

Diffractive–refractive optics: (+,−,−,+) X-ray crystal monochromator with harmonics separation

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A new kind of two channel-cut crystals X-ray monochromator in dispersive (+,−,−,+) position which spatially separates harmonics is proposed. The diffracting surfaces are oriented so that the diffraction is inclined. Owing to refraction the diffracted beam is sagittally deviated. The deviation depends on wavelength and is much higher for the first harmonics than for higher harmonics. This leads to spatial harmonics separation. The idea is supported by ray-tracing simulation.

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1. Introduction

X-ray crystal monochromators for synchrotron radiation deliver monochromatic radiation which is contaminated by higher harmonics as follows from the Bragg law. To reject higher harmonics, various approaches have been developed. Except for removing higher harmonics by mirror, the most frequently used approach is a slight ‘de-tuning’ of crystals (Hart & Rodrigues, 1978). Both crystals set in non-dispersive (+,−) position are slightly de-tuned from parallel position such that the Darwin–Prins (DP) curves for higher harmonics no longer overlap whereas the overlapping of DP curves for the first harmonic is still high enough for sufficient intensity throughput. It is obvious that this method does not remove higher harmonics completely and the de-tuning also partly decreases the diffracted intensity of the first harmonic. If both crystals are asymmetrically cut so that the asymmetry indices are different on both crystals, the harmonics rejection effect may even be improved (Bonse *et al.*, 1976). Matsushita & Hashizume (1983) showed that even a channel-cut crystal monochromator with different properly chosen asymmetry indices on both walls may reject higher harmonics in a narrow wavelength region. As discussed by Hrdý & Hrdá (2008), the harmonic free wavelength region may be significantly extended if, for example, one wall of the channel-cut crystal monochromator is properly curved. If the double-crystal monochromator forms a so-called slightly dispersive setting which happens, for example, if the crystals are different but the d spacing is similar, then harmonics are angularly separated and could be shielded by a slit (Bonse *et al.*, 1976). This is the case when the combination of Ge and Si crystal is used. The diffracted beam for the Ge–Si combination is deviated from the incident beam direction but this deviation is small (of the order of degrees). In the same paper (Bonse *et al.*, 1976) it is shown that the combination of symmetrical Laue and Bragg diffraction yields a good rejection of harmonics, but at the cost of absorption in the Laue crystal.

A completely different approach was presented by Zhong (2000). He placed a prism between two crystals set in a non-dispersive (+,−)

arrangement. The prism angularly separated the harmonics, owing to a different refractive index. The individual harmonics are then diffracted from the second crystal at different angles of rotation of the second crystal. This is a combination of refraction and diffraction using two optical elements (crystals and prism). Diffractive–refractive optics, which utilizes refraction in crystals during Bragg or Laue diffraction, allows for separation of harmonics without any prisms. In all of these cases the harmonics suppression or separation happened in the meridional plane and the diffraction was coplanar.

In this paper we propose a new kind of two channel-cut crystals X-ray monochromator in (+,−,−,+) position which spatially separates harmonics owing to the diffractive–refractive effect. The diffracting surfaces are oriented so that the diffraction is inclined and the separation occurs in the sagittal plane. The device is described in the following section and its properties are discussed. The discussion is followed by ray-tracing simulation.

2. Monochromator design

The method proposed is based on the sagittal deviation of the diffracted beam from the inclined surface. As was shown by Hrdý (2001), the sagittal deviation δ is given by

$$\delta = K[(2 + B + 1/B)/\cos \alpha] \tan \beta, \quad (1)$$

where

$$B = \sin(\theta - \alpha)/\sin(\theta + \alpha). \quad (2)$$

Here, α is the angle of asymmetry, β is the inclination angle, θ is the Bragg angle and, for Si,

$$K = 1.256 \times 10^{-3} d_{h,k,l} [\text{nm}] \lambda [\text{nm}]. \quad (3)$$

A new monochromator acting as an X-ray splitter was proposed by Hrdý (2010) and it was shown that this device also separates the first harmonic from the higher harmonics. However, its roof-shape is somewhat complicated and more demanding for fabrication. For only

