1 of 1

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A Ray-Tracing Study of Inclined Double-Crystal Monochromators

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Third generation synchrotron X-ray sources such as the Advanced Photon Source (APS) under construction at Argonne National Laboratory will place severe heat load demands on the first beamline optical element. A cooled, inclined double-crystal monochromator is one of the methods being developed at the APS to handle these high heat loads while retaining the brilliance of the source. Using a modified version of the 1989 VAX/VMS SHADOW code, we examine the properties of the exit beam for two inclined double-crystal monochromator geometries.

Introduction

The inclined geometry double crystal monochromator (see fig. 1) has been developed in recent years as one of the most attractive methods for handling the high on-axis power densities ($\sim 150 \text{ W/mm}^2$ 30 m from the source) expected at the Advanced Photon Source (APS) [1][2]. In this geometry the crystal surfaces are cut at a large angle β with respect to the atomic planes corresponding to the reciprocal lattice vector $\mathbf{H}$. By orienting the crystal so that the rotation axis Ω corresponding to β lies in the plane of incidence formed by $\mathbf{H}$ and the incident wavevector $\mathbf{k}_i$, one can obtain considerable spreading of the incident beam on the surface of the first crystal while retaining a nearly symmetric ($b \simeq -1$) reflection. This gives a larger range of energy tunability than a conventional asymmetric cut crystal, and avoids the beam walk associated with the general asymmetric geometry. Using our modifications [3] to the 1989 VAX/VMS SHADOW ray-tracing program [4], we examine some of the subtleties inherent in inclined geometry monochromators.

Exit beam displacements

For a well collimated X-ray beam incident on an inclined crystal at an angle θ_i corresponding to the center of the single-crystal rocking curve, the index of refraction effects deflect the reflected beam $\mathbf{k}_H$ out of the plane of incidence of the first crystal with an azimuthal Bragg angle ρ_r as shown in fig. 1 [5]. (The size of the horizontal deflection is exaggerated for illustrative purposes.) The reflected polar Bragg angle is θ_r . If the second crystal is positioned so that a symmetrically reflected beam would intercept its surface at the average position $x = 0$,

$$z = h = a \tan(\theta_i), \quad (1)$$

then, ignoring the small quantity $\theta_r - \theta_i$, the true reflected beam intercepts the surface of the second crystal at the average position

$$x \simeq \frac{a \tan(\rho_r \cos(\theta_r))}{\left[1 - \frac{\tan(\beta) \tan(\rho_r \cos(\theta_r))}{\sin(\theta_r)}\right]}, \quad (2)$$

$$z \simeq h + x \tan(\beta).$$

If the well collimated incident beam makes an approximately oval footprint (shown in white in fig. 1) on the surface of the first crystal, then the reflected beam will make a similar oval footprint (also shown in white) on the surface of the second crystal.

At the high inclinations ($\beta \simeq 85^\circ$) of interest for high-heat-load monochromators, small variations in the incident angle θ_i produce large variations in ρ_r [5]. Therefore, if the incident beam is poorly collimated in the vertical direction and originates close to the surface of the first crystal, then the reflected beam will produce a footprint on the second crystal similar to the shaded rectangle of fig. 1. Note the significant difference in orientation between this footprint and that produced by a well collimated incident beam.

The inclined geometry quickly becomes asymmetric ($b \neq -1$) for non-zero incident beam azimuthal angles ρ_i , and therefore a horizontally divergent beam will suffer significant shifts in both θ_r and ρ_r . In this case the exit beam shape is not simply the diverged image of the incident beam shape as it would be with a symmetric double-crystal monochromator.

Using our modified version of SHADOW, we separate the affects of the incident beam divergences on the exit beam for a simplified APS undulator-A-like source and the nominal APS Si (1,1,1) high heat load inclined double-crystal monochromator (IDCM) tuned to 4.000 keV. The IDCM is assumed to be ~ 30 m downstream of the source. The source distributions are assumed to be uniform with a full width at half maximum (FWHM) horizontal and vertical source size of $\Delta x_s \simeq 0.73$ mm and $\Delta z \simeq 0.20$ mm, and a FWHM horizontal and vertical source divergence of $\Delta\theta_{xs} = 57 \mu\text{rad}$ and $\Delta\theta_{zs} = 25 \mu\text{rad}$. The incident beam FWHM spot size immediately upstream of the IDCM is therefore $\Delta x \simeq 1.86$ mm by $\Delta z \simeq 0.78$ mm. Figure 2 shows the coordinate systems used.

We ray traced a 4.000 keV monochromatic X-ray beam through the IDCM set for a nominal offset of $h = 35$ mm. Figures 3a and b show the exit beam 1 m

downstream of the IDCM resulting from a point source at the surface of the first crystal with FWHM divergences of (a) $\Delta\theta_{xs} = 0 \mu\text{rad}$ and $\Delta\theta_{zs} = 25 \mu\text{rad}$, and (b) $\Delta\theta_{xs} = 57 \mu\text{rad}$ and $\Delta\theta_{zs} = 0 \mu\text{rad}$. Figure 3c shows the exit beam 1 m downstream of the IDCM resulting from a perfectly collimated source with FWHM dimensions of $\Delta x_s = 1.86 \text{ mm}$ and $\Delta z_s = 0.78 \text{ mm}$. The incident beam divergences lie within the peak of the single-crystal rocking curve of the two crystals and so we have plotted the ray intercepts rather than the photon intensity. In all three cases, the ρ_r -kick from the second crystal compensates the ρ_r -kick from the first crystal and so there are no significant changes in the exit beam divergences.

