Sagittal Focusing of Synchrotron X Radiation
with Curved Crystals*

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ABSTRACT

We describe the sagittal focusing of x rays with singly bent crystals that accept the meridian plane divergence from a similar but flat crystal to form a pair in a nondispersive two-crystal Bragg monochromator. Curved crystals can intercept from 5 to 20 times the sagittal divergence of curved mirrors at x-ray energies above 10 keV. Anticlastic (transverse) bending of the crystal is made negligible in the meridian plane with reinforcing ribs cut parallel to the plane of scattering. Results show that at energies of 10, 20, and 30 keV the bent crystal performs efficiently and images the source size at the Cornell High Energy Synchrotron Source.

1. INTRODUCTION

MASTER

Because of the divergence of synchrotron radiation and the large distances between the sample and source, it is desirable to focus the radiation to increase the useful intensity. It is most worthwhile to focus the horizontal divergence which can contribute 100 times more to

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the intensity than focusing the vertical divergence. Previously, variable radii crystals have been curved in their meridian (scattering) plane to focus the horizontal divergence from synchrotron radiation. Such an arrangement contributes to an unfavorable polarization loss, and precludes their use in a two-crystal Bragg monochromator. This construction requires operation at fixed energies or motion of the sample.

Sagittal focusing of synchrotron x radiation with a mosaic crystal of fixed radius has been used for fluorescent excitation [1]. A cylindrically curved crystal at a magnification, M , near one-third has been shown to satisfy the Bragg condition of the central vertical rays exactly for a horizontal radiation fan of arbitrary divergence angle, Ψ_H [2]. More recently, a crystal curved to approximate a conical surface has been shown to intercept large horizontal divergences with a satisfactory match to the Bragg condition for M from 1/3 to 2. This crystal caused less focal aberrations at $M \sim 1$ than obtained with the cylindrical crystal at $M=1/3$, [3]. A crystal bending device was built to test both the cylindrical and conical geometries at the Cornell High Energy Synchrotron Source, CHESS. The bending device will be described in another article [4].

The geometry for focusing is shown in fig. 1. Relationships among the different variables are:

$$N_S = 2F_1F_2\sin\theta/(F_1 + F_2) ; \quad (1a)$$

$$R_m = \frac{[(F_1 + F_2)^2 - 4F_1F_2\sin^2\theta]^{1/2}}{\sin 2\theta} ; \quad (1b)$$

$$\text{Magnification, } M = F_2/F_1 , \quad (1c)$$

where N_S and R_m are the sagittal and meridional radii of curvatures of the crystal planes and are normal to the Bragg reflecting planes. The width of the horizontal divergence intercepted by the curved optic cannot be greater than the diameter, and a practical limit is the sagittal radius of curvature, N_S . As crystals have Bragg scattering angles, θ_B , that are typically 20 times the critical angles of reflection for mirrors, N_S will be 20 times larger for crystals than for mirrors, eq. (1). If the physical size of the optical element were not limiting, crystals might intercept 20 times the horizontal divergence intercepted by mirrors.

In general, the horizontal divergence from storage ring bending magnets is about 50 mrad. At 10 m from the source, crystals limited to 20 cm in width, L_S , will intercept 20 mrad of this horizontal divergence. Singly curved mirrors set at critical angles to reflect 10 to 40 keV x rays intercept from two to ten times (respectively) less horizontal divergence when no restrictions are placed on their physical size. Practical manufacturing limits of 60 cm lengths, L_m , for curved mirror surfaces reduce the horizontal divergences intercepted by an additional factor of two. In addition, the larger penetration depth of x rays diffracting from crystals lessens the effect of both surface contamination and imperfections which can reduce the intensity of specular reflection from mirrors.

Here we report on the intensities, rocking curve widths, and focusing from bent silicon (111) crystals.

Anticlastic Bending Effect

Pure bending of even thin rectangular plates (thickness $\ll$ radius of curvature) results in a transverse curvature of the plate. This

transverse curvature, $\overline{R_m}$, of a plate subjected to pure bending in a plane of symmetry is related to the intended radius, N_s , by

$$\overline{R_m} = N_s / \sigma , \quad (2)$$

where σ is Poisson's ratio [5]. With the aid of the diagram shown in fig. 2, the anticlastic curvature of the crystal, $\overline{R_m}$, is shown to produce an error, $\Delta\theta_E$, which increases for the more vertically divergent rays. The error in Bragg angle for a small vertical divergence is given by

$$\Delta\theta_E = F_1 \phi_v / 2 \overline{R_m} \sin\theta , \quad (3)$$

where ϕ_v is a typical opening angle for 90% of the radiation from a 2.5 GeV storage ring. For maximum intensity this error, $\Delta\theta_E$, should be smaller than the angular range over which the crystal diffracts, $\Delta\theta_B$.

