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X-ray focusing using an inclined Bragg-reflection lens

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An experimental demonstration showing that a one-dimensional focus can be produced by using the principle of inclined diffraction from a perfect crystal is presented. By machining a groove with a controlled cross-sectional profile it is shown that it is possible to vary the out-of-plane deviations in a controlled manner and hence generate a focus. Also demonstrated is the use of four reflections in (−,+,+,−) dispersive geometry resulting in the cancellation of all beam-spreading in the orthogonal direction. The experiment used an energy of 15 keV with a source-to-crystal distance of 13.5 m and crystal-to-focus distance of 4.5 m. A focus of width 0.29 mm was produced from an incident beam of width 2.7 mm. It is clear from the measurements that a better surface finish would result in a smaller focal spot.

Keywords: inclined diffraction; sagittal focusing; X-ray lens; X-ray monochromator.

1. Introduction

In earlier papers, Hrdý has shown that the extension of the usual dynamical diffraction theory to properly include the third dimension, *i.e.* the out-of-plane behaviour of the dispersion surface, leads to additional angular deviations of the diffracted beam if the surface of the crystal is miscut in a direction out of the diffraction plane (the so-called inclined geometry). Hrdý (1998) discusses the possibility of making a carefully profiled groove in the crystal surface such that all the diffracted beams from within this grooved region pass through a point at some distance from the crystal, *i.e.* forming a focus. This paper describes experiments performed at NSLS to demonstrate this effect.

2. The inclined Bragg-reflection lens (IBRL)

When the surface of the crystal is inclined with respect to the diffracting crystallographic planes in such a way that the surface normal is inclined out of the diffraction plane (this is different from the more usual asymmetric geometry), then the diffracted beam is slightly deviated in the sagittal direction away from the surface. If two such surfaces create a longitudinal groove then the diffracted beams are convergent. If the profile of the groove is parabolic then the groove behaves as a sagittally focusing lens. This idea was presented by Hrdý (1998), where the shape of the groove was calculated and properties of various arrangements were discussed. In that paper the device was called an X-ray inclined lens. The effect is closely related to normal refraction. If the refractive index were equal to unity, there would be no focusing. The effect of sagittal beam concentration using a simple groove with a linear V profile was experimentally observed by Hrdý *et al.* (1998).

Hrdý (1998) showed that, when using a single parabolic groove, two effects play a negative role. The first one is the increase in the vertical dimension of the diffracted beam which may deteriorate the effect of focusing. The second effect is that the focus has a finite horizontal (sagittal) dimension which is connected with the finite width of the single-crystal diffraction pattern. The first effect may be completely removed using crystals with identical grooves in the dispersive (−,+,+,−) arrangement. Another well known advantage of this dispersive arrangement is that it represents a fixed-exit device. However, there is a third advantage which was not mentioned in the previous paper. To understand it we refer to Fig. 1, taken from Hrdý (1998). The monochromatic beam is diffracted in a certain angular region determined by the single-crystal diffraction pattern. The beam diffracted on the first crystal at the beginning of the diffraction region (smaller θ) is deviated sagittally less than the beam that would be diffracted at the end of the diffraction region. The same beam, when impinging on the second crystal with the same inclination angle β and in the dispersion position with respect to the first crystal, will be diffracted at the end of the diffraction region (higher θ) and thus its sagittal deviation will be larger. In other words, the deviation of the beam from the value corresponding to the middle of the reflection region on the first crystal is compensated by the reflection on the second crystal. The resulting sagittal deviation is the sum of the deviations on both crystals and is equal to 2δ, where δ is the deviation caused by a single crystal for the beam at the centre of the diffraction region. The sagittal broadening of the deviated beam typical for a single groove is, in the case of two

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crystals in the dispersive setting, completely cancelled and the focus should be sharp. From the above it is seen that the function of the IBRL for synchrotron radiation is optimal if it is composed of four crystals in the (−,+,+,−) arrangement and if the parabolic grooves are cut into the first and the fourth crystals or into the second and the third crystals or into all four crystals.