Qualitatively, one can see that the affect of the undulator vertical divergence on the exit beam shape should be negligible compared to the affect of the incident beam size. The horizontal divergence, however, should produce a small distortion of the exit beam shape. Exit beam shapes very similar to the one shown in fig. 3b have been observed during high-heat-load IDCM tests using the NSLS X-25 focused wiggler beam which has a significant horizontal convergence [2].

Since the incident beam x and z positions and divergences are correlated, the actual profile obtained with an undulator source is not a simple convolution of these three simplified cases.

Mis-Orientation Sensitivity

A series of ray tracings were done in order to examine the deflection of the exit beam from an IDCM for mis-orientations about each of the crystal default optic coordinate system axes of fig. 2. The IDCM was again set to optimally reflect 4.000 keV X-rays.

Figure 4 shows the smoothed exit beam image on a screen 60 m from the source for a white X-ray beam incident on the IDCM with no mis-orientations. The source size and divergences were modeled as Gaussian with FWHM's as given above. The exit beam image has roughly the expected FWHM width and height,

with some slight distortions – possibly due to the source divergences. (5000 rays were traced and so the statistical fluctuations are not negligible.) Ray tracings were performed for various small mis-orientations of the first and second crystals about the x_O , y_O , and z_O axes. Mis-orientation of up to the FWHM of the rocking curve ($80 \mu\text{rad}$) about the Bragg angle axes x_{O1} and x_{O2} produce a linear vertical exit beam deflection at the image screen of the same size as one would expect for a symmetric crystal ($\sim 53 \mu\text{m}/\mu\text{rad}$). However, unlike the symmetric case, there is also a significant linear horizontal deflection of $\sim 600 \mu\text{m}/\mu\text{rad}$ due to the dependence of ρ_r on θ_i . (The linear horizontal deflection is also $\sim 600 \mu\text{m}/\mu\text{rad}$ at 10 keV.)

The vertical and horizontal deflections corresponding to mis-orientations of the first and second crystals about the y_O and z_O axes are shown in figures 5a and b. After the x_O axes, the IDCM is most sensitive to rotations about the y_O axes.

Sagittal Focusing with the Second Crystal

Ice and Sparks have proposed that bending the second crystal of an inclined double crystal monochromator about the y_{O2} axis (see fig. 2) to a sagittal radius of

$$R_s = \frac{2u_1 u_2 \sin(\theta)}{(u_1 + u_2) \cos(\beta)} \quad (3)$$

will produce sagittal focusing of the beam [6]. (u_1 and u_2 are respectively the source to optic and optic to focus distances.) They have ray traced an 85° inclined, sagittally focusing monochromator followed by a cylindrically bent, vertically focusing mirror using an APS undulator-A-like source at 10 keV *assuming* that the reflection is symmetric. They find no significant aberrations at 1:1 and 6:1 magnification. We have repeated their calculations using the source model from above at 10 keV, a fixed position 85° inclined double crystal monochromator at 35 m with the second crystal bent for 1:1 and 6:1 focusing ($R_s = 79.42\text{m}$ and 22.69m respectively.) Using our modified code that properly treats the asymmetric aspects of the inclined geometry we find no significant aberrations in the image for either 1:1 or 6:1 focusing. Figure 6 shows the result for 1:1 focusing.

Conclusions

Using a modified version of the SHADOW ray tracing code which includes new subroutines which treat general asymmetric dynamical Bragg diffraction, we have examined the performance of the inclined double crystal monochromator geometry. We find that it is somewhat more sensitive to misalignment than the symmetric geometry, but so far we have found nothing peculiar to the inclined geometry that would prevent its use as a high heat load monochromator at the APS. As suggested by Ice and Sparks, the inclined geometry can be used to provide sagittal focusing with the second crystal with relaxed constraints on the sagittal bending radius. Conversely, the same effect makes the inclined geometry more sensitive to defocusing of the exit beam due to thermally induced convex sagittal curvatures in the first crystal. In the future we hope to examine the effects of thermal bumps and random strain fields (mosaic spreads) in the first crystal.

Acknowledgements

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Figure Captions

Figure 1: Intercepts of a well collimated and a divergent beam on the surfaces of the first and second crystals of an inclined double crystal monochromator. See the text for details.

Figure 2: Source, default optic, and image screen coordinate systems used to discuss the SHADOW ray-tracing results.

Figure 3: Exit beams 1 m after an inclined-double-crystal monochromator for (a) a point source on the first crystal with a typical APS undulator-A vertical divergence, (b) a point source on the first crystal with a typical APS undulator-A horizontal divergence, and (c) a parallel incident beam with typical APS undulator-A beam size.

Figure 4: Smoothed photon intensity contour plot (arbitrary units) of the exit beam from a Si (1,1,1) inclined-double-crystal monochromator (IDCM) for an APS-undulator-A-like source. The IDCM is at 30, m from the source, the image screen is at 60, m.

Figure 5: Average vertical z_I (a) and horizontal x_I (b) beam displacements 60 m from the source for mis-orientations of θ_{y1} (squares), θ_{z1} (diamonds), θ_{y2} (circles), and θ_{z2} (triangles). See fig. 2 for definitions of the angles.

Figure 6: Smoothed photon intensity contour plot (arbitrary units) of the focus of an inclined-double-crystal monochromator with the second crystal bent to a sagittal radius of $R_s = 79.42$ m.

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FIG. 1

FIG. 2

FIG. 3a

Fig. 3b

Fig. 3c

FIG. 4

FIG. 5a

Fig. 5b

Fig. 6

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