For magnification of one, a Si (111) crystal located 10 m from the source has a sagittal focusing radius, N_s , calculated as a function of photon energy from eq. (1a) listed in table 1. Using 0.25 as Poisson's ratio for Si, we then calculate the anticlastic radii, $\overline{R_m}$, assumed by a thin rectangular Si (111) plate bent to the radii, N_s . These anticlastic radii, $\overline{R_m}$, listed in table 1 are used to calculate $\Delta\theta_E$ from eq. (3) for the most extreme rays. As shown in table 1, $\Delta\theta_E$ is larger than the acceptance angle $\Delta\theta_B$ by a factor of 5 at 5 keV, 22 at 10 keV and 641 at 40 keV. Thus, the attempt to use unreinforced crystals for sagittal focusing of synchrotron radiation would result in a reduction of the vertical divergence accepted by just the ratio $\Delta\theta_E/\Delta\theta_B$. To ensure that diffraction occurs, we have chosen to limit the error, $\Delta\theta_E$, to about one-fifth of the angular range of the crystal reflecting width. These permissible anticlastic radii were calculated using eq. (3) and are listed in table 1.

To reduce the anticlastic curvature, ribs transverse to the bending curvature were attached to the back surface of the crystal with various glues. These ribs significantly reduced the anticlastic bending without seriously stiffening the crystal in the direction of the desired bending radius, N_S . However, the glue caused appreciable distortions in the crystallographic planes. To eliminate these distortions, ribs were machined integral with the crystal from a thick monolithic Si block. Such a crystal is shown schematically in fig. 3. The height, h , spacing, s , and width, w , of the ribs determine the resistance of the crystal to anticlastic bending. In the thin plate approximation and assuming an elastically isotropic material, the relationship between the bending radius, N_S , and the resulting anticlastic radius, R_m^- , for a ribbed crystal can be shown to be,

$$R_m^-/N_S = -\frac{1}{\sigma} \left(\frac{h}{t}\right)^3 \left(\frac{w}{s-w}\right) \left[1 - \left(\frac{w}{s-w}\right) \left[1 - \left(\frac{t}{h+t}\right)^3\right]\right] \left\{1 + \frac{t(s-w)(12Z_x^2 + t^2)}{w(1-\sigma^2)h} + \left[\frac{1/2(h+t) - Z_x}{h}\right]^2\right\}, \quad (4)$$

where the notation is given in fig. 3, and the distance between the middle plane of the plate and the mean neutral surface is

$Z_x = wh(h+t)/2(st+wh)$ [5,6]. An adequate approximation to eq. (4) is

$$R_m^-/N_S \approx -\frac{1}{\sigma} \left[1 + \frac{w}{s} \left(\frac{h}{t}\right)^3 (1 - \sigma^2)\right]. \quad (5)$$

The plate's resistance to anticlastic bending depends on the rib height cubed. Let the width of the ribs and the thickness of the crystal be 0.5 mm with a rib repeat distance of 2.5 mm. The silicon crystal with a

Poisson's ratio of 0.25 is located 10 m from the source. Using eq. (5), we calculate the height of the ribs for that anticlastic bending radius given in table 1 which is sufficiently large so that the error in $\Delta\theta_E$ is only 1/5 the diffraction width of a nearly perfect Si (111) crystal. Results are listed in table 1. As seen from table 1, the necessary height of the ribs increases with increasing x-ray energy. As the crystal surface under the ribs does not bend, the minimum horizontal focal width that can be achieved even for a point source at an M of one is $2W$. Thus, the source size will influence the choice of rib width, height and spacing.

Experimental Arrangement

For the test results presented here, Si crystals were machined with rib heights of 1 and 1.4 cm, with radii at their base of 0.12 mm to lessen their stress sensitivity. Syton polished Si (111) crystals were machined with a diamond impregnated blade to the shape shown in fig. 3. They were 7.6 cm long and 3.5 cm wide with $t = 0.5$ mm, $w = 0.5$ mm and $s = 2.5$ mm. After machining, a chemical etchant, consisting of 95 wt % HNO_3 and 5 wt % HF in an ice bath, was used to remove 35 to 75 μm from the machined surfaces. Etch pit measurement of dislocation densities gave $\sim 10,000 \text{ cm}^{-2}$. The ribs came to within 2 mm of the inner bending rods which are spaced 4.2 cm apart. The outer bending rods were spaced 6.6 cm apart, and all bending rods were 9.4-mm diam.

A nondispersive (1,-1) double-crystal monochromator was arranged with a flat Si (111) crystal followed by the ribbed crystal mounted in a bending device as sketched in fig. 4. The first crystal was located 11 m from the photon source at CHESS. Three mrad of horizontal divergence

and 90% of the vertical divergence was intercepted by the bent crystal. Each crystal was mounted on independent axes for θ rotation. They were displaced from each other by 5 cm in the vertical direction. An ionization chamber was inserted between the first and second crystal and another immediately following the second crystal. Because of the high radiation background in the first ionization chamber, the efficiency of the bent second crystal as an element in a two-crystal monochromator was obtained by comparing the output of the second chamber when the second crystal was unbent to the output when the crystal was bent for optimum focus.

Visual observations of the focusing were made at a point 21 m from the source with a ZnS fluorescent screen, TV camera and monitor. Rocking curves of the bent and unbent crystals were made to measure the distortions introduced by bending.

