s = 3.24 \times 10^{-5}$.]

From (1) and (2) it is seen that the angle of incidence ($\theta_B + \Delta\theta_0$) and the angle of reflection ($\theta_B + \Delta\theta_h$) are different and their difference δ is given by

$$\delta = \Delta\theta_0 - \Delta\theta_h. \tag{6}$$

Substituting (1), (2) and (5) into (6) gives

$$\delta = 2\Delta\theta_s \tan\theta_B \tan\alpha/(\tan^2\theta_B - \tan^2\alpha). \tag{7}$$

This situation is shown schematically in Fig. 2. The two parallel beams impinging on the two different walls of the V-shaped groove create two convergent beams after diffraction. It is obvious that to concentrate the diffracted beam into a small spot the profile of the groove must be more complicated.

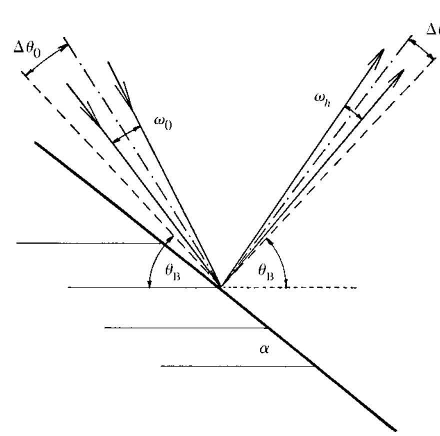

Figure 1
Geometry of Bragg asymmetric diffraction for monochromatic radiation.

Let the profile of the groove be described by a function $y = f(x)$ (see Fig. 3). Let us suppose that the impinging radiation is parallel. In order that the beam impinging on the wall of the groove at a point $A(x,y)$ be diffracted to the focus F, the deviation δ must be

$$\delta = [-x\sin(\theta_B + \Delta\theta_0) + y\cos(\theta_B + \Delta\theta_0)]/F, \qquad (8)$$

where F is the focusing distance.

Taking into account that here $\tan\alpha = -f'(x)$ (first derivative) and neglecting $\Delta\theta_0$ in (8), then (7) and (8) give the differential equation

$$[x\sin\theta_B - f(x)\cos\theta_B]/F = 2\Delta\theta_s \tan\theta_B\, f'(x) / \left\{\tan^2\theta_B - [f'(x)]^2\right\}, \qquad (9)$$

which describes the shape of the transversal groove.

The numerical solution for $\lambda = 0.15$ nm with an Si(111) monochromator and $F = 5$ m is shown in Fig. 4. Fig. 5 shows the dependence of α on x. It is seen that the angle $|\alpha|$ approaches asymptotically the angle of incidence (the angle between the impinging beam and the diffracting planes) for large and small x and only differs noticeably from it at -2 mm $< x < 2$ mm. This region represents the width of the groove that is feasible and it is obviously compatible with the vertical size of a synchrotron radiation beam. It is interesting to note that the groove is asymmetrical. Its shape obviously depends on λ and F. In order that this focusing monochromator could be used for a broad wavelength region, it is necessary to produce either several parallel grooves for various λ or only one groove whose shape changes transversally. The focusing conditions will be then adjusted by the translation of the crystal.

The differential equation (1) was solved under the assumption that θ_B is a constant, independent of x. This is not exactly true even if the impinging radiation is parallel. For every x, and thus every α, the crystal chooses a particular wavelength to be diffracted. To estimate the error in the determination of δ due to this simplification we calculated the wavelength which is diffracted at $\alpha = 10°$ and obtained the value $\lambda = 0.1469$ nm. (The wavelength diffracted at $\alpha = x = 0$ is $\lambda = 0.015$ nm.) The corresponding value δ is only higher by 5%, which is acceptable.

