Ray-tracing analysis of diffractive–refractive X-ray optics

Nikolay Artemiev,[a]* Jaromir Hrdý,[b] Serguei Peredkov[c] and Alexander Artemev[d]

[a]Laboratoire d'Optique Appliquee – ENSTA, Ecole Polytechnique, France, [b]Institute of Physics, Academy of Sciences, Czech Republic, [c]MAX-lab, Lund University, Sweden, and [d]Russian Research Centre, Kurchatov Institute, Russia. E-mail: artemiev@ensta.fr

Ray-tracing simulations of mistuned sagittal diffractive–refractive X-ray lenses (DRXL) are presented. In this article, firstly the characteristic aberrations for various types of crystal misalignments within one-crystal and four-crystal DRXLs are considered, and the sensitivity of such an optical system to the mutual misalignment of its components is discussed. The simulations reveal that a DRXL is not too sensitive to the adjustment of its components. In the second part of this article the performance of such lenses with ideal and approximate profiles is examined. Comparative analysis of parabolic and cylindrical DRXLs showed that, in the case when the linear source size is comparable with the acceptance of the lens, the performances of parabolic and cylindrical DRXLs are practically the same.

Keywords: ray-tracing; diffractive–refractive X-ray lens; X-ray focusing; X-ray monochromator.

1. Introduction

Application of the refraction effect for focusing synchrotron radiation in the X-ray band is now well established. Compound refractive lenses (Snigirev *et al.*, 1996) are similar to ordinary lenses for visible light. Such lenses are relatively simple to produce and work well in the hard X-ray region. For longer wavelengths, however, gain in the focus decreases due to absorption in the lens material. To overcome this, some sophisticated solutions have been proposed (Lengeler *et al.*, 1999; Piestrup *et al.*, 2000).

An alternative focusing method based on refraction was proposed by Hrdý (1998). He proposed using the diffractive–refractive effect, which is the refraction phenomenon occurring during Bragg diffraction. It was shown theoretically (Hrdý, 1998) and experimentally (Hrdý & Siddons, 1999) that X-rays that are diffracted from a parabolic longitudinal groove machined into a single-crystal monochromator are sagittally focused. Fig. 1 shows a schematic view of such a one-crystal lens, and also a four-crystal $(-,+,+,-)$ lens (see insert in the left upper corner), which produces the most sharp and aberration-free focus. Here the grooved crystal acts as an X-ray monochromator and a focusing X-ray lens simultaneously. Moreover, the focusing distance may also be fixed in a relatively broad energy region when using asymmetrically cut crystals (Hrdý, Artemiev *et al.*, 2001).

Our experiments (Artemiev *et al.*, 2001; Hrdý, Artemiev *et al.*, 2001; Hrdý, Ziegler *et al.*, 2001) show that by using this method it is possible to reach a focal width of the order of 100 µm without any special treatment of the diffracting surface. These focusing monochromators are simple and compact; their focusing distance remains practically constant within a certain energy range. Owing to the dispersive four-bounce configuration, they also keep the position of the exit beam fixed.

2. Objectives

The ideal profile of an optical element, *e.g.* a paraboloid of revolution or ellipsoid, is usually very complicated to produce, and thus the following major questions arise. What if the working surface has an approximate shape? How can the profile be simplified while at the same time not spoil the performance too much?

Another important question concerns the sensitivity of the optical system to the misalignment of its components. Moreover, if the optical system consists of more than one element it would be very helpful to understand the role of each element in the formation of the focus and the influence of their mutual misalignment on the aberration of the focal spot.

In this article we attempt to provide answers to these questions for sagittal DRXLs. Under the term diffractive–refractive X-ray lens we define a crystal device that utilizes the refraction phenomena occurring during X-ray diffraction to focus or collimate the diffracted beam. One or more crystals with grooves, machined into their working surfaces, set sequentially along the optical path, form a sagittal DRXL. The grooves should have a concave profile and must be cut in the longitudinal direction.

Ray-tracing simulations of mistuned DRXLs, which are produced here, helped us to tune such lenses during our experiments. Comparative analysis of parabolic and cylindrical DRXL focusing properties is supported by the experimental data.

The ray-tracing calculations presented in this article have been performed with the help of the program *DRTRACE*, which was developed in our laboratory especially for studying diffractive–refractive X-ray optics.

