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Compensation of Aberration of Inclined X-ray Monochromators

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Inclined double-crystal monochromators for synchrotron radiation suffer from aberration that is connected with the horizontal divergence of the synchrotron radiation beam. Two different methods are proposed to compensate for this aberration. The first method introduces slightly different angles of inclination for the first and the second monochromator crystals. The condition for the difference of the angles of inclination is Bragg angle dependent and also depends on the projection of the distance of both crystals onto the direction of the normal to the diffracting planes. The second method uses an additional inclined double-crystal monochromator cut such that the aberration introduced by the first pair of crystals is nearly completely compensated by the second pair of crystals. This method is independent of wavelength. Both methods are illustrated by ray tracing.

Keywords: aberration; inclined monochromators; X-ray monochromators.

1. Introduction

The inclined-geometry double-crystal X-ray monochromator has been independently proposed in Sincrotrone Trieste (Hrdý, 1990, 1992) and APS (Khounsary, 1992) as one of the most attractive methods for handling high radiation power densities. In this geometry the crystal surfaces are cut at a large angle with respect to the atomic diffracting planes such that the plane determined by the normal to the surface and the normal to the diffracting crystallographic planes is perpendicular to the plane determined by the impinging and diffracted beams. By orienting the crystal in this way one can obtain considerable spreading of the incident beam on the surface of the first crystal whilst retaining nearly symmetric diffraction (Macrander, Haeffner & Cowan, 1992; Hrdý & Pacherová, 1993). This gives a larger range of wavelength tunability as compared with the asymmetrically cut crystal. The second crystal must be cut in the same way to give the exit beam nearly the original shape.

The inclined monochromator has been successfully tested by the APS group (Macrander, Lee *et al.*, 1992; Lee *et al.*, 1992) and its properties have been discussed in a number of papers (Macrander & Lee, 1992; Lee & Macrander, 1992; Macrander, Khounsary & Graham, 1992; Macrander, Haeffner & Cowan, 1992; Hrdý & Pacherová, 1993; Rogers & Macrander, 1993; Macrander & Blasdell, 1994; Blasdell, Macrander & Lee, 1994). It has also been shown (Ice & Sparks, 1992) that in the inclined geometry the second crystal may be sagittally bent to focus the monochromatic radiation.

In order to increase the spreading of the incident radiation on the surface of the first inclined crystal further, one may decrease the angle between the incident beam and the surface of the crystal by turning the monochromator around the normal to the diffracting planes (Smither & Fernandez, 1994; Blasdell & Macrander, 1994). The resulting position is a combination of 'pure' inclined and 'pure' asymmetric geometry, although the 'pure' asymmetric position does not exist if the angle of inclination is higher than the Bragg angle. This was called a general asymmetric position by Smither & Fernandez (1994), although the name general inclined seems to be more appropriate. This approach has been adopted for SPring-8 (Kamiya *et al.*, 1995; Uruga *et al.*, 1995) where the geometry was called a rotated-inclined double-crystal monochromator.

Recently (Hrdý & Pacherová, 1993; Hrdý, Busetto & Bernstorff, 1995), we have shown that the inclined double-crystal monochromator introduces a certain distortion of the profile of the exit beam which manifests itself as a deformation of the shape of the virtual source. This distortion is connected with the horizontal divergence of the synchrotron radiation beam. The real point source is transformed into a virtual source that has the shape of a vertical line. A similar observation was also reported by Blasdell, Macrander & Lee (1994). We have analyzed this kind of aberration both analytically and by ray tracing. In this paper we propose two different ways in which it can be suppressed.

2. Different angles of the first and second crystals

In the symmetric double-crystal (+, −) monochromator, the gap (defined as the distance between the diffracting planes on the first and the second crystals for a given beam) is independent of the direction of the beam. Here the gap is equal to the distance between the planes containing the diffracting surfaces of both crystals. In this case the crystals behave as mirrors (from the geometrical point of view only) and thus no aberration is observed. A real point source is here transformed into a virtual point source.

As was shown recently (Hrdý, Busetto & Bernstorff, 1995) the situation in the case of an inclined double-crystal monochromator and horizontally divergent radiation is different (Fig. 1). The gap is equal to the projection g_0 of the distance between the crystals onto the normal to the diffracting planes only for the central beam ($X = 0$). Let the horizontal deviation of a beam from the central beam be determined by a variable X. The corresponding angular deviation ε may be determined from

$$\tan\varepsilon = X/L \tag{1}$$

where L is the distance of the monochromator from the source S. From Fig. 1 it is seen that the gap g_x corresponding to the deviated beam decreases with X. For $X > 0$ the gap $g_x < g_0$ and for $X < 0$ the gap $g_x > g_0$. This variation of the gap with X (or ε) is the main reason for the above-mentioned aberration because the change of gap causes the shift of the exit beam and consequently increases the vertical dimension of the virtual source.

