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A proof-of-principle experiment of a novel harmonics separation optics for synchrotron facilities

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A proof-of-principle experiment of a novel harmonics separation optics for synchrotron facilities is presented. The harmonic separator is a Si crystal cut in an inclined geometry in which the impinging beam undergoes a diffractive–refractive effect owing to the dispersive nature of X-ray refraction. A polychromatic beam containing higher-order energies is spatially separated behind the separator into individual monochromatic diffraction spots. A synchrotron experiment at a bending-magnet beamline with 7 keV fundamental energy is presented. The spot of the third-order harmonic of 21 keV is deviated from the fundamental by 0.35 mm at a distance 1 m behind the device.

Keywords: harmonics separation; diffractive–refractive optics; inclined geometry; higher order.

1. Introduction

The contamination of experimental data by higher-order harmonics represents a problem at synchrotron beamlines. In the past decades several approaches have been developed in the field of methods and instrumentation to overcome this problem. The first attempt was made using two different crystal materials instead of one crystal material, forming a double-crystal monochromator (DCM) (Bonse *et al.*, 1976). Using a system made of a Si and a Ge crystal, the diffracting angles of the higher-order harmonics at the Si crystal do not coincide with the angles for the Ge crystal. The diffracting angle of the Ge is matched to the fundamental energy diffracted from the Si crystal. At the same time the diffraction conditions are not fulfilled for the higher orders. In this way only the fundamental energy is diffracted. The next approach was undertaken by de-tuning two crystals forming a DCM (Hart & Rodrigues, 1978). The Darwin–Prins diffraction curve has different FWHMs for the fundamental energy and for the higher-order harmonics. By rocking or de-tuning one of the two crystals of a DCM the narrower Darwin–Prins curves of higher-order harmonics are shifted away from each other, until they no longer overlap or only overlap by a very little. A drawback of this method is the loss of flux owing to the simultaneous de-tuning of the Darwin–Prins curve of the fundamental energy. In the 1980s a method based on an asymmetric crystal set-up was introduced (Hashizume, 1983; Matsushita & Hashizume, 1983; Hrdá & Hrdý, 2006; Treimer & Hildebrandt, 1989). By applying an asymmetric geometry the diffracting angles of the higher-order diffractions no longer coincide. A different case is when the asymmetry is achieved by a curved surface; here the higher-order harmonics separation is achieved for a broad range of Bragg angles (Hrdá & Hrdý, 2006). A different approach was used by Zhong (2000), who used acrylic blocks as refractors and thus the higher-order harmonics were spatially separated.

In this paper we show that the inclined higher-order separator (Fig. 1) has several advantages compared with the previously introduced methods. First, it has no flux loss owing to de-tuning or use of different crystal structures. Second, filtering of the unwanted higher orders can be carried out using a simple slit system. Finally, the inclined separator, when operated in the dispersive two channel-cut crystal mode, can

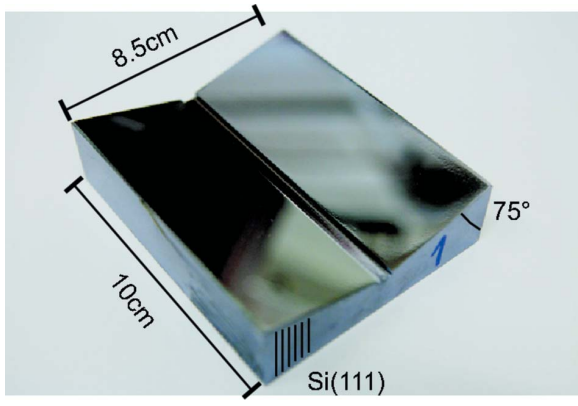

Figure 1
The inclined Si(111) higher-order separator. The inclination angle β is 75°. The gap in the middle is for better access for the polishing tool.

replace the beamline's monochromator owing to its energy-selective nature. A theoretical description of the inclined separator has already been presented elsewhere (Hrdý *et al.*, 2011).

2. Experimental preparation

The experiment was performed at the optics beamline at the Swiss Light Source (Paul Scherrer Institute) (Flechsig *et al.*, 2009). As a source we used a bending magnet (BM), set to a (fundamental) energy of 7 keV. This energy was used because the BM increases higher-order contamination at this energy by ~17%. The inclined separator was mounted on a goniometer. The dimensions of the crystal separator (in mm) are 100 × 85 × 25 (L × H × T) and the inclination angle is $\beta = 75^\circ$ (Fig. 1). Because of the atypical surface geometry (V-shaped crystal) it was difficult to polish the inclined surface to optical quality using a polishing machine, therefore the crystal was hand polished. The surface roughness was measured using a white-light interferometer (Zygo NewView 5010 profiler). The peak-to-valley values at different points at the surface were between 150 nm and 300 nm. This surface quality is due to the strong etching which was performed on the crystal as part of the production process. After the strong etching process there were visible artifacts left on the surface of the crystal separator which were difficult to smooth out by polishing without reducing the crystal thickness too much.