3. Discussion

Synchrotron radiation monochromators usually consist of two crystals set in an $(n, -n)$ position. The combination of a symmetrical and an asymmetrical diffraction in this position leads to 'detuning' of the diffraction regions in both crystals (Matsushita & Hashizume, 1983) such that only part of the radiation is diffracted from both crystals. For example, while for $\alpha = 0$ the reflected crystal function of the first crystal perfectly overlaps the incident crystal function of the second crystal, for $\alpha = 8.7°$ these functions overlap only at a half-maximum height. This undesirable effect becomes less important for large F which needs only a shallow groove with small values of α. This is different from the sagittal focusing based on inclined diffraction, where the inclined diffraction is not influenced by a symmetrical or inclined diffraction on previous crystals.

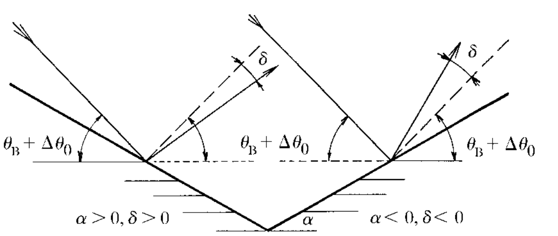

Figure 2
The deviation δ is such that a parallel beam diffracted on a V-shaped transversal groove becomes convergent.

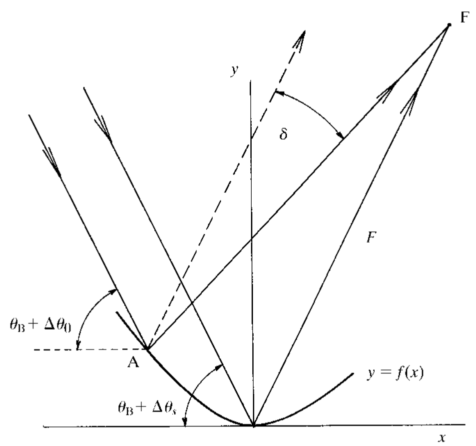

Figure 3
Geometry of focusing on the groove described by the function $y = f(x)$.

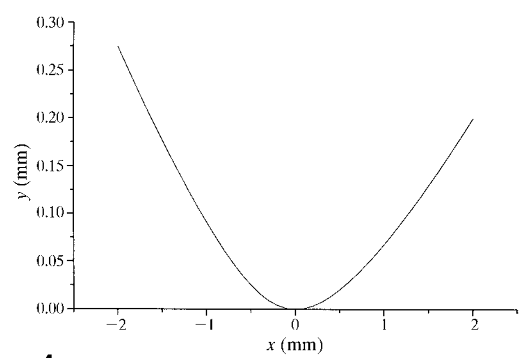

Figure 4
Shape of the groove in an Si(111) crystal for $\lambda = 0.15$ nm and focusing distance $F = 5$ m.

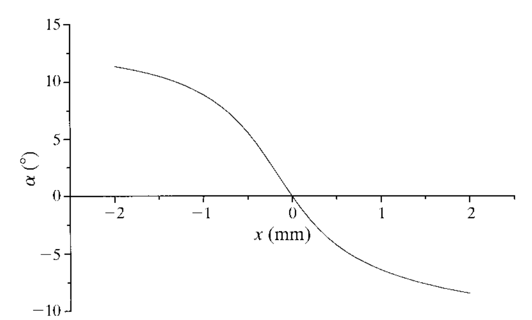

Figure 5
Dependence of the asymmetry angle α of the groove from Fig. 4 on x.