3. Ray tracing

Analytical studies of the focusing properties of DRXLs have led us to develop a ray-tracing program which takes into account the refraction during Bragg diffraction on perfect crystals and is able to trace diffracted beams from profiled crystals. In order to estimate the focusing properties and aberrations of sagittal and meridional DRXLs of various arrangements and parameters, we created a simple

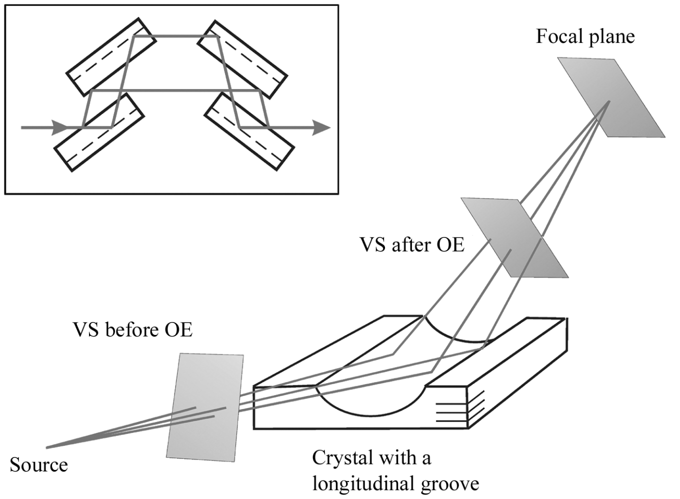

Figure 1
Schematic view of a one-crystal sagittal DRXL. A side view of a four-crystal $(-,+,+,-)$ DRXL is inset in the left upper corner of the figure.

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program called *DRTRACE* which works with profiled, but not bent, crystals. Our aim was not to develop a universal program for all possible cases, such as *SHADOW* (Welnak *et al.*, 1994), for example, but rather to create a very simple code quickly which would be able to perform such calculations.

DRTRACE simulates the imaging properties of a diffractive–refractive optical system. Randomly or regularly the program creates a set of rays, emulating a light source, and traces them through an optical system according to the laws of geometric optics. Diffraction of a 'ray' on an arbitrarily oriented crystal surface is calculated on the basis of the dynamical theory of diffraction. Obviously we cannot talk about diffraction of a ray – it would be more correct to say that on the basis of the dynamical theory of diffraction of X-rays on perfect crystals we calculate the diffraction of a plane incident wave, the wavevector of which is represented by the ray. The boundary conditions are considered at the point where the ray hits the crystal surface.

The diffraction of X-rays on a crystal surface is calculated in accordance with some simplifications of the dynamical theory of X-ray diffraction, described by Hrdý & Hrdá (2000), Hrdý & Pacherova (1993) and Hrdý (2001).

An optical element (OE) is a perfect crystal, which may have a flat inclined and/or asymmetric working surface with respect to the crystallographic planes as well as a cylindrical and parabolic shape. Additionally, in the case of a meridional DRXL, the free profile of a groove could be imported as an ASCII file. The number of optical elements is unlimited. The program calculates the sagittal and meridional deviations of a ray on an inclined and/or asymmetrical surface of an optical element.

4. Alignment of optical elements in a DRXL

In the following section we will consider one of the most important questions: how is a DRXL sensitive to the misalignment of the optical elements it consists of? For this purpose, in the ray-tracing program *DRTRACE* we introduced the possibility of shifting and turning any optical element independently around its ideal position. For practical reasons we will discuss one- and four-crystal $(-,+,+,-)$ DRXLs.

Moreover, not all degrees of freedom should be taken into account, only two. It is simple to realise that only the shift across the incident beam in the sagittal direction and the rotation around the vertical axis perpendicular to the incident beam have to be considered.

There are six degrees of freedom for each optical element: three rotations and three translations. One rotation and one translation are supposed to be responsible for the degradation of the focusing properties of a lens; the other four could be simply tuned experimentally or do not affect the focusing at all:

(i) The rotation (rocking) of a crystal around the horizontal axis perpendicular to the incident beam is the so-called θ or Bragg rotation, which is very sensitive to the incident angle. There is no problem tuning this misalignment with microradian precision. It is sufficient to look at the intensity of the Bragg reflection.

(ii) The rotation (tilt) of a crystal around the axis, which is parallel to the diffracting planes and lies in the diffraction plane, also affects the intensity of the Bragg reflection and could also easily be tuned.

(iii) The translation of a crystal in the meridional direction could be controlled by viewing the diffracted beam on an X-ray TV monitor. By shifting each crystal up and down, one can easily position the optical element by visual interception of the beam.

(iv) A short translation of the crystals along the beam does not affect the focusing but changes the arms of the optical layout.

4.1. One-crystal DRXL

In Fig. 2 a sequence of images on a virtual screen (VS), installed immediately after the OE (see Fig. 1), and in the focus in real and angular space are shown. The lens is rotated in the sagittal plane by 0.001, 0.01 and 0.1 rad. The corresponding images are shown in the upper, middle and lower rows, respectively.

