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Rotated-inclined double-crystal monochromator for synchrotron radiation: aberration and its compensation

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A rotated-inclined double-crystal X-ray monochromator was designed for high-power undulator beamlines for SPring-8 to reduce the impinging radiation power density. Recently, it has been shown that an inclined double-crystal monochromator suffers from a certain type of geometrical aberration that may be relatively easily compensated. In this paper, it is shown that a similar aberration exists also in the case of rotated-inclined monochromators and that as in the inclined case the aberration may also be compensated.

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

1. Introduction

The use of inclined and asymmetric double-crystal monochromators is proposed as one of the attractive methods for handling the high radiation power density of new synchrotron radiation sources (see *e.g.* the survey of Busetto & Hrdý, 1995). The asymmetric monochromator is based on the well known asymmetric diffraction. The inclined monochromator may be created by the rotation of the asymmetric monochromator about the normal to the diffracting crystallographic planes by an angle of 90°. The area of the footprint of the radiation on the surface of the crystals may be, for both types of monochromator, substantially larger compared with that of symmetric monochromators and consequently the radiation power density impinging on the surface of the crystals will be lower.

The horizontal divergence in an inclined double-crystal X-ray monochromator and the vertical divergence in an asymmetric double-crystal X-ray monochromator cause distortion of the exit beam, which manifests itself as a deformation of the virtual source (hereafter called aberration). This was thoroughly discussed by Hrdý *et al.* (1995). This aberration may be observable in the case of sufficiently divergent radiation like the radiation from wigglers or bending magnets, provided that sufficiently large crystals are used. (The dimensions of the crystals available at the present time restrict the usage of the inclined monochromator for rather narrow beams from undulators.) In subsequent work, Busetto & Hrdý (1995) showed that there exist two possible ways to compensate for this aberration in the inclined case. The first one uses slightly different angles of inclination for the two crystals and the second one uses two double-crystal inclined (noncompensated) monochromators with opposite angles of inclination with respect to each other.

In order to increase further the spread of incident radiation on the surface of the first crystal of the inclined monochromator, 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. This approach, based on that of Smither & Fernandez (1994), has been adopted for SPring-8; the geometry was called a rotated-inclined monochromator (see *e.g.* Kamiya *et al.*, 1995). The purpose of this paper is to show that the results obtained by Busetto & Hrdý (1995) for the inclined double-crystal monochromator are essentially also valid (with some modifications) for the rotated-inclined double-crystal monochromator. This paper represents an extension of the work by Busetto & Hrdý (1995) and uses the same symbols and takes into consideration only a real point source. The effect of variable asymmetry within the horizontally divergent beam has been studied by Macrander & Lee (1992) and will not be taken into account here. Also, the effect of refraction is not included in the calculation.

2. Theory

The rotated-inclined geometry is derived from the inclined geometry by the rotation of the crystals about the normal to the diffracting crystallographic planes by an angle ξ. This is essentially equivalent to the inclined case studied by Busetto & Hrdý (1995) with the beam horizontally deviated from the direction that would represent 'pure inclined diffraction' by the angle ξ. To follow the procedure described by Busetto & Hrdý (1995), we must introduce the parameter X for the characterization of the impinging beam (Figs. 1 and 2). For practical reasons, it is advantageous to introduce also the auxiliary parameter X' with the origin at O'. The central beam is now characterized by the parameter $X' \neq 0$, where $X' \simeq L\cos\theta\sin\xi$ ($C \simeq L\cos\theta$) and L is the distance of the monochromator from the X-ray source. Let the horizontal dimension of the beam (in the place of the monochromator) be $2h$ and the vertical dimension be $2v$. Then the horizontal and vertical divergences of the beam are 2ε and 2φ, respectively, where $\tan\varepsilon = h/L$ and $\tan\varphi = v/L$. The beam deviated from the central beam in the horizontal direction by $\pm\varepsilon$ may be characterized by the parameter $X' \pm \Delta X'^h$ and similarly the beam deviated from the central beam in the vertical direction by $\pm\varphi$ may be characterized by the parameter $X' \pm \Delta X'^v$. It may