As was shown by Hrdý (1998), the basic formula which gives the relationship between the deviation δ and the inclination angle β (not valid for β close to 90°) is

$$\delta = K \tan \beta, \tag{1}$$

where, for silicon, $K = 1.256 \times 10^{-3}\, d_{hkl}$ [nm] λ [nm]. The shape of the parabolic groove is determined by

$$y = ax^2, \tag{2}$$

where y and x are in mm and where a (mm^{-1}) may be determined from the number N of diffraction events on the grooves, source-to-lens distance S (mm) and lens-to-focus distance f (mm) (focal distance) as follows:

$$a = (S + f)/2NKfS. \tag{3}$$

These equations give the complete information needed for the design of the inclined diffraction lens. For typical useful parameters, the width of the parabolic grooves becomes rather small and thus this focusing method is best suited to narrow beams, such as those produced by an undulator. As an example, we consider the following set of parameters. We choose an energy of 15 keV, a source-to-optic distance of 13.5 m and an optic image distance of 4.5 m, parameters appropriate to beamline X6A at NSLS. From (3), for an optic with four reflections we calculate a = 1.142 mm^{-1}. This produces a groove with a depth of 1.142 mm and a width at its mouth of 2 mm. Thus, the sagittal angular acceptance of this optic at 13.5 m from the source is ~150 μrad.

The purpose of this paper is to demonstrate the operation of an inclined lens using the above discussed (−,+,+,−) dispersive arrangement.

3. Experiments

Taking the parameters calculated above, two monolithic silicon devices were machined, each one having the parabolic groove milled into opposing faces [Fig. 2(*a*)]. The crystals were fabricated by Polovodice a.s. (Semiconductors) of Prague using a specially manufactured diamond-cutting wheel having the correct parabolic cross section. One consequence of this technique is that the parabolic groove does not extend across the full face of the crystal, so care must be taken to ensure that the beams fall on the proper part of the crystal. The two monoliths were mirror images of each other, and were arranged in dispersive mode (Beaumont & Hart, 1974), with the inter-crystal angle fixed such that the monochromator transmitted a beam of energy 15 keV [Fig. 2(*b*)].

Our experimental set-up was in two parts. First, using a white-beam hutch (beamline X12A), we set up a goniometer stage with axes to adjust the Bragg angle and the yaw. The two crystals were mounted on a common mounting plate. One was rigidly fixed to the plate, and the other was attached by a three-point kinematic mount which permitted rotation of the crystal about the roll and yaw