These calculations show that angular misalignment of the order of 1 mrad, which is many times larger than the precision of modern X-ray equipment, does not affect the focusing at all. Moreover, a 10 mrad angular mismatch hardly disturbs the focal spot. Finally, a 0.1 rad mistuning of the lens and incident beam axis, which is roughly 5.7°, is recognized in all three images.

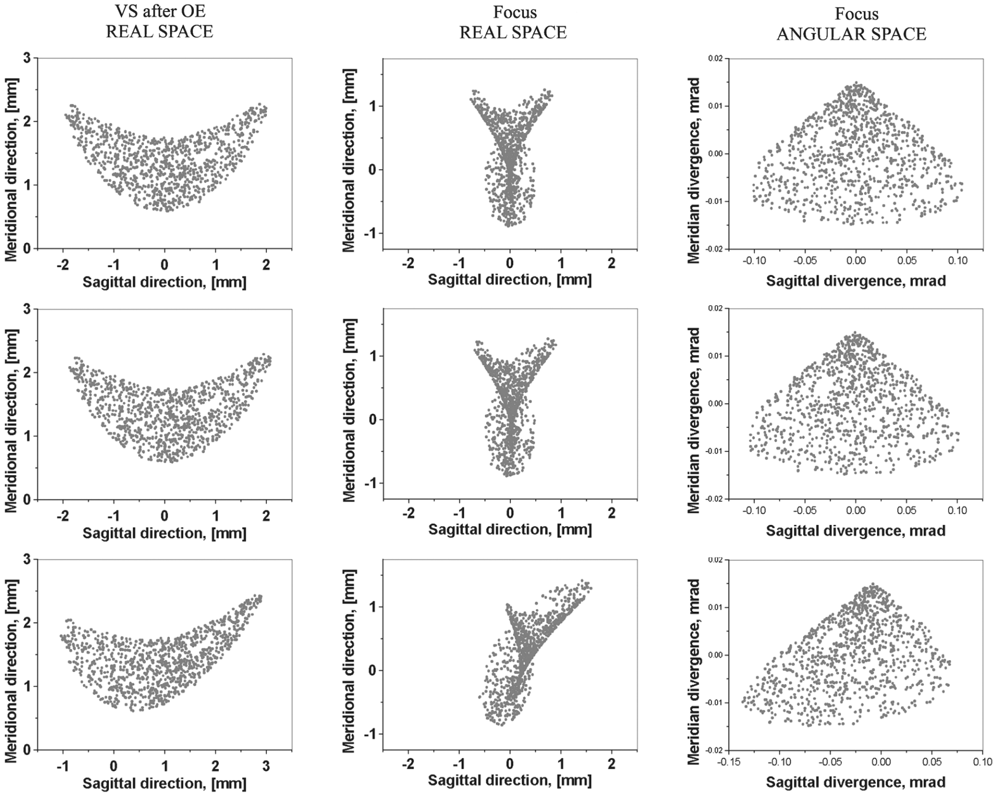


Figure 2

Real- and angular-space distributions of the beam when the lens is rotated in the sagittal plane by 0.001, 0.01 and 0.1 rad (upper, middle and lower rows, respectively).

Fig. 3 presents images of the diffracted beam distributions in the same order but for various values of sagittal shifts of the lens. Here again we see that considerable aberration appears when the lens is shifted by 100 µm off the incident beam axis. The aberration appears somewhat different from the rotational misalignment and in this way it would not be too difficult to understand how to tune a lens. Also it would not be difficult to decode even a combination of these 'pure' cases step by step, translating or rotating the crystal and observing *via* an X-ray monitor.

4.2. Four-crystal DRXL

Obviously the case of a four-element lens is much more complicated. For the sake of simplicity, let such a lens consist of two pairs of crystals, each of which holds two crystals in parallel (non-dispersive) order. From our experience it follows that such pairs could easily be manufactured from one piece of crystal, forming a so-called 'channel-cut' crystal. The crystals in such a pair are perfectly aligned and rigidly fixed with respect to each other. In this way we need only to explore the different kinds of mistuning of such pairs, which considerably simplifies the task. For the reasons described above, we need only to consider mutual one-dimensional shifts and rotations and their combinations.