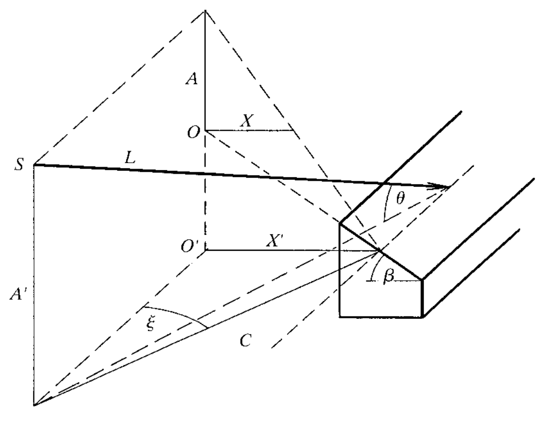

Figure 1
Perspective schematic view of rotated-inclined double-crystal monochromator. For simplicity, the second crystal is not shown. S is the radiation source.

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be shown that

$$\Delta X'^h \simeq h\cos\xi = L\tan\varepsilon\cos\xi \quad (1)$$

and

$$\Delta X'^v \simeq v\sin\xi/\sin\theta = L\tan\varphi\sin\xi/\sin\theta, \quad (2)$$

where θ is the Bragg angle.

It was shown in our previously mentioned papers that the aberration is caused by the variation of the gap within the divergence of the beam. (The gap here means the distance between the diffracting crystallographic planes of the first and the second crystal for the beam under consideration.) If the gap was constant, then the real point source would be transformed into a virtual point source and there would be no aberration as in the case of an ordinary $(n, -n)$ double-crystal monochromator based on symmetrical diffraction. It should be noted that, for the determination of X' and the gap, only the projection of the beam into the plane determined by the normals to the diffracting planes and the surface of the crystals is important (Fig. 2). The variation of the gap for a divergent beam in the rotated-inclined monochromator is obviously given by (see Busetto & Hrdý, 1995)

$$\Delta g_x = g_0A/\{A + k[X \pm (\Delta X^h + \Delta X^v)]\}, \quad (3)$$

where $A = A' - X'\tan\beta$, $A' = L\sin\theta$, $k = \tan\beta$ and β is the angle of inclination, *i.e.* the angle between the diffracting crystallographic planes and the surface of the crystal, which so far is equal for the two crystals. It is obvious that for the *central beam*

$$X/A = X'/A', \quad (4)$$

$$\Delta X/\Delta X' = X/X', \quad (5)$$

and thus the following expressions may be used for the estimation of the gap variation:

$$A = L\sin\theta(1 - \sin\xi\tan\beta/\tan\theta), \quad (6)$$

$$X = L\cos\theta\sin\xi(1 - \sin\xi\tan\beta/\tan\theta), \quad (7)$$

$$\Delta X = \Delta X'(1 - \sin\xi\tan\beta/\tan\theta). \quad (8)$$

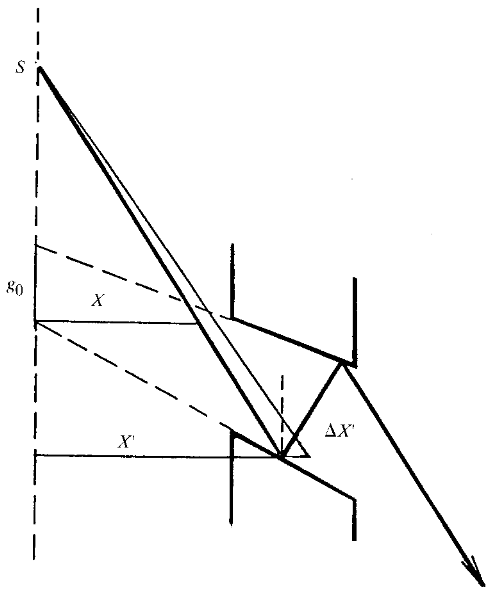

Figure 2
Front schematic view of rotated-inclined monochromator with different angles of inclination on the two crystals. (Diffracting crystallographic planes are situated horizontally.)

From equation (3), it is seen that for the pure inclined case ($\xi = 0$) only the horizontal divergence causes the variation of the gap and for the asymmetric case ($\xi = 90°$) only the vertical divergence causes the variation of the gap. For these two extreme cases, formula (3) is consistent with the estimation given by Hrdý *et al.* (1995). As was mentioned earlier, if the gap was constant, then all exit beams would originate in the point virtual source. The variation of the gap Δg causes the shift of the exit beam Δs, which is given by

$$\Delta s = 2\Delta g\cos\theta, \quad (9)$$

which is the approximate estimation of the smearing of the virtual source.

