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SIMULATED HIGH HEAT LOAD PERFORMANCE OF AN INCLINED CRYSTAL MONOCHROMATOR*

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ABSTRACT

Thermal distortions of an inclined silicon crystal subjected to the high heat loads expected for a 2.5 m long undulator at the Advanced Photon Source were simulated, and the distortions were then used to calculate (111),(111) (+,-) double crystal rocking curves. The inclination angle for all the simulations was either 80° or 85°. The first crystal was assumed to be a slab that was uniformly cooled on its underside with liquid gallium. For some of the simulations, the undulator gap was set to 11.5 mm corresponding to $K=2.2$, and the crystals were oriented to diffract the first harmonic energy at 4.2 keV. For $K=2.2$, the total x-ray power incident on the crystal is 3.8 kW, and the peak power density transverse to the beam is 148 W/mm². Rocking curve broadening in these cases was found to be no more than 0.42 arcsec. Simulations for the third harmonic at $K=2.2$ were also performed, and the broadening was found to be no more than 1.87 arcsec. In other simulations the undulator gap was widened, and rocking curves for the third harmonic at $K=1.5$ (19.9 keV) and the first harmonic at $K=1.2$ (8.2 keV) were obtained. Only weak broadening was found for these cases as well. Finally, rocking curves at 4.2 keV were not altered if a slit that passed only the central cone of the undulator was placed in front of the first crystal.

1. INTRODUCTION

A recent optical innovation for x-ray synchrotron monochromators called an inclined crystal^{1,2} monochromator has been tested under severe heat loads from an undulator beam³ and from a focused wiggler beam⁴. A dramatically improved performance compared to a noninclined monochromator was found in both cases. In the inclined geometry (shown in Fig. 1a), the beam is incident at a small angle thereby spreading out the beam footprint as shown in Fig. 1b. A significant reduction in the surface power density can be achieved without sacrificing the tuning range of the monochromator.

Numerical results for the temperature and deformation of a silicon crystal subjected to the heat load from a type A undulator at the Advanced Photon Source (APS) were simulated using computer modeling, and the resulting surface deformations were used to compute rocking curves. The calculations of the thermal deformations were obtained in the same manner as described previously,¹ and the rocking curve computations were obtained by tailoring a procedure previously used for a noninclined monochromator⁵ to an inclined monochromator.

Fig. 1a. The inclined crystal geometry. The top portion of the figure shows a perspective view. The inclination angle is denoted as β .

Fig. 1b. The footprint on the crystal surface in the inclined geometry resulting from a horizontal beam having a rectangular cross section. The top portion is a perspective view.

2. CONDITIONS FOR THE VARIOUS CASES

The beam parameters for the cases that we have treated are listed in Table 1. These parameters are for 100 mA current in the storage ring. The $K=2.2$ cases correspond to an undulator gap of 11.5 mm and a peak power density of 148 W/mm² at 30 m from the undulator. The crystal parameters for the above cases are listed in Table 2.

Table 1. Undulator beam parameters. K is a dimensionless parameter proportional to the magnetic field strength and the undulator period. The slit is placed at 30 m from the undulator and has a 1.8 mm vertical opening and a 3.6 mm horizontal opening. The total power in the undulator beam is denoted as P_{tot} ; beam dimensions (FWHM) at 30 m for the vertical and horizontal frequency integrated power are denoted as FIP_v and FIP_h , respectively; the undulator harmonic used for diffraction is indicated as HARM; and the beam dimensions at 30 m for the central cone of the harmonic are denoted as CC_v and CC_h .

CASE #	K	SLIT	P_{tot} (kW)	FIP_v (mm)	FIP_h (mm)	HARM.	CC_v (mm)	CC_h (mm)
1	2.2	no	3.8	2.33	7.99	3	0.73	1.88
2	2.2	yes	0.8	2.33	7.99	3	0.73	1.88
3	1.5	yes	0.5	2.33	5.52	3	0.70	1.86
4	1.2	yes	0.4	2.33	4.42	1	0.78	1.88
5	2.2	yes	0.8	2.33	7.99	1	0.87	1.93
6	2.2	yes	0.8	2.33	7.99	1	0.87	1.93
7	2.2	no	3.8	2.33	7.99	1	0.87	1.93

Table 2. Crystal parameters. The inclination angle, β ; the energy of diffraction, E ; Bragg angle, Θ ; and the length and width of the crystal are listed.

CASE #	β (deg)	E (keV)	Θ (deg)	Length (mm)	Width (mm)
1	85	12.6	9.0	952	131
2	80	12.6	9.0	151	31
3	80	19.9	5.7	233	31
4	85	8.2	14.0	183	51
5	85	4.2	28.0	91	51
6	85	4.2	28.0	293	151
7	85	4.2	28.0	293	151

3. TEMPERATURE AND DISPLACEMENT RESULTS

As shown in Fig. 2, the crystal was divided into finite elements in order to compute temperatures and the accompanying displacements. The footprint of the beam (frequency integrated power) on the crystal is highlighted in Fig. 2. All the radiation was assumed to have been absorbed at the surface. (The effect of thermal distortion within the depth of the crystal was found previously to have a negligible influence on rocking curves.) The crystal was assumed to be 10 mm thick, and it was assumed to have a flat underside in contact with liquid gallium. This cooling arrangement corresponds to a heat transfer coefficient of $5 \text{ W/cm}^2\text{-K}$. The crystals were not physically constrained, that is, they were assumed to be free standing.