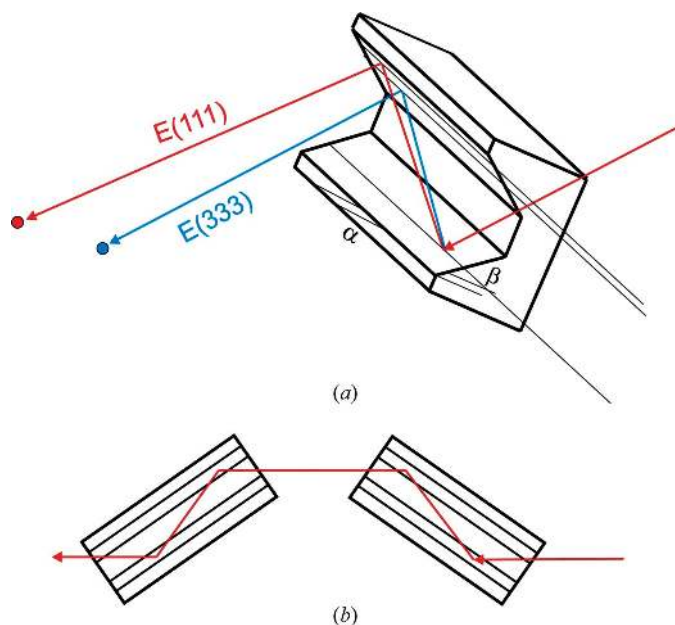


Figure 1
 (a) A channel-cut crystal with inclined diffracting surfaces. (b) The monochromator consists of two such crystals set to a dispersive position. The grooves of the crystals are on the same side, pointing towards the reader (denoted as a '>>' arrangement).

the harmonics separation (*i.e.* no splitting) a much simpler design is sufficient. Fig. 1 shows the shape of the channel-cut double-crystal monochromator which we propose. Both diffracting surfaces are inclined with the inclination angle β . The inclination causes the sagittal deviation of the diffracted beam. This deviation depends on the refraction, which for higher harmonics is smaller than for the first harmonic. We can thus suppose that the higher harmonics are practically not deviated and are diffracted in the direction of the incident beam. Only one crystal shown in Fig. 1(a) extends the beam cross section in the vertical direction and thus it is necessary to use two such crystals set in dispersive (+, -, -, +) position (Fig. 1b). This cancels the vertical and reduces the horizontal (sagittal) spread of the diffracted beam. The crystals must be oriented so that the second channel-cut crystal doubles the sagittal deviation caused by the first crystal, thus the total deviation is four times the value given by equation (1). Fig. 2 shows the calculation of the deviation of the first harmonic from the straight direction of the incident beam at a distance of 10 m from the monochromator. In this calculation the crystals have the asymmetry angle $\alpha = 0^\circ$, *i.e.* the crystals are inclined but symmetrical. As may be seen, the value of deviation is relatively high, *i.e.* the harmonics can be easily separated by slits. As follows from Hrdý (2010), the deviation may be substantially enhanced if asymmetric crystals are used. However, the asymmetry may delimit the usable wavelength range of the monochromator. The inclined crystal, *i.e.* the crystal with an inclined diffraction, works as an optical prism spreading the beam in the sagittal plane. [Similarly, a highly asymmetric crystal spreads the beam in the plane of diffraction, as was shown by Kohn *et al.* (2009). This may obviously also be used for harmonics separation in a very narrow energy region.]

It should be pointed out that owing to the (+, -, -, +) arrangement the monochromator described is a fixed-exit device and the inclined diffraction is advantageous from the point of view of heat load because it decreases the impinging radiation density. A similar crystal geometry for the heat load problem solution has already been proposed by our group (Oberta *et al.*, 2008).

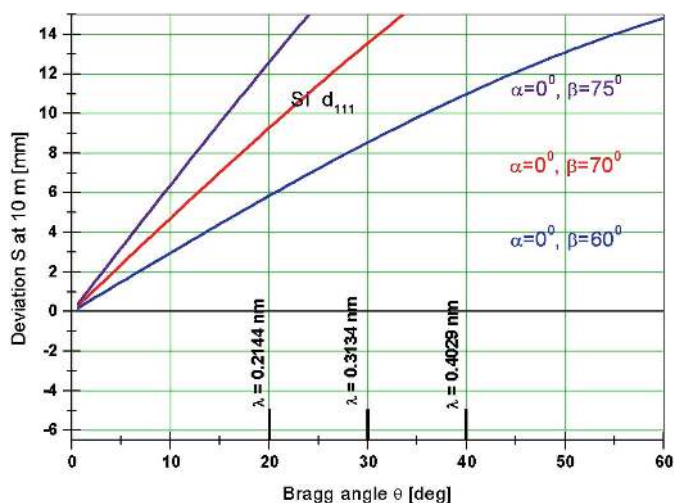


Figure 2
 Sagittal deviation of the first harmonics at 10 m behind the double channel-cut crystal (+, -, -, +) monochromator shown in Fig. 1(b). The deviation of the next (third) harmonic is substantially smaller. The diffraction is on a Si(111) crystal.

The following section will demonstrate the performance of the monochromator by ray-tracing simulation.