It was shown by Busetto & Hrdý (1995) for the inclined case ($X = 0$ for the central beam) that in the general case when the angle of inclination β' ($k' = \tan\beta'$) on the second crystal is different from the angle of inclination β on the first crystal, the gap g_x is given by

$$g_x = \{A/[(A - kX)(A + k'X)]\}\{X[A(k - k') - kg_0] + g_0A\}, \quad (10)$$

where g_0 is the gap for $X = 0$.

It was shown that, if

$$A(k - k') - kg_0 = 0, \quad (11)$$

then for small X the variation of the gap with X is minimal.

In the rotated-inclined case, the parameter X may be large and formula (11) may give (for $X > 0.268A/k$ as may be shown from a detailed calculation) worse results than in the noncompensated case, *i.e.* $k = k'$. Nevertheless, it is possible to find the optimal k' for given X by minimizing the first derivative of (10). The simpler procedure is to plot (10) for various k' from the value given by (11) to $k' = k$. Such a plot is seen in Fig. 3 for $A = 909.166$ mm ($L = 25\,000$ mm, $\theta = 20°$, $\xi = 5°$), $k = 3.732$ ($\beta = 75°$) and $g_0 = 100$ mm. The value of k' calculated from (11) is 3.321 56. From this graph, it is seen that for given X it is possible to find k' for which the variation of the gap within ΔX is minimal. For instance, for the central beam, $X = 217.7$ mm and thus the most suitable k' is about 3.729. Once the crystal is manufactured, the k' cannot be changed. However, from (10) it follows that any change of θ requires the change of k'. Fortunately, as in the inclined case, instead of changing k', the appropriate change of g_0 may minimize the gap variation for given X.

Synchrotron radiation experiments usually require that the position of an exit beam remains fixed. The fixed-exit double-

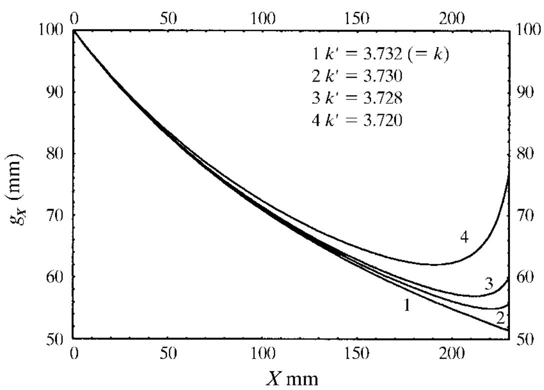

Figure 3
The dependence of the gap g_x on X for various k' (see text).

crystal monochromator is based on the proper change of the gap with the change of Bragg angle. The procedure described above requires the change of the gap with the change of Bragg angle to minimize the gap variation within ΔX. Unfortunately, it is not possible to fulfil both conditions at the same time. It is also interesting to note that from (1) and (3) it follows that even in the noncompensated case ($k' = k$) the influence of h on the variation of the gap decreases with the increase of ξ.

The second method of the aberration compensation in the inclined case consists of the usage of two double-crystal inclined monochromators cut in such a way that the angles of inclination β in the first monochromator and the angles of inclination in the second monochromator differ in sign. In this case, the change of the gap on the first monochromator is compensated by the change of the gap on the second monochromator. As was stated above, the rotated-inclined monochromator is essentially the inclined monochromator with large X. If the crystals create a $(-,+,+,-)$ setting, then the configurations of both monochromators and the beam are similar. [It is advantageous to imagine that the second monochromator is turned around the impinging beam by 180°. Then the resulting configuration corresponds to the first monochromator with the opposite sign of X and β that does not change (3).] This means that if for instance the increase of X leads to the decrease of the gap on the first monochromator then it also leads to the decrease of the gap on the second monochromator and, owing to the $(-,+,+,-)$ geometry, the resulting displacement of the beam is zero for any X.

If the crystals create a $(-,+,-,+)$ setting, then the situation is somewhat different. The sign of X remains unchanged but instead of k in (3) for the second monochromator, there will be $-k$. Then according (3) the resulting gap G is given by

$$G = Ag_0/(A + kX) + Ag_0/(A - kX), \qquad (12)$$

which may obviously substantially change with X for large X and thus this crystal arrangement is less suitable for the aberration compensation as compared with the $(-,+,+,-)$ arrangement.

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