First observation of meridional focusing of an X-ray beam using diffraction by a crystal with a transverse groove

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The possibility of concentrating a synchrotron X-ray beam using diffraction by a single crystal with a properly designed transverse groove on its surface, suggested earlier, has been studied experimentally. Here, the first experimental demonstration of this effect is reported, performed on beamline BM5 at the ESRF. The experimental result confirms the theoretical model.

Keywords: X-ray focusing monochromators; meridional focusing; asymmetric diffraction.

1. Introduction

Sagittal focusing of synchrotron radiation by means of diffraction by a single crystal with a parabolic longitudinal groove on its surface has been presented in earlier studies (Hrdý, 1998; Hrdý & Siddons, 1999). The focusing effect was demonstrated experimentally. When using a cylindrical hole instead of a parabolic groove (Artemiev *et al.*, 2001; Hrdý *et al.*, 2001), a significant focusing effect has also been observed. This type of focusing is based on a diffractive–refractive phenomenon or, in other words, on the refraction effect occurring during Bragg diffraction. Single crystals with longitudinal grooves in $(-,+)$ or better $(-,+,+,-)$ arrangement can act as a sagittally focusing synchrotron radiation monochromator.

As an analogy to the above-mentioned sagittal focusing, Hrdý & Hrdá (2000) studied the possibility of the meridional focusing of a synchrotron radiation beam by means of X-ray diffraction by a single crystal with a properly designed transversal groove on its surface. They demonstrated theoretically that focusing should be possible and described the procedure to calculate the groove profile for parallel incident radiation.

The refraction effect on which meridional focusing is based is shown in Fig. 1. When an incident polychromatic and parallel beam is diffracted by an asymmetrically cut crystal it is deviated from the direction of specular reflection by an angle δ and at the same time it is angularly spread. The angular spread $\Delta\delta$ and the deviation δ are given by

$$\delta = \Delta\theta_0 - \Delta\theta_h \tag{1}$$

and

$$\Delta\delta = |\omega_0 - \omega_h|, \tag{2}$$

respectively, where $\Delta\theta$ is the angular deviation of the centre of the Darwin–Prins curve (crystal function) from the Bragg angle, ω is the width of the Darwin–Prins curve, and the indices 0 and h refer to the incident and reflected beams, respectively. Through a proper design of the groove it is possible to generate a δ value for each point of the crystal surface such that all diffracted central beams (centres of the angular spread) converge into a focus. The value of the angular spread is zero for symmetrical diffraction (at the bottom of the groove) and increases with the angle of asymmetry α. It is obvious that this angular spread creates a smearing of the focus and results in imperfect focusing. (In the case of sagittal focusing on a longitudinal groove, the angular spread is cancelled by using two grooved crystals in dispersive position.) The relative spread $\Delta\delta/\delta$ is proportional to a structure factor F_{hkl} which means that the focus should be sharper when using diffracting planes with higher (h,k,l). The relative spread $\Delta\delta/\delta$ is also proportional to $b^{1/2}/(1+b)$, which implies a decrease of $\Delta\delta/\delta$ when increasing the absolute values of the angle of asymmetry $|\alpha|$. The factor of asymmetry b is here defined as $b = \sin(\theta-\alpha)/\sin(\theta+\alpha)$ with α positive at grazing incidence.

To take into account the finite divergence of an impinging beam, the differential equation given by Hrdý & Hrdá (2000), which describes the profile of the groove, must be modified in the following way,

$$x\sin\theta_B(1/S+1/f) + f(x)\cos\theta_B(1/S-1/f) = 2\Delta\theta_s\left[f'(x)/\tan\theta_B\right]/\left\{1-\left[f'(x)/\tan\theta_B\right]^2\right\}, \tag{3}$$

where f is the focusing distance, S is the distance of the groove from a synchrotron radiation source, $f(x)$ is a function describing the shape of the groove and $f'(x)$ is the first derivative of $f(x)$.