To begin, it is worth looking at the behaviour of a pair of crystals. As may be seen from Fig. 4(*a*), a 100 µm sagittal shift of such a pair hardly shows any noticeable aberration of the focal spot. Moreover, a 0.5 mm shift does not change the focus considerably (Fig. 4*b*). However, one should be careful when combining a shift and a translation of such a crystal pair. Fig. 4(*c*) shows a combination of the 0.5 mm translation and 0.1 rad rotation of a crystal pair. It seems like the rotation somehow compensates the translational aberration of the focal spot. The situation is not so difficult to understand if we look at Fig. 4(*d*), where the pair is rotated in the opposite direction. The spot shape looks different and an experimenter with minimal skill could easily distinguish these cases.

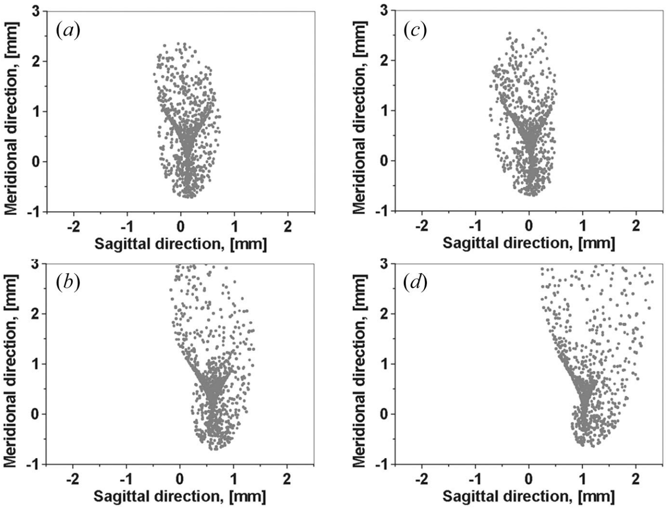


Figure 4
Real-space beam distributions of a mistuned pair of crystals: (*a*) the pair is shifted by 0.1 mm in the horizontal direction; (*b*) the pair is shifted by 0.5 mm in the horizontal direction; (*c*) the pair is shifted by 0.5 mm and rotated by −0.1 rad in the horizontal direction; (*d*) the pair is shifted by 0.5 mm and rotated by 0.1 rad in the horizontal direction.

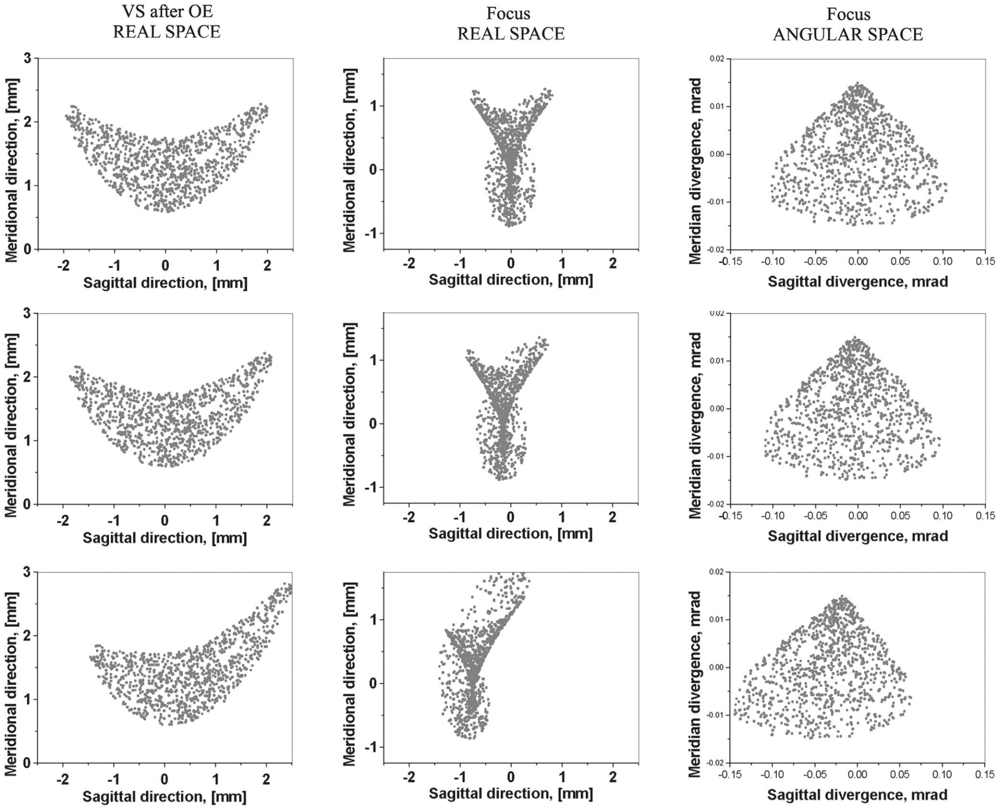


Figure 3
Real- and angular-space distributions of the beam when the lens is shifted in the sagittal plane by 0.01, 0.1 and 0.5 mm (upper, middle and lower rows, respectively).