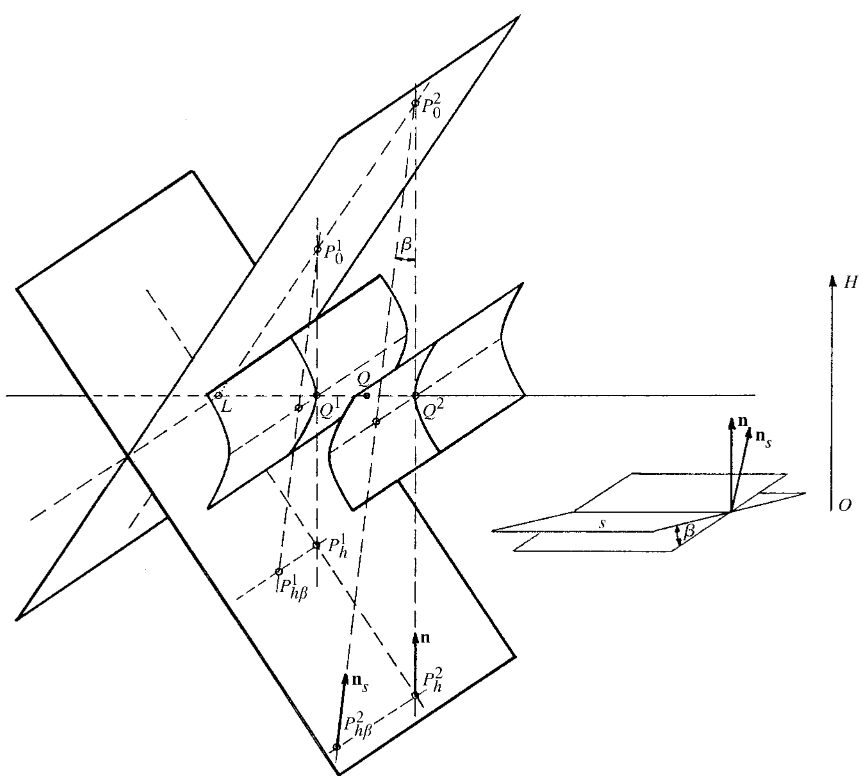

Figure 1
Part of a diffraction diagram in reciprocal space. The spheres of incidence and reflection are approximated by planes and the dispersion surfaces by hyperbolical cylinders. $\mathbf{n}$ and $\mathbf{n}_s$ are the normals to the diffracting planes and surface, respectively. $P_{h\beta}$ and P_0 are the starting points of the wave vectors of reflected and incident radiation, respectively.

directions and translation perpendicular to the beam direction. This permitted the two crystals to be aligned such that the focii of the parabolic grooves were coplanar. The diffraction plane in this case was vertical. The incident white beam was collimated by slits to roughly 0.5 mm (v) × 10 mm (h), and filtered through a 1.6 mm aluminium plate to avoid problems with beam heating. We could thus illuminate simultaneously the grooved and flat regions of the monoliths. Alternatively, by displacing only one of the monoliths by a distance larger than the groove width, it was possible to observe the grooved region of each of the two monoliths independently, and hence separately align each one to be parallel to the same beam direction and mutually coplanar. In this manner we produced an assembly of two monoliths fixed to a metal plate, well aligned with respect to each other. Fig. 3 shows a photograph of this assembly.

The second part of the experiment took place at beamline X6A, another white-light beamline, but this time having easy access to the beamline (X12A is rather crowded, and modifications to the beamline structure are difficult). It required the mounting of the assembly described above in a vacuum tank mounted at the proper distance from the hutch. This step was necessary because the focal length of the device was over 4 m, and no white-beam hutch was available at NSLS which could enclose both the monochromator and its focus. Since adjustments of the relative orientation of the two monoliths would now involve venting and re-pumping a significant volume of vacuum enclosure, we took considerable care over our pre-alignment. The crystal assembly was located 13.5 m from the source and the calculated image plane was 4.5 m from the crystals. Again, beam-heating effects were avoided by the insertion of a 1.6 mm-thick aluminium filter upstream of the monochromator. Small adjustments could be made to the monochromator by moving its entire vacuum enclosure using the kinematic mounting arrangement provided for normal monochromator adjustments. In particular, adjustment of the yaw angle was possible, as was translation to place the beam on the grooved region or on the flat region of the device.

The detector we used to observe the beam profiles during this phase was a high-resolution YAG scintillator/CCD camera combination originally developed for X-ray microtomography (Dowd *et al.*, 1998). With this combination our spatial resolution at the detector was ~2 pixels, or 35 μm. The scintillator and lens combination was not very efficient and a typical exposure time was ~10 s.

For this stage of the experiment we switched our dispersion plane from vertical to horizontal. This was performed because of the highly anisotropic nature of the NSLS source. Currently, NSLS dipole sources have an effective source size of 0.1 mm in the vertical direction and 1.0 mm in the horizontal (FWHM). Thus, to provide a good test of the focusing action of the monochromator, it was better to image the vertical source dimension. The penalty for this geometry is low intensity, since the source subtends roughly 5 Darwin widths in this direction, thus, for any particular setting, only one-fifth of the source is contributing to the diffracted intensity. Fig. 4(*a*) shows the output beam of the four-reflection device when the beam strikes the flat areas of the monoliths, *i.e.* no focusing is expected. The shape is produced by two mechanisms. In the vertical plane the size is limited by slits in the white beam to a value