The inclined double-crystal monochromator discussed above has the same angles of inclination β for both crystals, *i.e.* the diffracting surfaces of both crystals are parallel. Now we will decrease the inclination angle β' on the second crystal to see how the variation of the gap will be affected (Fig. 2). (The angles β and β' shown in Fig. 2 are taken as positive.) It may be shown (see *Appendix*) that

$$g_x = \frac{A}{(A - kX)(A + k'X)}\,\{X[A(k - k') - kg_0] + g_0 A\} \tag{2}$$

where $A = L\sin\theta$, $k = \tan\beta$, $k' = \tan\beta'$ and θ is the Bragg angle.

It is obvious that in all practical cases the absolute values of kX and $k'X$ are much smaller than A and thus the fraction in (2) is approximately equal to $1/A$. Now it is clearly seen that if

$$A(k - k') - kg_0 = 0 \tag{3}$$

or

$$k' = k(L\sin\theta - g_0)/L\sin\theta \tag{4}$$

the gap will be practically independent of X (or ε). Unfortunately, from (4) it follows that k' depends on θ and thus also on the wavelength λ. Fortunately, it also depends on g_0. This means that for a certain k', determined from (4) for some θ, the influence of the subsequent change of the Bragg angle may be compensated by the change of g_0, *i.e.* the component of the distance of the crystals in the direction of the normal to the diffraction planes. In this way the inclined double-crystal monochromator may be kept free of aberration for a certain θ interval. For $k' = k$

$$g_x = Ag_0/(A + kX) = g_0\sin\theta/(\sin\theta + \tan\beta\tan\varepsilon). \tag{5}$$

The previously detailed procedure may be illustrated by the following example. Let us suppose that $L = 25\,000$ mm, $\beta = 75°$ ($k = 3.732$), $\theta = 20°$, $g_0 = 100$ mm, and X is changed from -50 to $+50$ mm. Provided that $k = k'$, the gap g_x changes from 102.23 to 97.86 mm. If we change the angle of inclination of the second crystal according to (3) or (4) we get $k' = 3.68835$ ($\beta' = 74.83°$) and the gap changes in the interval 99.996–100.072 mm, *i.e.* 57.5 times less than in the previous case. If we now wish to change the Bragg angle from 20 to 30° (for the same k'), we will have to increase g_0 to 146.2 mm to keep the variation of the gap suppressed. This example is only a theoretical case because its realization would require very large crystals. Fig. 3

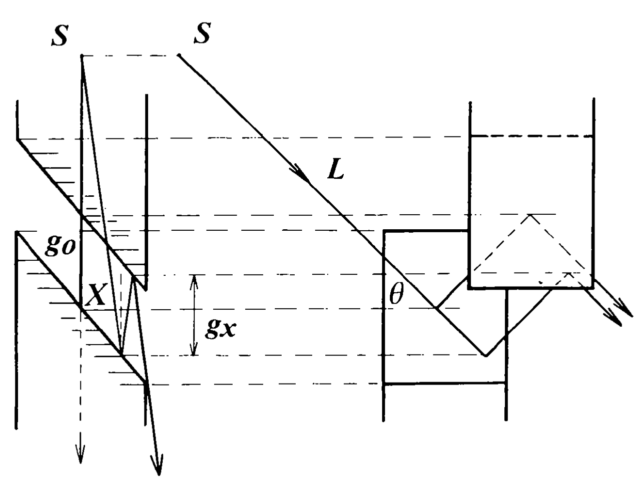

Figure 1
Front and side view of horizontally divergent synchrotron radiation from a point source S impinging on an inclined double-crystal monochromator. (In contrast to the real situation, the picture is oriented in such a way that the diffracting planes are horizontal and thus the synchrotron beam is not horizontal.)