Regarding the crystal pair alignment, it is worth mentioning the positioning of the crystals within such a pair or, in other words, the manufacturing precision. Fig. 5 shows two sample calculations of the crystals misalignment. In Fig. 5(*a*) the sagittal groove is shifted by 0.5 mm and in Fig. 5(*b*) it is rotated by 0.1 rad with respect to the other. The shift does not affect the focal spot considerably while the angular mistune affects it considerably. In the following section we will show that a four-crystal lens is more sensitive to mistuning, but this example just points out that the grooves in a pair should be cut with a precision much greater than these values.

Up to this point considerable aberrations of the focal spots followed from rather a large mismatch of the lens and the incident beam axis, which is far from the precision of standard X-ray equipment. As expected, the changes of the focal spot profile somehow give an indication of the lens alignment. The situation becomes more difficult when aligning two pairs of grooved crystals in one DRXL. The focal spot in this case becomes 50 times thinner sagittally and two to three times shorter meridionally. As a consequence, such a DRXL is roughly ten times more sensitive to the positioning of the optical elements. Moreover, the number of elements increases which complicates the situation on the whole.

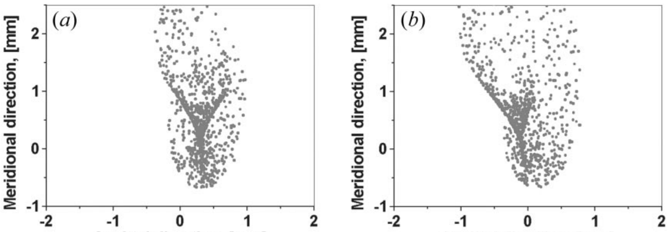


Figure 5

Real-space beam distributions of crystals within a pair of crystals: the first crystal is (*a*) shifted by 0.5 mm and (*b*) rotated by 0.1 rad with respect to the second crystal.

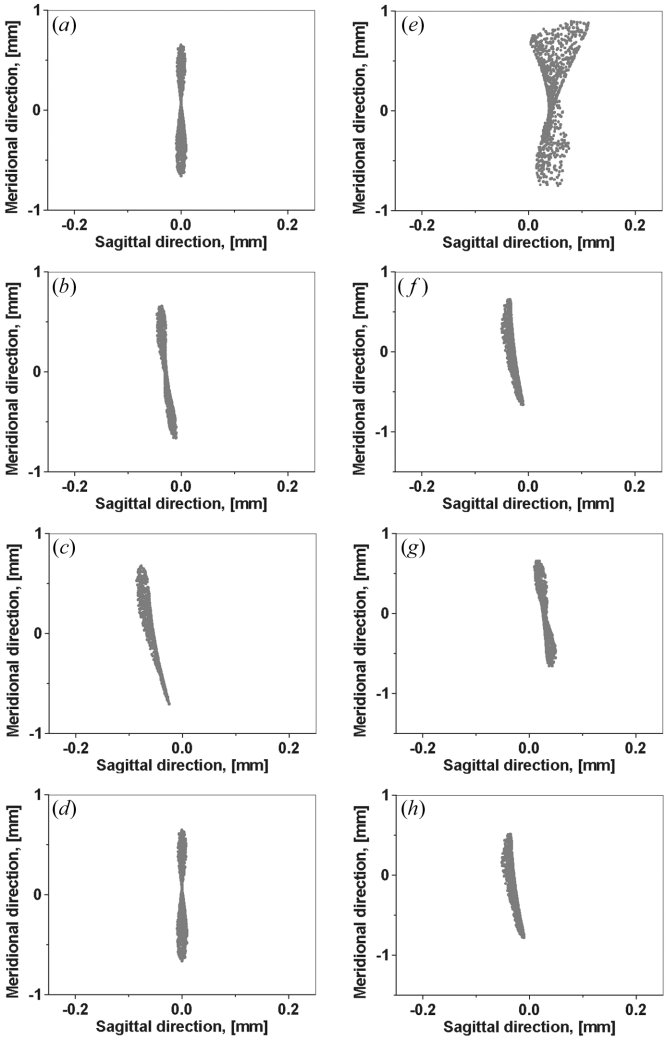


Figure 6

Real-space distributions of a mistuned four-crystal DRXL. (*a*) Ideal alignment of all four crystals. (*b*) First crystal is shifted by 0.1 mm. (*c*) First and second crystals are shifted by 0.1 and −0.1 mm, respectively. (*d*) First and second crystals are shifted by 0.1 mm (the first pair is shifted). (*e*) First crystal is rotated by 0.1 rad. (*f*) First pair is rotated by 0.01 rad. (*g*) Second pair is rotated by 0.01 rad. (*h*) First pair is rotated by 0.01 rad and shifted by 0.5 mm.