From the properties of asymmetrical diffraction it follows that the size of the focus cannot be ideally sharp. The impinging parallel beam is diffracted with a certain wavelength interval $\Delta\lambda$ which corresponds to the width ω_0 of the crystal function. The reflected beam, however, has a divergence $\Delta\omega = |\omega_0 - \omega_h|$, which increases with α ($\Delta\omega = 0$ for $\alpha = 0$). It implies that the side beams are diffracted into the focus F with the maximum divergence $\Delta\omega_{\alpha\,\max}$ and the beam impinging on the bottom of the groove ($\alpha = 0$) is diffracted into the focus with zero divergence. Thus the dimension of the focus (half-maximum width) may be very roughly estimated as $\Delta\omega_{\alpha\,\max}F/2$. The size of the region from which the radiation is squeezed is $2\delta_{\alpha\,\max}F$. (For simplicity here we suppose that $\alpha_{\max}$ is the same on both sides of the groove, which is not true because the groove is not symmetrical.) Obviously the intensity spread in the focus is not uniform and its maximum value may be estimated as $2\delta_{\alpha\,\max}/0.5\Delta\omega_{\alpha\,\max}$. [This situation is similar to the case of diffraction on a single longitudinal groove (Hrdý, 1998). As was shown by Hrdý & Siddons (1999), the broadening of the focus in that case is cancelled by diffracting radiation from two longitudinal grooves on crystals arranged in a dispersive position. The possibility of a similar procedure for meridional focusing is being investigated.]

The surface of the footprint of the impinging radiation on the groove is larger than the surface of the footprint on the flat crystal would be, but the radiation density across the groove is not uniform. From the point of view of the heating of the crystal by synchrotron radiation the situation on the left-hand part of the groove (Fig. 3) is better than on the right-hand part of the groove (where the radiation density is even higher than it would be for a flat crystal). Obviously the groove may be situated such that most of the radiation impinges on the left-hand part of the groove. Then the lattice deformation induced by the radiation may be even smaller than for a flat crystal.

The main advantage of the Bragg-diffraction asymmetric (and also inclined) lens is that it has the function of both dispersing and focusing elements which does not need any bending of crystals and thus it is compact and simple. X-ray monochromators with flat crystals need an additional element to focus the radiation and this element is a source of partial intensity loss due to absorption and scattering. For this reason, for example, the X-ray refractive lens (Lengeler *et al.*, 1999) is efficient only for short wavelengths ($E > 15$ keV for an Al lens; this region may be extended towards lower energy with a Be lens). On the other hand, as compared with Bragg asymmetric lenses, it may create a very small two-dimensional focus which is of the order of micrometers. Also, mirrors or capillary lenses (Bilderback & Thiel, 1995; Thiel, 1998), both based on a specular reflection, may create a small focus but with partial loss of intensity. Moreover, X-ray mirrors are expensive and capillaries create a relatively divergent beam at the focus. In some ways a similar conclusion may be stated for other focusing elements such as, for example, multilayers.

The idea of two-dimensional focusing on the depression combines the sagittal focusing due to the inclined diffraction (Bragg-diffraction inclined lens) with the meridional focusing due to the asymmetric diffraction (Bragg-diffraction asymmetric lens). It is a compact device which should provide a concentration of radiation in both the sagittal and meridional directions. Another approach might be to use the four-crystal (−,+,+,−) arrangement with longitudinal grooves on the second and third crystals and the transversal groove on the fourth crystal. This arrangement may create a sharp focus in the sagittal direction and a concentration of radiation in the meridional direction. Moreover, it may allow the tuning of λ and the focal distance by the translation of crystals, as mentioned above. These devices may compete with other methods for longer wavelengths where the losses of intensity due to absorption in those methods are significant and where the fine focus is not needed. The longer the focusing distance F, the more intensity passes through the monochromator and the higher the angular acceptance.

The tuning of λ or the focusing distance requires rather a complicated shape of the crystal surface. However, the problem of production of such a precise, smooth and namely 'single-crystal' shape has been solved only partially and further research is still required.

Precise comparison with other methods requires a ray-tracing method which may take into account a general shape of the crystal surface. Such a program is being developed in our laboratory. Also, some experimental tests are necessary. So far only a Bragg-diffraction inclined lens has been tested successfully (Hrdý & Siddons, 1999) and even in this case additional experiments are required to determine the limits in the focus production.

4. Conclusions

The above discussion is somewhat simplified and it shows that a meridional focusing of synchrotron radiation on the transversal groove is possible and further theoretical and experimental work is desirable. From this work and from the previous results on sagittal focusing on a longitudinal groove it is obvious that a properly designed depression in the surface of the diffracting crystal should generate a two-dimensional focusing of the diffracted radiation.

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