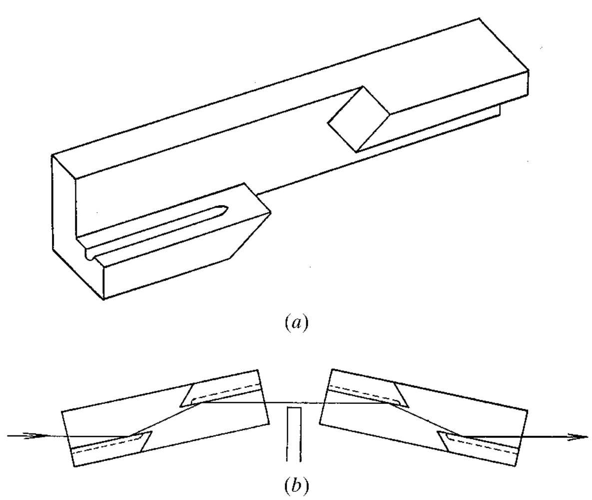

Figure 2
(*a*) The channel-cut monochromator with parabolic grooves machined into its reflecting faces and (*b*) the dispersive arrangement of two such devices used in these experiments.

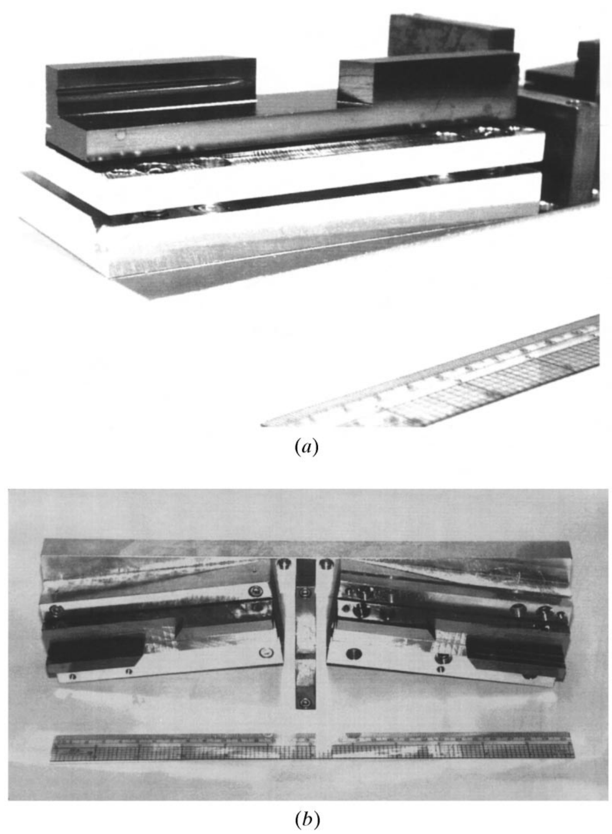

Figure 3
(*a*) A photograph of the grooved crystal and (*b*) of the pre-aligned assembly of two crystals.

slightly less than the natural beam divergence. It is roughly 3.3 mm in the detector plane (18 m from the source). The intensity profile in that direction is a truncated Gaussian. In the horizontal plane the monochromator is highly dispersive and, as a result, only rays within 1 Darwin width of the forward direction are transmitted. Thus the horizontal size of the transmitted beam in the detector plane is simply the horizontal source size convolved with the Darwin width for Si(111) at 15 keV (roughly 3.5 arcsec) projected into the imaging plane. The observed profile is 1 mm FWHM. The profile in this direction is also a Gaussian function, and the horizontal slits were opened wide enough such that any truncation was negligible. Since, in this geometry, the region of the crystal which is active depends on the orientation of the crystal relative to the source, measurements were always preceded by an alignment step involving closing down the horizontal slits to identify a particular spot on the first crystal, then adjusting the Bragg angle to