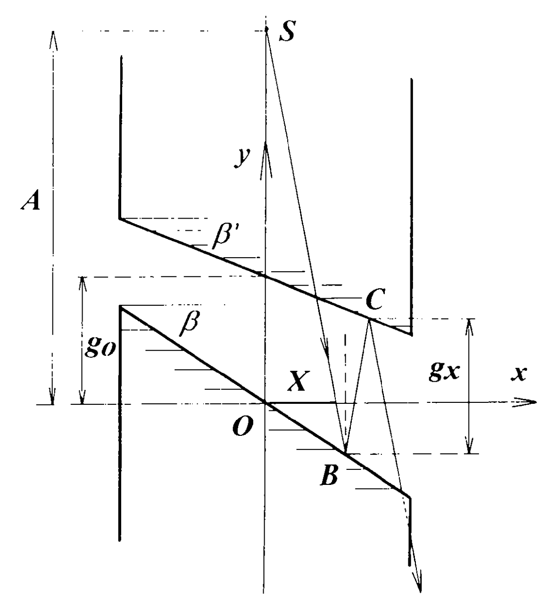

Figure 2
Inclined double-crystal monochromator with different angles of inclination for the two crystals to compensate for aberration.

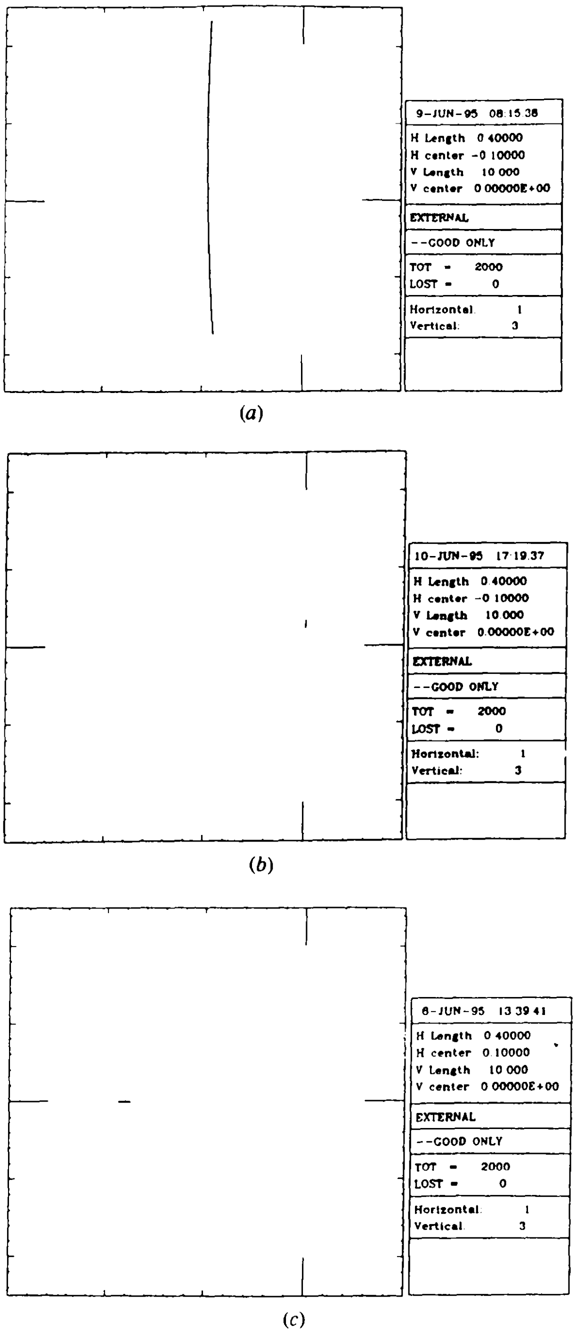

Figure 3
Virtual source generated by the ray-tracing program *SHADOW* for a real point source and horizontally divergent radiation. (*a*) The virtual source created by the inclined double-crystal monochromator with $\beta = 75°$, $\theta = 20°$, $g_0 = 100$ mm, $L = 25\,000$ mm and -50 mm $< X < +50$ mm. (Here the aberration is not compensated.) (*b*) The virtual source of the same monochromator with a slightly different angle of inclination on the second crystal calculated according to (4) to compensate for the aberration. (*c*) The virtual source for two inclined double-crystal monochromators creating the $(+, -, -, +)$ arrangement and with the same parameters as in (*a*) but the angles of inclination on the second monochromator have opposite signs with respect to the first monochromator (see Fig. 4). The curvature, the horizontal dimension and the horizontal displacement of the virtual source are due to the refraction. All three diagrams are drawn to the same scale: the horizontal length of the diagrams corresponds to 0.4 mm and vertical length to 12.5 mm.

shows a simulation of the virtual source for the above example using the *SHADOW* ray-tracing program (Lai & Cerrina, 1986).