In a double-crystal $(+,-)$ monochromator composed of a grooved crystal and a flat crystal, the intensity of the diffracted beam should be smaller than in the case of a single grooved crystal. This is due to the decreasing of the overlap of the Darwin–Prins reflectivity curves (crystal functions) of both crystals with increasing α.

2. Experiment

We have designed a groove transverse to the beam direction for an experiment on beamline BM5 at the ESRF and for a wavelength λ of 0.15 nm. The focusing distance was 2 m and the source-to-groove distance was 40 m. The groove was machined into an Si(111) single crystal, and was designed for diffraction of the first order. Fig. 2 shows the calculated profile of the groove. The beam impinged from the left-hand side. One can see that the groove is slightly asymmetric. The

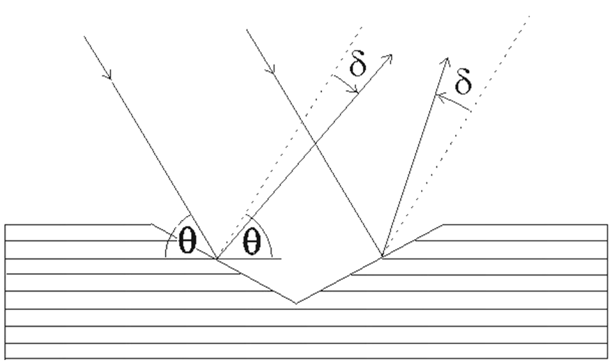

Figure 1
Principle of meridional focusing using a transverse groove.

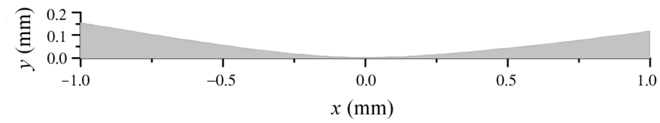

Figure 2
Calculated profile of the transverse groove. The beam impinges from the left-hand side.

groove-manufacturing procedure was as follows. First we ordered a tool in the form of a disc with a profile almost identical to the profile of the groove. We took into account that the groove had to be polished and etched. After cutting the groove, the surface was repeatedly polished and optically measured until minimal deviation was obtained between the profile after final etching and the calculated shape.

For the experiment, the beam was monochromated using the Si(111) monochromator of the beamline. The monochromator crystals were slightly detuned to decrease the contamination of higher harmonics. The grooved crystal was glued to a crystal holder and attached to a HUBER goniometer with its axis horizontal. The image of the diffracted radiation was recorded by a CCD camera, first at the focal distance (2 m from the grooved crystal) and then at 10 cm from the crystal. When the camera was located at 2 m from the grooved crystal, we placed a tube filled with He between the crystal and the camera to minimize the absorption of the radiation by air. For both positions of the camera we took a number of photographs at various angles θ around the main reflection, at intervals of 1.8 arcsec. This allowed us to determine the shape of the rocking curve. The opening of the vertical slit was large enough that the reflection from the flat parts of the crystal could also be seen on both sides of the groove.

An image of the diffracted radiation taken at 2 m from the groove is shown in Fig. 3. The sharp horizontal line is the focused diffracted radiation. The much weaker images above and below are the images of the radiation diffracted from the flat parts of the crystal. The figure is oriented such that the radiation impinges from above. It is obvious from the geometry of the diffraction set up that a large part of the radiation was diffracted by the right-hand part of the groove (see Fig. 2) and was concentrated after diffraction due to the asymmetry ($\alpha < 0$). Also, the image of the beam diffracted from the bottom of the groove ($b = 1$) must be obviously off the centre of the groove image. Thus it is clear that in Fig. 3 also the image of the focused radiation appears off the axis of the image of the groove. Here, the term 'image of the groove' means the dark part between the images of the flat parts of the crystal on both sides of the groove. If the beam was diffracted from the flat part of the crystal instead of the groove, it would have created an image of meridional size 0.75 mm at a distance of 2 m. Owing to the geometry of the experiment and the focusing effect, however, the beam diffracted from the groove was squeezed to about 0.1 mm. This value was close to the resolution of the CCD camera used and the real size of the focus might have been even smaller. The peak intensity at the focus, however, is only about 3.3 times higher than the intensity of the radiation diffracted from the flat part of the crystal.