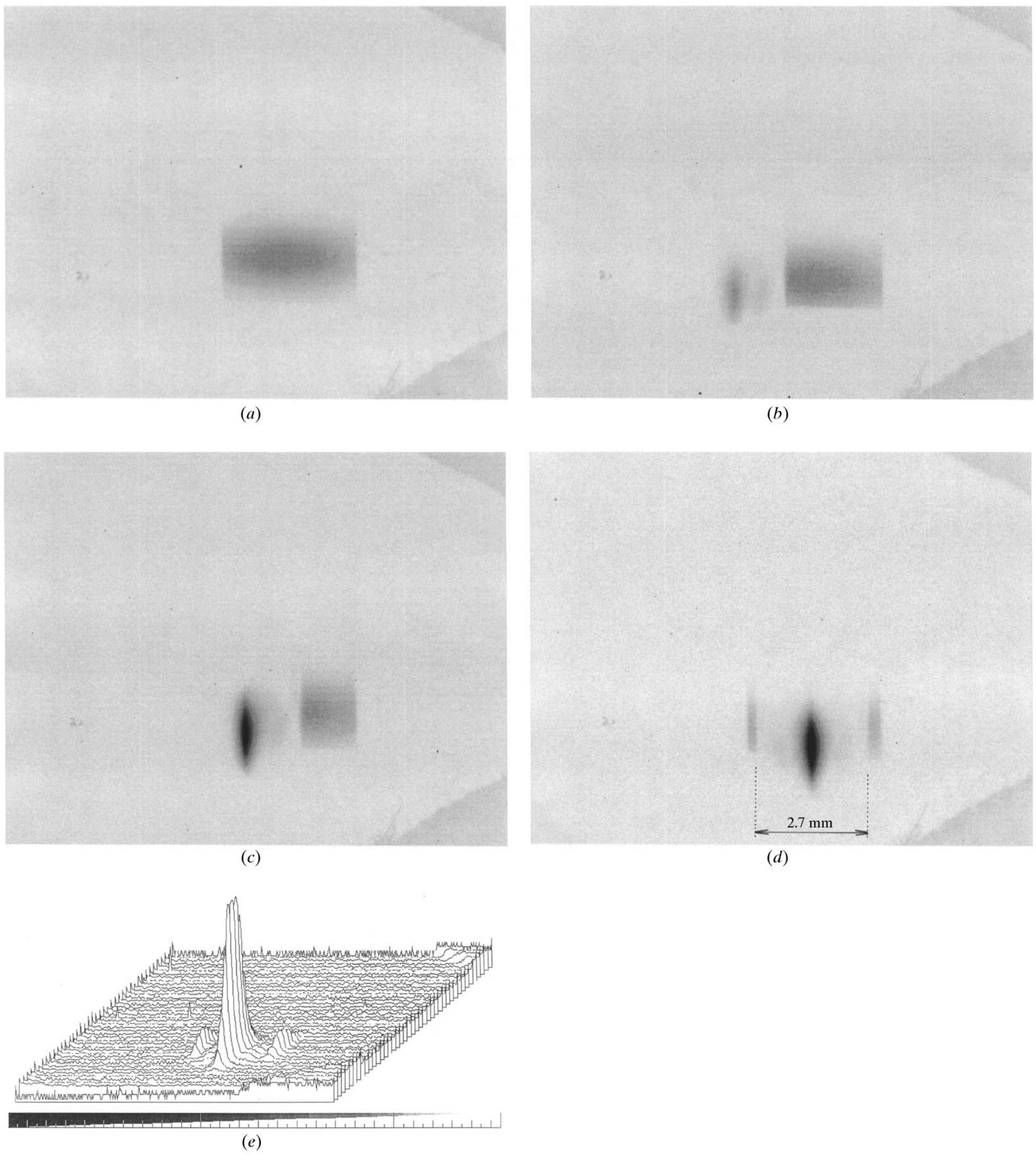

Figure 4
(*a*) Image of the beam transmitted by the flat regions of the monochromator. (*b*), (*c*) Images when the crystals are progressively moved to bring the groove into the beam. (*d*) Image when the groove is centred on the beam profile. (*e*) The same data as (*d*) presented as a three-dimensional plot of intensity *versus* position.

optimize the reflected intensity. After this was accomplished, the horizontal slits were opened wide for the measurement. This was necessary because of the finite extent of the properly paraboloidal region in the crystals along the beam direction.