In Fig. 6 the most common focal images of a mistuned four-crystal DRXL are shown. All images are on the same scale. From this figure it is shown that a shift of an OE by 0.1 mm and/or a rotation of 0.5° off the incident beam axis do not spoil the focus too much, and at the same time the shape and the tilt of the focal spot reveal the character of the crystals mistunings.

4.3. Longitudinal distance between crystals

At the end of this section the distortions of the focal spot due to the finite distance between the crystals will be discussed. Obviously it is not possible to decrease this distance to zero and consequently this factor influences the minimal size of the focus.

In order to get a feel of the scale of the problem let us construct an ideal DRXL of minimal length considering a more or less real optical scheme (see Fig. 7): source-to-lens distance = 40 m, source half-divergence = 50 μrad in the sagittal and 15 μrad in the meridional direction, focusing distance of the lens = 8 m, parabolic parameter of the sagittal groove machined into the working surfaces of the crystals = 3.5 mm. From these values it follows that the beam size at the lens position is 1.2 mm (vertical) × 4 mm (horizontal). To accept the beam the grooves opening should not be less than 4 mm sagittally; consequently the grooves depth is 0.5 mm and the length is about 2.5 mm. The Bragg angle for an incident photon energy of 8 keV is about 14°. From this it follows that the minimal distance between the bottoms of the first and the second, the third and the fourth crystals is about 2×0.5 mm/sin $\Theta_{\rm B} \simeq 4.1$ mm. The distance between the second and the third crystals could not be less than double the longitudinal half-size of the beam spot on a crystal groove, which is roughly 0.6 mm/sin $\Theta_{\rm B} \simeq 2.5$ mm. These simple calculations show that the minimal lens size for the given parameters could not be less that 11 mm. In reality, however, these distances are larger, for the following reasons. First, there are manufacturing difficulties when a DXRL is constructed of two crystal pairs and the crystals within the pair cannot be produced too close to each other. Second, there are always installation problems as the crystal holders and adjusting stages are usually bigger than the crystals described above. Third, once a DRXL plays a twofold role, *i.e.* focusing and monochromatization, the crystals should be suitable for a reasonably large range of incident angles and in this way their longitudinal size could be larger than the values calculated above. From this it follows that the real length of the lens should be a few times larger than the minimal calculated value of 11 mm.

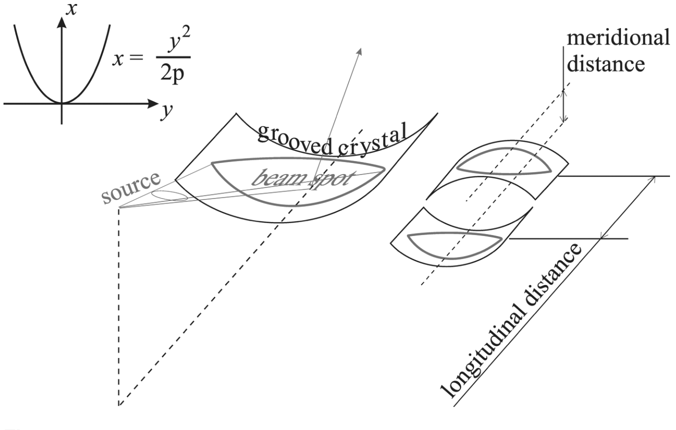


Figure 7

Factors which influence the minimal distance between crystals with longitudinal grooves.

Fig. 8 shows two focal spots calculated for a DRXL of ideally minimal size (Fig. 8*b*) and for a lens constructed from the same crystals but where the distances between them have more or less reasonable values (Fig. 8*a*). The sagittal focal spot size from a hypothetical lens of minimal length is roughly ten times smaller than the spot from the practically shortest lens. In reality, these distances could be even larger and the focal spot size is also thicker.

To avoid this aberration, a DRXL must be constructed from crystals with slightly different grooves. In this case, the parabolic profile of the grooves remains untouched but the parabolic parameter of each consequent groove must be slightly larger than the previous one. Unfortunately the changes in the grooves are so small that it does not seem really feasible either to produce or to control them with sufficient accuracy.

As a conclusion concerning the misalignment of crystals within a DXRL we can say that the positioning of optical elements in the 100 μm and 0.5° range does not considerably spoil the focusing. However, the minimal possible sagittal focal spot size is about 10 μm, which is related to the geometrical parameters of the lens.