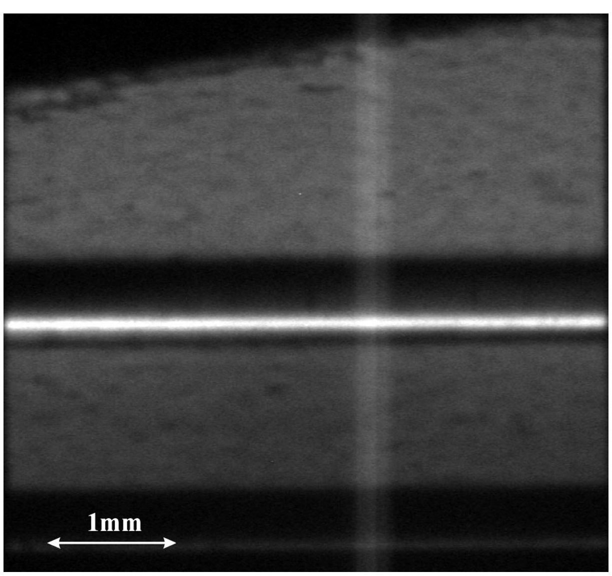

Figure 3
Image of the radiation diffracted on the crystal with a transverse groove taken at 2 m from the crystal.

3. Discussion

The images recorded at the focal distance for various angles θ showed that the crystal was slightly bent, probably due to gluing, such that its surface was convex with a focusing distance of about -20 m. Moreover, the FWHM of the rocking curve when measured at the peak of the focused radiation was $10''$. This was slightly more than the theoretical value and might have been caused by the bending or insufficient etching of the crystal. Both these effects may have had a slight defocusing effect on the diffracted radiation.

As mentioned above, the synchrotron radiation beam was mostly diffracted from the right-hand part of the groove, and was concentrated due to the asymmetric diffraction. This implies that the beam exiting from the groove was much narrower than when diffracted from a flat symmetrical crystal. On its way to the focus, this beam had a tendency to become narrower due to the focusing (δ) and, at the same time, to become broader due to the angular spread $\Delta\delta$. As for (111) diffraction, the values of both effects are comparable (δ is somewhat larger) and tend to cancel each other out. This means that, up to the focus, the beam height slightly decreased, which is what we observed. Fig. 4 shows an image taken at 10 cm from the groove. The sharp image of the beam diffracted from the groove (concentrated beam) is practically superimposed on the image of the radiation diffracted from the flat part of the crystal, because the shift due to the deviation δ was very small at this short distance.

As mentioned above, the FWHM vertical size of the beam impinging on the groove decreased at the focus by about 7.5 times, whereas the intensity at the centre of the focus increased by only 3.3 times as compared with the intensity of the beam diffracted from the flat part of the crystal. There are three reasons for this.

First, owing to the asymmetric diffraction, the right-hand side of the groove had a smaller wavelength acceptance than that of a symmetrically diffracting crystal. For example, the right-hand side of

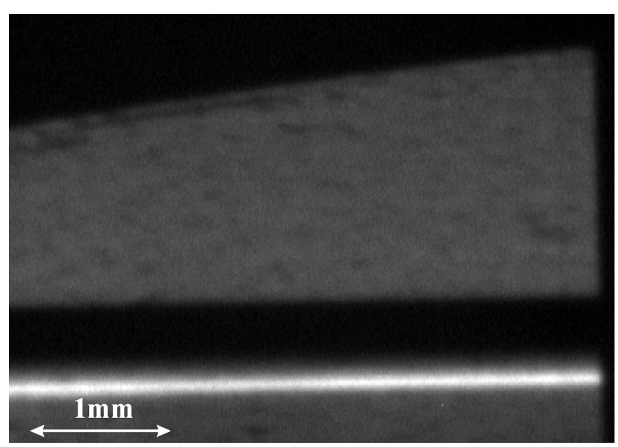

Figure 4
Image of the beam diffracted by the groove taken at 10 cm from the groove.

the groove near the edge (α = 10.8°) has a 2.7 times smaller acceptance than a symmetrically diffracting crystal. Owing to this effect, the right-hand side of the groove reflects about 1.8 times less radiation than a flat crystal would diffract.