As is evident from Fig. 1, the surface displacement relevant for diffraction is not the displacement occurring in planes that contain the surface normal. Rather, it is the displacement in vertical diffraction planes that determine the rocking curve. As an example, the amplitude of this displacement for case 7 plotted as a function of position on the crystal is shown in Fig. 3. Cursory results for all the cases are summarized in Table 3. The on-surface peak power densities are also listed in Table 3. In the inclined geometry the peak power density normal to the beam is reduced by the spreading factor for the footprint area. This factor is given by $\cos\beta \sin\Theta$ (see ref.3).

Table 3. The value of the peak power density on the surface, the maximum surface temperature rise, displacement (in the diffraction plane), and slope.

CASE #	on-surface peak power density (W/mm^2)	ΔT_{max} (deg K)	displmax (μm)	slopemax (arcsec)
1	2.0	39	5.5	5.2
2	4.0	58	1.9	13.6
3	2.6	23	1.9	8.0
4	3.1	21	3.5	3.0
5	6.1	92	0.6	18.7
6	6.1	70	1.0	10.0
7	6.1	142	3.2	24.0

4. ROCKING CURVE RESULTS

The slope values listed in Table 3 are not indicative of rocking curve broadening. This follows because only a small portion of the entire crystal surface is irradiated by radiation from the central cone and because over this small region the slope remains fairly constant. The net result is that rocking curve centers are offset in angle, but they are not greatly broadened.

The surface was cut along rows of elements (i.e., elements that lie along the z direction in Fig. 2) corresponding to a single vertical diffraction plane, and

Fig. 2. Schematic illustration of a crystal showing the elements used in the numerical simulations and the footprint of the frequency integrated power.

Fig. 3. Thermal displacements normal to the Bragg planes.

the displacement profiles along these cuts were fit using a spline fitting procedure.⁶ Each spline fit was differentiated to obtain slope errors, and separate rocking curves were calculated using these slope errors. These separate rocking curves were obtained by breaking the slope error profile for each cut into 250 segments and calculating a rocking curve for each segment using dynamical theory for a perfect crystal. A rocking curve for each cut was obtained by adding up the rocking curve amplitudes for each segment after offsetting them in angle by the slope error for that segment and applying the appropriate photon flux as a weighting factor. This flux was computed using the vertical Gaussian distribution for the central cone⁷ stretched out by a factor of $1/\sin\theta$. Finally, an overall rocking curve was obtained by adding rocking curves for all the cuts after weighting them according to the horizontal Gaussian distribution for the central cone stretched out by a factor of $1/\cos\beta$.

Rocking curves are shown in Figs. 4-10, and FWHM and amplitudes of the rocking curves are listed in Table 4. Also listed are FWHM values for the

Table 4. Rocking curve summary.

CASE #	FWHM (arcsec)	FWHM (arcsec)	peak amplitude
	with displacement	without displacement	with displacement
1	6.52	6.31	0.960
2	8.19	6.31	0.709
3	5.02	3.94	0.709
4	10.24	10.05	0.973
5	22.33	22.33	0.983
6	22.75	22.33	0.980
7	22.63	22.33	0.985

case of no displacement. That is, we also calculated rocking curves with the same procedure as was used for the thermally distorted surfaces but with an ideally flat surface. The amount of thermal broadening can be determined by comparing the two FWHM values for each case. The peak rocking curve amplitude for the zero displacement cases were also used to normalize rocking curves for the nonzero displacement cases. That is, we simply divided rocking curve amplitudes for the nonzero displacement cases by this peak value. The last column in Table 4 lists the peak value obtained after applying this normalization procedure. The lowest diffraction efficiency is seen to be 70.9%.

Fig. 4. The FWHM is 6.52 arcsec. The FWHM of an ideal crystal in this case is 6.31 arcsec.

Fig.5. The FWHM is 8.19 arcsec. The FWHM of an ideal crystal in this case is 6.31 arcsec.

Fig.6. The FWHM is 5.02 arcsec. The FWHM of an ideal crystal in this case is 3.94 arcsec.

Fig.7. The FWHM is 10.24 arcsec. The FWHM of an ideal crystal in this case is 10.05 arcsec.

Fig.8. The FWHM is 22.33 arcsec. The FWHM of an ideal crystal in this case is 22.33 arcsec.

Fig.9. The FWHM is 22.75 arcsec. The FWHM of an ideal crystal in this case is 22.33 arcsec.

Fig.10. The FWHM is 22.63 arcsec. The FWHM of an ideal crystal in this case is 22.33 arcsec.

5. SUMMARY AND CONCLUSIONS

Cases 7 and 1 are for the first and third harmonic of the undulator without any slit, that is, with the crystal exposed to the entire undulator beam. Only a very slight effect on the rocking curve is found for both cases.

However, although the crystal size required for the first harmonic, 31 by 151 mm, appears reasonable, the crystal size required for the third harmonic, 131 by 952 mm, is unreasonable. In order to permit a smaller crystal to be used in case 2, a decreased inclination angle of 80° was applied, and a slit was placed in front of the first crystal. The rocking curve in this case became asymmetric (see Fig. 5) and was thermally broadened by 1.87 arcsec. The peak diffraction efficiency decreased to 70.9%.

Case 4 was for the third harmonic at 19.9 keV. The higher energy implies a narrower ideal rocking curve with a FWHM of 3.94 arcsec. The observed rocking curve has a width that is only 1.08 arcsec broader.

From the other runs, it is clear that rocking curves for the first harmonic at 8.2 and at 4.2 keV are hardly affected at all. Comparing the results for cases 6 and 7, we conclude that the presence of a slit does not have a significant effect at 4.2 keV.

In conclusion and in agreement with our experimental results (see refs. 3 and 4), these simulations show that the inclined crystal arrangement is very effective in handling high heat loads from undulators and, in particular, is promising for undulator monochromators at the APS.

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