Between the BM and the inclined separator was a low-vacuum pipe and two 100 µm CVD (chemical vapour deposition) windows. As detectors we used a silicon photodiode (AXUV100) and X-ray film from the FOMA company. The photodiode was used for the adjustment of the Bragg diffraction. The detectors were mounted on the 2Θ arm of the goniometer (Fig. 2). The X-ray beam, consisting of the fundamental energy of 7 keV and higher-order energies, impinges on the inclined surface and is diffracted–refracted. The refractive effect is energy-dependent; higher-order energies are less deviated. The spectral dependence of the deviation distance calculated according to Hrdý *et al.* (2011) is shown in Fig. 3. This deviation is also called the sagittal deviation because it is in the sagittal plane. The deviation distance is the offset from the geometrical path that the diffracted beam would follow if diffracted from a plane surface in a coplanar geometry. One can see that the deviation distance is different for the fundamental energy (7 keV) and the higher-order diffraction (21 keV). The difference is the spatial separation of these two energies. The calculation shown in Fig. 3 is made for an inclination angle $\beta = 75^\circ$ at a distance of 1 m from the two inclined surfaces (one channel-cut crystal).

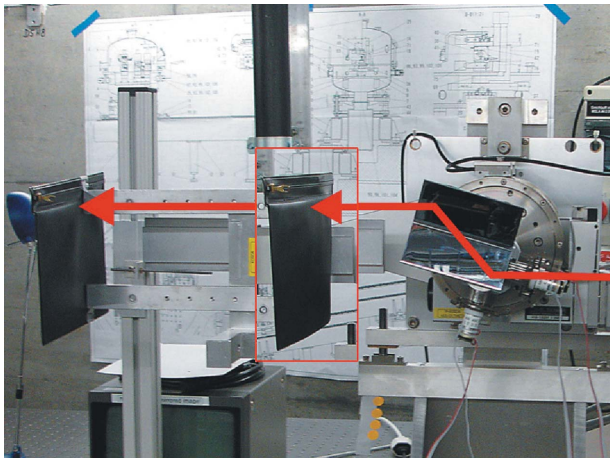

Figure 2
Experimental set-up. The inclined separator is mounted in the Θ-arm of the goniometer. The detector (X-ray film) is mounted on the 2Θ-arm. The X-ray beam is twice diffracted–refracted from the two inclined walls. The X-ray film was mounted at two different distances from the inclined separator. The arrows indicate the propagation path of the X-ray beam.

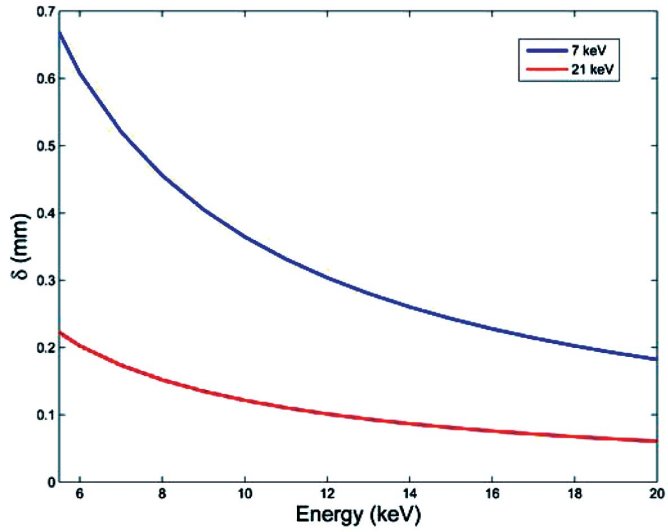

Figure 3
Plot of the deviation distance (δ) *versus* energy for the fundamental energy [black line (blue online)] and the higher order [grey line (red online)]. The deviation is calculated at 1 m after two diffraction events on one channel-cut crystal with inclination angle $\beta = 75^\circ$.

3. Results and discussion

The experimentally obtained results are shown in Figs. 4 and 5. Fig. 4 shows the fundamental and higher-order harmonics separation after one inclined crystal wall. The line shape of the beam is due to the inclined geometry of the diffracting wall. The X-ray film was placed at a distance of 1 m from the inclined separator. One can see that the higher-order separation from the fundamental energy is 0.17 mm, corresponding to half of the value seen in Fig. 3 which is calculated for a double-diffraction event. The stronger line spot is the fundamental energy diffraction and the weaker and narrower line is the higher-order diffraction. The damaged shape (the cut-off at the lower side) of the higher-order diffraction is probably due to the poor surface quality of the inclined separator.