Figs. 4(*a*)–4(*d*) show the observed images as the optic is translated to move the beam across the grooved region of the crystals. It is seen that the beams which fall on the grooved region are steered into the focus, as expected. We observe a small meridional displacement of the focus compared with the unfocused radiation. This is a consequence of the fact that the two grooves are not exactly identical and, as a result, the cancellation of the meridional displacements produced by each of the monoliths is not exact. Fig. 4(*e*) shows a three-dimensional plot of the same data as Fig. 4(*d*).

Fig. 4(*d*) shows the beam profile which occurs when the crystal assembly is translated to bring the grooved section into the centre of the incident beam profile. In this case the image consists of three regions. The central intense region is the focus and the two weak regions on either side are the beams from the flat parts of the crystal on either side of the groove, *i.e.* the incident beam slightly overfills the groove. It is clear that the focusing action works. We attempted to locate a focal line minimum by translating our detector along the beam direction. We were able to move it by roughly 1 m, but no significant change in the line width could be detected. The beam just downstream of the monochromator could not be seen easily due to a rather inefficient fluorescent flag coating, but it could be determined that the beam was at that point unfocused. Our earlier experiments in X12A gave us confidence that beams incident on the entire groove profile were efficiently transmitted through all four reflections.

From the geometry of our arrangement we would expect to produce an image of the NSLS vertical source profile reduced by 3 whose size is (after the reduction) 30 µm. We attempted to optimize the observed focus by tilting the monochromator to optimize the alignment of the groove axis with the beam centreline. The minimum size we observed was 0.23 mm, but for this orientation the image was visibly skew. The setting which produced a symmetric image gave a size of 0.29 mm. This discrepancy is not yet fully understood, although there are doubtless sources of aberration in this highly off-axis imaging system. The fact that we did not observe any sharp minimum in the line width as a function of position of the detector is an indication that we see an extended caustic waist, rather than a good focus.

In order to assess the efficiency of this device we can make two observations. The full width at half-maximum of the focal line is 0.29 mm. This compares with 2.7 mm which is the height of the groove projected into the detector plane. If the groove were uniformly illuminated, we should thus expect the peak intensity in the focus to be 9.3 times that in the unfocused beam. We find, in fact, that the ratio is closer to five times. This is partly explained by the Gaussian illumination profiles. One must properly integrate the intensity across the profile to obtain a good estimate. We can make a simple calculation: if $\sigma_{\rm horiz}$ = 0.6 mm, then FWHM = 1.0 mm. We can integrate over this 1 mm and compare the result with the integral over the central 0.1 mm (*i.e.* one-tenth of the FWHM). The ratio is 7.4, closer to the experimental value of 5.

To obtain more information about the aberration, the size of the vertical slit was set to 0.3 mm and the slit was moved step by step (0.3 mm) to scan over the profile of the grooves. At the same time the position and the width of the focal spot was measured. The first information obtained was that the detector is not set at the real focus and the real focus was found at 5.7 m from the monochromator. (The size of the demagnified image of the source for this focal length was 42 µm.) Then the detector was set to the real focus and the whole procedure was repeated. Now the beams diffracted from various parts of the groove produced an image centred at the same place but having varying widths. The beam diffracted from the centre of the groove created a focal spot of width 0.107 mm while the beam diffracted from the steepest part of the groove created a diffuse focal spot of width up to 0.6 mm. This indicates that the surface roughness of the groove may be responsible for the width of the focal spot observed (0.23 mm). This roughness causes local errors in the inclination angle β which cause large changes in the deviation, hence smearing out the image. Towards the edges of the groove, the angle between the beam and the surface of the groove is small and so the influence of any deviation from the ideal surface may become important. Another reason may be that the horizontal broadening of the diffracted beam is not completely compensated by the second channel-cut crystal due to misalignment, or to the small difference between the depths and widths of the grooves. In any case, it is obvious that the performance of the device would be improved by making the surface of the parabolic groove smooth, *e.g.* by chemical-mechanical polishing.