Up to now we have considered only DRXLs with parabolic grooves. It is also applicable, however, to DRXLs with cylindrical grooves or holes, with the only difference being that, owing to larger aberrations, cylindrical DRXLs are even less sensitive to misalignments of its components. Moreover, a DRXL with a hole is free of the problem of the manufacturing precision of a crystal pair with two parabolic grooves that could be mistakenly cut with a shift and/or tilt to each other.

5. Comparative ray-tracing analysis of parabolic and cylindrical DRXLs

The first experimental test using a parabolic DRXL showed good results (Hrdý & Siddons, 1999). However, a cylindrical DRXL resulted in rather good sagittal focusing and moreover appeared to be much more feasible in comparison with a parabolic lens (Artemiev *et al.*, 2001). Some aspects of parabolic and cylindrical DRXLs are discussed in this section.

When the focusing distance is much smaller than the distance from the source to the lens, aberrations of a lens play a crucial role in the focus formation. In such optical systems, where the demagnification factor is large and the minimal focus size is larger than the demagnified image of the source, the real size of the source does not influence the focus too much (see for instance Artemiev *et al.*, 2001). On the other hand, in optical systems with comparable arms and with a source whose size is comparable with the beam it delivers to an optical element, aberrations play a less important role. We can say that the minimal focus which could be achieved is just an image of a point source in the focal plane of the optical system.

In the case of one-dimensional sagittal focusing, an ideal parabolic DRXL should image a point source into a fine vertical line. However, for the reasons described above we will not consider an *ideal* parabolic DRXL and instead will focus our attention on a *nearly ideal* DRXL, which consists of four crystals with identical parabolic grooves. The distances between the crystals are more or less real. The following analysis will show that in most cases a DRXL with cylindrical grooves or holes results in rather good focusing, and production of such a lens is much more simple and accurate than for the parabolic lens.

In 2001 we performed an experiment using a symmetrical cylindrical DRXL at the APS on the 5ID beamline. The results of the experiment were published by Hrdý, Artemiev *et al.* (2001). Here we would like to recalculate the same optical scheme and to justify using the cylindrical lens. The parameters of this beamline are particularly interesting for our analysis. The sagittal source size, 764 μm (σ_x = 325 μm), is quite large and the sagittal beam size accepted by the DRXL was just about 2 mm. The source-to-DRXL and DRXL-to-focus distances were 55 m and 20 m, respectively. The DRXL consisted of two Si(111) crystals with cylindrical holes, arranged into dispersive position. The diameter of the holes was 4.5 mm, which corresponded to a focal distance of 20 m for 13 keV radiation.

Fig. 9 shows how the focusing properties of parabolic and cylindrical DRXLs differ when imaging a point source. The weaker intensity and large wings of the cylindrical lens focus make such a lens unsuitable for use in optical schemes with a small source. The intensity at the focus is 40% smaller for a cylindrical lens than for a parabolic lens. However, the situation considerably changes when comparing parabolic and cylindrical lenses focusing a large source.

Fig. 10 shows the ray-tracing calculations of the same optical scheme as in Fig. 9 but using the real source size. Here we see that the parabolic DRXL results in a simply demagnified source image equal to 290 μm (FWHM) while the performance of the cylindrical lens is

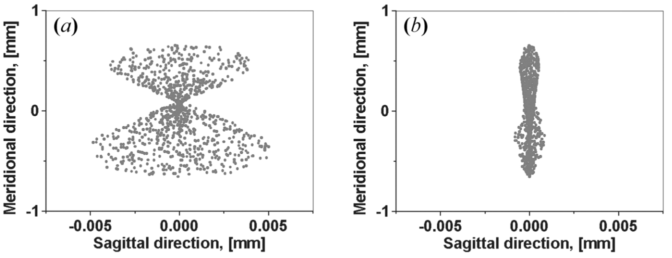
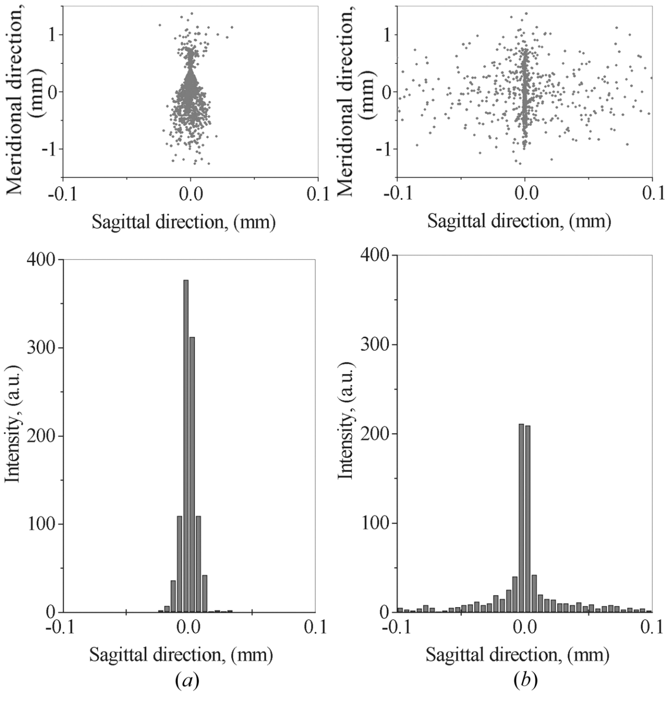