After adjusting the crystal in such a way that the impinging beam was diffracted from both inclined walls, we took an

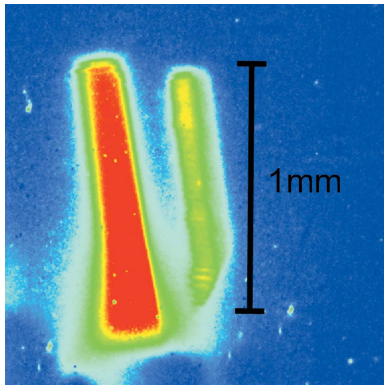

Figure 4
X-ray film image showing the separation of spots of the fundamental energy (7 keV) and the higher-order diffraction (21 keV) after one diffraction event. The spatial separation is 0.17 mm at a distance of 1 m.

image of the separated spots at two different distances (Fig. 5). Fig. 5 shows the separation of the higher order after a distance of 0.5 m (top left) and 1 m (top right). The spot shape is circular owing to the three-dimensional geometry of the sequent non-coplanar diffractions. Fig. 5 shows a clear increase in the separation distance of the fundamental energy and the higher-order diffraction. Owing to the sensitivity of the X-ray film, the two spots were saturated in the peak intensity and a FWHM calculation from the intensity distribution was not possible. The increase in separation distance from 0.17 mm to 0.34 mm after 0.5 m and 1 m between the fundamental energy and the higher-order (third harmonic) is clearly resolved. At the bottom of Fig. 5 is a ray-tracing simulation of a diffraction spot after two diffraction events at a distance of 1 m. The ray-tracing simulation confirms the minimal distance of 111 and 333 maxima corresponding to the measured value, while the simulated 111 spot is more elongated. If the crystal separator is used in a dispersive DCM set-up made out of two channel-cut crystals, then the spatial separation would be even higher, because of the four diffraction events introduced by the four diffraction surfaces. At most beamlines the distance between the monochromator and the experimental hutch is several tens of metres. This additional increase of distance makes the spatial separation of the two diffraction spots even higher, up to several millimetres. In such a case the higher orders can be easily separated by a slit system.

4. Conclusion

In this paper we have presented experimental proof of a novel harmonics separation optics. The optical device is made from a silicon crystal and is cut in an inclined geometry. If arranged in a dispersive set-up the optical device can be operated as a monochromator, making it a multiple-purpose crystal optics. The higher-order separation is based on the diffractive–refractive effect. The diffractive–refractive effect deviates the propagation path of the X-ray beam. The longer the wavelength (the lower the energy) the higher the deviation. Owing to the dispersive nature of the diffractive–refractive effect,

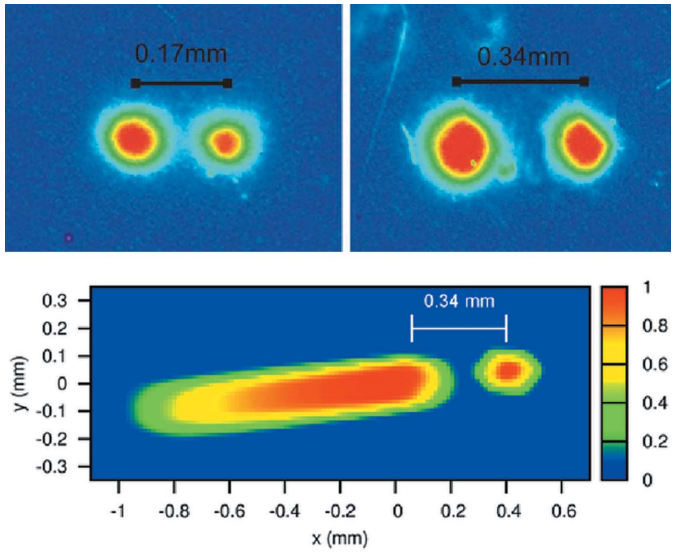

Figure 5
X-ray film images of spot separations of the fundamental energy (7 keV) and of the higher-order diffraction (21 keV) after two diffraction events at two different separator-to-detector distances. The spatial separation between the two diffraction spots increases from 0.17 mm at a distance of 0.5 m to 0.34 mm at a distance of 1 m. At the bottom is a ray-trace simulation of a diffraction spot after two difraction events at a distance of 1 m.

rays with individual energies (higher orders) embraced in an X-ray beam corresponding to the fundamental energy are deviated differently and thus spatially separated. At distances common for synchrotron beamlines, *i.e.* tens of metres, the spatial separation is of the order of several milimetres. Using a simple slit system one can easily block the unwanted harmonics. The advantage of this monochromator compared with other higher-order separation methods is that it does not introduce any flux loss, it is easy to align and it can be implemented in the mechanics of the present monochromator chambers.

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