3. Two inclined double-crystal monochromators

The gap in an inclined double-crystal monochromator with $\beta = \beta'$ is given by (5). As the absolute value of kX is very small when compared with A, the relation (5) may be approximated by a line and it holds that

$$(g_x - g_0) \doteq -(g_{-x} - g_0). \qquad (6)$$

Let us suppose that the beam, determined by a parameter X, passes through the first inclined double-crystal monochromator cut as shown in Fig. 4(*a*) and then through the second inclined double-crystal monochromator cut according to Fig. 4(*b*). (The first monochromator has an angle of inclination β and the second one $-\beta$.) The beam with parameter X in the first monochromator is, in the second monochromator, in the same situation as a beam with parameter $-X$ in the first monochromator. Thus, from (6) it follows that the change in the gap caused by the first monochromator is almost completely compensated in the second monochromator for any θ. Here we suppose that both monochromators form a so-called non-dispersive or $(+, -, +, -)$ setting, *i.e.* all the diffracting planes are parallel and the beam impinges first on the lower crystal and then on the upper crystal.

The first monochromator ($k_1 = k$) causes a change in the gap of

$$\Delta g_1 = g_0 - Ag_0/(A + kX) \qquad (7)$$

and the second monochromator ($k_2 = -k$) causes a change in the gap of

$$\Delta g_2 = g_0 - Ag_0/(A - kX). \qquad (8)$$

(In fact A and X are slightly larger on the second monochromator when compared with the first monochromator but the value of the fraction remains the same.)

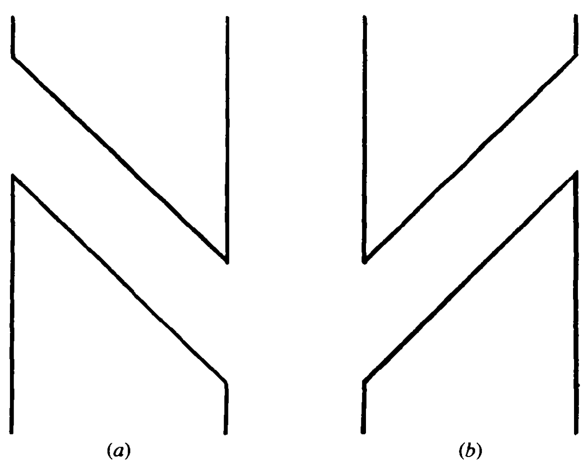

Figure 4
(*a*), (*b*) Schematic diagram of two inclined double-crystal monochromators with opposite angles of inclination.

The resulting gap change is given by

$$\Delta g = \Delta g_1 + \Delta g_2 = 2g_0[1 - A^2/(A^2 - k^2X^2)]. \quad (9)$$

The absolute value of the term in square brackets is of the order of 10^{-3} in the worst extreme, or much smaller, which means that the resulting change in the gap is insignificant. Both monochromators may be also arranged in such a way that they create the so-called dispersive $(+, -, -, +)$ setting having a high resolution. However, in this case the beam diffracted from the upper crystal of the first monochromator impinges first on the upper crystal of the second monochromator and then on the lower one. To compensate for the influence of gap variation on the position of the exit beam it is necessary that both monochromators be cut in the same way as in the previous $(+, -, +, -)$ case.

APPENDIX

For a given X the gap g_x may be determined as the difference $Y_2 - Y_1$, where Y_1 and Y_2 are the y coordinates of the points B and C, respectively (see Fig. 2). The point $B[X_1, Y_1]$ is the intersection of the horizontally deviated beam with the surface of the first crystal. Its coordinates may be determined by solving the system of equations

$$y = -(A/X)x + A \quad (10)$$

$$y = -kx, \quad (11)$$

where the first equation describes the beam impinging on the first crystal and the second equation describes the projection of the diffracting surface of the first crystal. This gives

$$Y_1 = -kAX/(A - kX) \quad \text{and} \quad X_1 = AX/(A - kX). \quad (12)$$

The coordinates of the point $C[X_2, Y_2]$, *i.e.* the intersection of the beam diffracted from the first crystal with the surface of the second crystal, may be determined by solving the system of equations

$$(y - Y_1) = (A/X)(x - X_1) \quad (13)$$

$$y = -k'x + g_0, \quad (14)$$

where the first equation describes the beam diffracted from the first crystal and the second describes the projection of the diffracting surface of the second crystal.

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