Figure 8
Two focal spots calculated for (*a*) a real size lens and (*b*) an ideally minimal longitudinal size of a DRXL.



(*a*) (*b*)

Figure 9
Scatter plots and corresponding histograms of sagittal focuses calculated for a point source for (*a*) a nearly ideal parabolic DRXL and (*b*) a cylindrical DRXL.

slightly worse, as in the case of a point source imaging. The intensity at the focus of the cylindrical lens is just 20% less and the focus size is 23% larger than that of the parabolic lens. The ray-tracing calculation shows that the size of the cylindrical DRXL focus is 350 µm (FWHM). In the experiment, however, the focus size was about 420 µm, which is 20% larger. The most probable reason for this discrepancy is related to the surface waviness and roughness.

For the analysis described above we did not have the technology of mechanical–chemical polishing of uneven crystal surfaces, and the holes were simply drilled into the crystals and etched normally. To check the influence of the working surface treatment we performed two experiments at the ESRF. The results evidently showed that mechanical–chemical polishing of DRXL working surfaces of crystals is essential (Artemiev *et al.*, 2003; Hrdá *et al.*, 2003). One more factor, smearing, which accompanies inclined Bragg diffraction (Artemiev *et al.*, 2000), also influences the focus size. In the case of a four-crystal DRXL this effect could be cancelled out but all four crystals or both holes must be produced identically. Here it means that the axes of the grooves or holes should form the same angles with the diffracting planes. If this condition is broken, the radiation falls under different angles onto working surfaces and the focus is distorted and smeared.

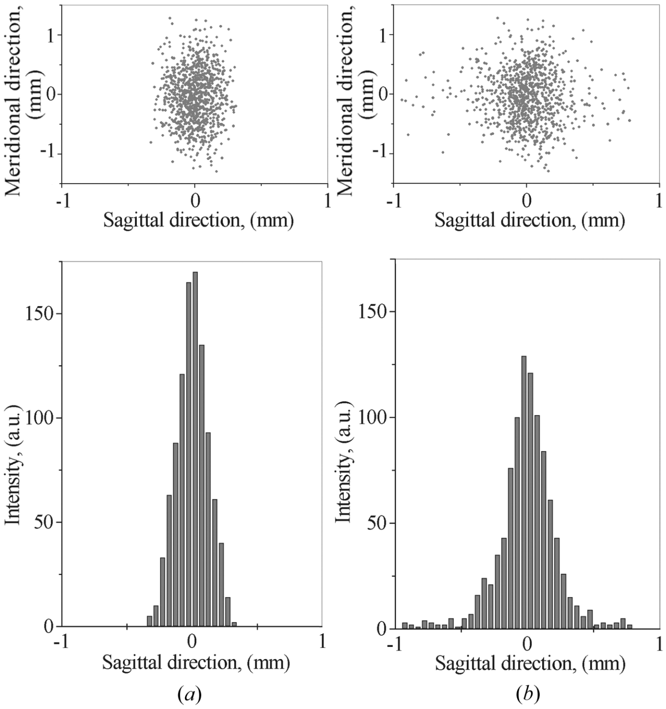


Figure 10
Scatter plots and corresponding histograms for sagittal focusing of (*a*) a nearly ideal parabolic DRXL and (*b*) a cylindrical DRXL, calculated for the real source size.

6. Conclusion

The ray-tracing simulations have shown that the focus aberrations of a mistuned sagittal DRXL unambiguously reveal the type of misalignment and, moreover, some combinations of various kinds of misalignment could easily be deciphered even in the case of a four-crystal DRXL. The comparison of parabolic and cylindrical DRXLs advocates the use of the latter in optical schemes with large source and small demagnification. The manufacturing process of a cylindrical DRXL is much more feasible and accurate, and the focusing properties are not too much worse than those of the parabolic DXRL.

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