The difference between the real and theoretical focal distance may be caused by the real shape of the groove. The shape of the parabolic cutter should be sufficiently precise, but after cutting the grooves the crystals had to be etched. This somewhat modified the profile of the grooves and may account for part of the observed focal length increase, but most likely not for all of it. For this reason we subsequently measured the profile of the grooves and obtained the following parameters a: 1.0299, 1.0203, 0.9876 and 1.0097. The average value is 1.0119 and gives a focal distance f = 5.3 m, which is much closer to our experimental value of 5.7 m.

For ideally perfect crystals, the penetration depth of the incident radiation in the highly reflecting region of the profile is essentially the extinction depth, which for our conditions is only 1.5 µm. Even a small amount of inhomogeneous strain in the surface region of the crystal can significantly increase this penetration depth. The effect of an increased penetration depth is to increase the observed focal length. We tested our crystals individually for throughput and found it necessary to perform an additional etch to bring the double reflectivity up to a reasonable value. We were reluctant to etch the crystals too heavily, since we needed to retain the profile shape. There therefore remains the possibility that some surface damage still exists and may contribute to the focus position we observe.

A third possibility exists, *i.e.* that the value of K in equation (1) is incorrect, either because of approximations in the theory or because of the effects of defects. More experimental tests need to be performed to determine the scale of any such effects.

A proper understanding of these aspects requires a ray-tracing calculation capable of incorporating the effects of the inclined geometry, which does not yet exist.

As in any crystal monochromator, Bragg's law allows higher-order reflections to take place at the same crystal orientation, for energies which are integer multiples (harmonics) of the wanted reflection. We carefully chose our operation conditions in such a way that harmonic contamination was not a problem. The first allowed order above (111) in silicon is (333), and would transmit a 45 keV component. The spectrum of the radiation emitted by NSLS is 200 times weaker at 45 keV compared with 15 keV. In addition, the Darwin width of the (333) reflection is more than ten times narrower than the (111) reflection. As a result, even after our 1.6 mm aluminium filter the harmonic contamination is less than 1%. The focusing distances for higher harmonics are generally much longer compared with a fundamental harmonic. If it were necessary to operate such a device in circumstances where this could present a problem, one could always detune the consecutive reflections in the channel-cut crystals to provide harmonics rejection (Hart & Rodrigues, 1978).

From the above it is seen that at the present time it is difficult to estimate the real size of the focus which may be practically reached by this method. Theoretically, the only limitation seems to be the demagnified image of a source and the penetration depth. The obtained focus size in this experiment is smaller than obtained by a sagittally bent crystal in many cases and, as was shown, it can be substantially decreased. On the other hand, Schulze *et al.* (1998) have demonstrated that a 20 μm focus size may be reached with a special crystal bender, and Freund *et al.* (1998) even claim that focusing down to a micrometre spot size should, in principal, be possible.

The sagittally bent monochromator efficiently focuses radiation only for $M = 1/3$, but is capable of accepting broad beams. The parabolic groove is effective for any M but particularly for short wavelengths it has a limited horizontal acceptance. Another disadvantage of the grooved crystal, however, is that the focal length moves with λ while for the sagittally bent crystal this effect may be corrected by dynamically changing the radius of bending. This drawback of the grooved crystal may be removed by fabricating several different parallel grooves into one crystal or even to fabricate one groove whose parameter changes in the longitudinal direction. The position of the focus may then be changed by translating the crystal in the transversal or longitudinal direction. On the other hand, sagittal bending mechanisms are complex and difficult to align. The grooved crystal is extremely simple mechanically and intrinsically stable.

4. Summary

We have successfully demonstrated that the inclined diffraction geometry can produce one-dimensional focusing in a four-reflection dispersive monochromator. This arrangement has the advantage of fully restoring the orthogonal spreading which occurs in non-dispersive arrangements of profiled crystals. We were able to focus a 2.7 mm broad beam into a 0.29 (0.23) mm spot. The focal line size achieved is not as small as a simple geometric calculation would imply, and work is underway to understand the aberrations involved in imaging real sources using these devices.

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