Second, the combination of the grooved crystal with the flat crystals of the main monochromator reduced somewhat the diffracted intensity from the groove. At the bottom of the groove the grooved crystal accepted all rays coming from the main monochromator. The right-hand side of the groove near the edge (α = 10.8°) accepted only about three-quarters of what it could have due to the mutual displacement of crystal reflection curves for α = 10.8° and α = 0°. This effect (for the right-hand side of the groove) could be minimized by a slight misalignment of the grooved crystal. This obviously increased the displacement of the crystal reflection curves on the left-hand side of the groove but, as was noted above, only a small part of the radiation (about 20% of the beam profile) was diffracted from this side.

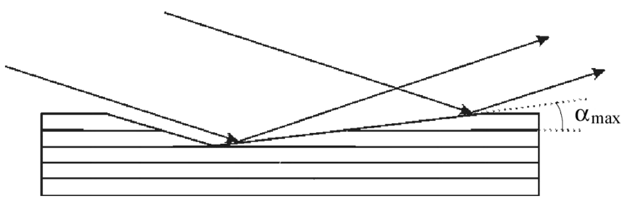

Figure 5
Hypothetical groove to be compared with the groove used in this experiment.

Third, the higher harmonics were not removed completely and thus might have created some background (see below) which was not subtracted.

Finally, one could speculate whether it would not be simpler to use a flat asymmetric crystal instead of the curved groove to squeeze the synchrotron radiation beam vertically. For this reason, let us compare our grooved crystal with the simple flat-asymmetric groove shown schematically in Fig. 5 (flat asymmetric concentrator).

The left-hand wall of the groove is parallel to the impinging beam, and the angle of asymmetry α on the right-hand wall of the groove is equal to the maximal value α of the right-hand side of the groove used in our experiment (α_{max} = 10.8°). The widths of both grooves are the same (3 mm).

As the crystal with the groove shown in Fig. 5 was not available, the comparison is performed by a ray-tracing method, which shows only the angular distribution of the diffracted radiation. Fig. 6(*b*) shows the radiation diffracted from the asymmetric concentrator (see Fig. 5) at 10 cm from the groove whereas Fig. 6(*d*) shows the same radiation at 2 m from the groove. For comparison, the simulations of the diffraction from the curved groove are shown in Figs. 6(*a*) (10 cm from the groove) and Fig. 6(*c*) (2 m from the groove). Here the influence of the flat-crystal main monochromator located before the grooved crystal is not included.

It is seen that close to the crystal the flat asymmetric concentrator may provide a better concentration of the radiation than the groove. At a focusing distance of 2 m, however, a better result is obtained by the groove. This is because in the case of the flat asymmetric concentrator the angular spread $\Delta\delta = 8 \times 10^{-5}$ (which is equal for all diffracted beams since $\alpha = \alpha_{max}$) is not compensated by a focusing