3. Ray-tracing simulation

Ray-tracing simulation of the device was performed using the *skl* program (Korytár *et al.*, 2003; Mikulík & Kuběna, 2010). Polychromatic divergent beam from a point source was collimated by a 1 mm \times 1 mm slit at 30 m from the source followed by the two crystals. They were adjusted to maximal throughput for diffraction 111 at 7 keV; the diffraction image was recorded after 10 m. Thus, three spots were intense on the screen 10 m after the crystals (see Fig. 3). The largest spot of diffraction 111 at 7 keV is the most intense. Spots of higher harmonics 333 (diffracting at \sim 21 keV) and 444 (diffracting at 28 keV) are partially overlapping but well separated from the 111

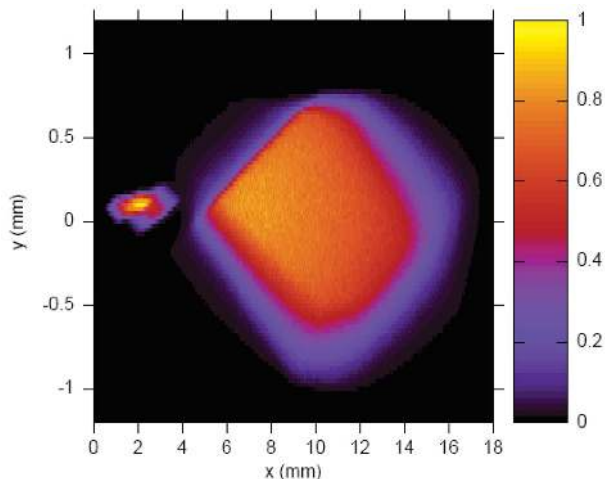


Figure 3
 Ray-tracing simulation of polychromatic radiation diffracted from the Si (111) monochromator described in the text. The horizontal axis shows the deviation of the beam from the straight direction at 10 m from the monochromator. The spot on the right corresponds to the first harmonic while the small spot on the left is unresolved third and fourth harmonics. The separation of the harmonics is easily visible. The simulation was performed for $\alpha = 0^\circ$ and $\beta = 75^\circ$.

spot. The bandwidth (400 eV) was chosen so that all wavelength that may be accepted by the monochromator be available.

The size and the shape of the spots shown in Fig. 3 follow from the DuMond diagram for the above crystals arrangement and from the construction of the sagittal deviation δ in the reciprocal space (Hrdý, 1998). The angular diffraction region of crystals in dispersive arrangement is given by the intersection of two bands representing the DP functions. As the DP function is narrower for higher harmonics, the diffraction region must also be narrower than that for the first harmonic. This explains why the vertical dimension of the higher harmonics in Fig. 3 is smaller. As follows from Hrdý (1998), the sagittal deviation of the beam in the inclined case is proportional to the distance of the DP curve from the exact Bragg angle, and the sagittal width (spread) of the beam is also proportional to the width of the DP curve. From this it follows that the sagittal width of the higher harmonics (*i.e.* its horizontal dimension in Fig. 3) is smaller. Thus the spot corresponding to the higher harmonics must be smaller in both directions.

The intersection of the DP bands in the DuMond diagram has a diamond-like shape. Both angular limits of the intersection correspond to one wavelength for which the sagittal deviation δ is the same (Hrdý & Siddons, 1999). (The small sagittal deviation on one crystal is compensated by the large sagittal deviation on the other crystal.) This corresponds to the upper and lower parts of the spots in Fig. 3 which are without the sagittal spread. The angular center of the intersection of DP bands, however, covers the finite region of wavelengths and the whole DP function and thus the sagittal spread is maximal. This explains the diamond-like shape of the spots.

As can be seen from Fig. 3, the sagittal deviation of the beam is accompanied by its sagittal spread. This, in our case, reduces the peak intensity of harmonics (as compared with non-inclined channel-cut crystals) by about five times. This is a drawback of this arrangement and it also concerns the X-ray splitter (Hrdý, 2010). The system behaves as a source with finite horizontal dimension (here 1 mm) and with divergent radiation (the sagittal spread). After choosing the desired harmonic, the radiation may be partially refocused by mirror.

The above-described arrangements of crystals may be schematically symbolized as '>>' (the grooves are pointing in the same

direction). The above crystals, however, may be arranged as '<<', *i.e.* the grooves are pointing in opposite directions. Then the sagittal spread is fully canceled by the second crystal. In this case the unwanted harmonics must be shielded before the second crystal. A detailed study is out of the scope of this article and will be part of a paper which is now under preparation.

4. Conclusion

The harmonics separation grows with wavelength. If the crystals are inclined but symmetrical ($\alpha = 0$), then the tunability is limited only by the shape and the dimensions of the crystals (see Fig. 2). If the crystals are inclined and asymmetrical, then in addition the Bragg angle θ must be larger than α .

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