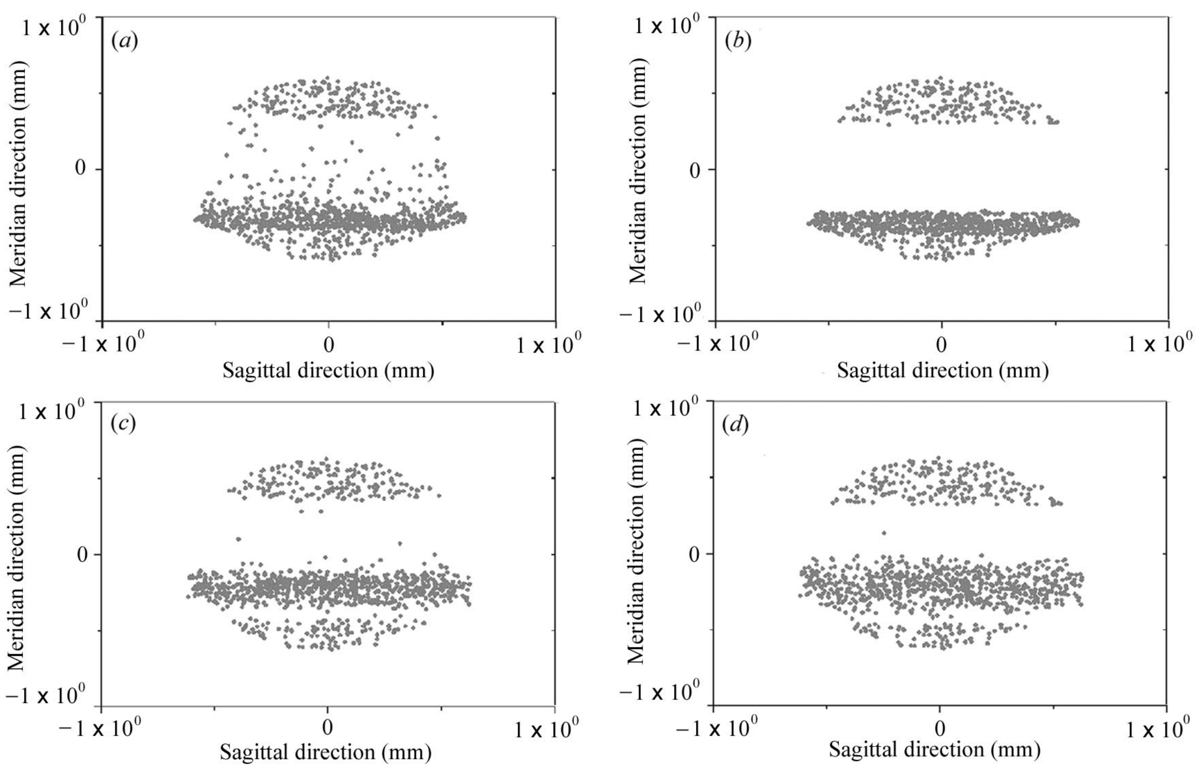

Figure 6
Comparative ray-tracing simulations of synchrotron radiation diffracted from the transversal grooves shown in Figs. 3 and 5. (*a*) and (*c*) show images of the radiation diffracted from the focusing groove at 10 cm and 2 m, respectively; (*b*) and (*d*) show images of the radiation diffracted from a triangular concentrator at 10 cm and 2 m, respectively.

effect. (The deviation $\delta = 1.2 \times 10^{-4}$ is also equal for all diffracted beams.) This leads to a broadening of the beam at 2 m from the crystal where the FWHM size of the beam would be about 0.95 mm. In the case of a curved groove, the angular spread is zero for a beam diffracted from the bottom of the groove and increases with α. Moreover, owing to the maximum constant asymmetry, the wavelength (angular) acceptance is minimal for all beams diffracted from the concentrator which should lead to a diffracted power from the concentrator that is 1.7 times lower than that from the groove. (This effect was not included in the ray-tracing simulation.)

Despite a modest increase of the intensity in the focus (factor 3.3), this experiment clearly showed that the focusing effect due to the diffraction on a transversal groove exists. From the above results it seems obvious that a curved groove is particularly advantageous if the meridional concentration of a synchrotron radiation beam is needed at a longer distance.

The crystal used in the above-described experiments was prepared by Polovodice a.s. in Praha. This research was partially supported by the Ministry of Industry and Trade of the Czech Republic (grant PZ-CH/22) and the Grant Agency of the Academy of Sciences of the Czech Republic (grant A1010104/01).

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 Received 12 July 2001 • Accepted 4 September 2001