Results

The precision of all necessary crystal bending device rod movements was 0.1 μm . Each end of the inner rods could be independently moved to apply the bending moment, and both the inner and outer rods could be moved relative to each other in the plane of the crystal plate to generate a conical surface. With these motions, both uniform and nonuniform bending moments as well as twist could be applied to the crystal. Our intent was to ensure that the crystal bending device would not be the limiting factor in the performance of the bent crystals. Because of the need to optimize many parameters, visual observation of the diffracted x rays with a fluorescent screen was very useful for determining which motion of the rods gave uniform diffraction from the bent crystal. Table 2 lists the radii, N_S , to which the crystals were bent, the measured width of the

rocking curves, $\Delta\theta$ unbent and $\Delta\theta$ bent, and the % of the radiation diffracted by the curved crystal compared to its unbent state.

Broadening of the rocking curve width of the bent crystal, $\Delta\theta_{\text{bent}}$, is obtained by comparison to the measured unbent value, $\Delta\theta_{\text{unbent}}$ (full-width half maximum). The unbent value is very near that expected for two flat Si (111) crystals in the (1,-1), geometry, $\sqrt{2} \Delta\theta_B$. Broadening observed on bending is small and commensurate with the high diffraction efficiency which approaches that from two flat crystals in a nondispersive orientation. At 30 keV, the reduction in diffraction efficiency resulted from a twist in the crystal as revealed by the two peaks in the rocking curve. The width listed in table 2 was determined by assuming a Gaussian peak shape and deconvoluting the double peak. Restrictions on beam time prevented us from correcting this misalignment and from evaluating the crystal at 40 keV. We are confident, however, of obtaining diffraction efficiencies of 70% at 30 keV for a properly bent crystal. Predictions from a ray tracing program were confirmed by the observed results. Even larger divergences than the 3 mrad used here can be intercepted. Ray tracing results for the diffracting efficiencies of sagittal focusing crystals intercepting 15 mrad of radiation predict values of 98% at 10 keV, 92% at 20 keV, 66% at 30 keV and 47% at 40 keV for the source size designed for the National Synchrotron Light Source. As the horizontal source width increases, the diffraction efficiencies decrease. The calculated variation in the Bragg spacing which results from the sagittal curvature could account for less than 1/6 the reflection width broadening observed here. X-ray topographs of the curved crystals revealed that anticlastic bending occurred between the ribs, and we believe this could account for the observed broadening.

To determine how well the bent crystals focused the radiation source at CHESS, a lead sheet containing three holes of approximately 1/4-mm diam spaced 1 cm apart was placed in the incident beam upstream of the first crystal as shown in fig. 4. At the location of this experiment, the 2σ (standard deviation) source size at CHESS is approximately 4.2-mm wide and 0.5-mm high. Thus, an actual size image of the source should be observed at $M=1$ if the curved crystal is not distorting the image. Polaroid film placed 21 m from the source and 10 m from the pinholes was used to record the source size for $M \approx 0.9$. An exposure was made through each pinhole separately to determine that each produced an image, and that the crystal focused uniformly. Results are shown in the upper part of fig. 5 and labeled A, B, and C for the three different pinholes. The exposure, ABC, is a composite taken when all three pinholes contribute simultaneously. Though we did not measure the focal spot sizes quantitatively with film, they are near the 2σ dimensions quoted earlier. In addition, the superposition of the three spots verified that the monochromator was focusing the horizontal divergence to the same central spot. With the pinholes removed and the ribbed crystal unbent, the horizontal width of the 3 mrad of radiation was 6 cm as shown by the center exposure of the unfocused beam in fig. 5. After focusing, the horizontal width was reduced to approximately the source width as shown by the exposure at the bottom of fig. 5. With no vertical focusing, the vertical dimension in the unfocused and focused exposures is determined by the opening angle of the radiation. If the anticlasic bending had not been negated by the rib structure, the vertical height of the horizontally focused beam and the rocking curve widths would not have approached the values for a flat crystal.

Conclusion

Ribbed crystals provide a solution to the problem of anticlassic bending. This permits the use of bent crystals to sagittally focus more of the large horizontal divergence of synchrotron radiation at energies above 5 keV than is possible with mirrors. These bent crystals match the meridian divergence from a first flat crystal and can be used with high efficiency as the second element of a (1,-1) two-crystal Bragg monochromator. As the energy resolution of this two-crystal monochromator is determined by the first flat crystal, there is no sacrifice in energy resolution from curving the second crystal. A mirror focusing in the meridian plane can be used for vertical focusing if desired. From our experience with these bent crystals, we predict that they can be used with good efficiency at energies up to 40 keV.

The simple bending technique of using a cantilevered triangular crystal [7] to generate a cylindrically curved surface would work with the ribbed crystal and permit its use for sagittal focusing of the horizontal divergence at $M \approx 1/3$. Our choice of the four point bending scheme permitted curving to the conical shape, the use of rectangular crystals to maximize the amount of radiation intercepted, and kept the center of curvature bisecting the horizontal divergence as the curvature is changed.

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Table 1

Rib heights, h , are given which restricts the anticlastic curvature so that the maximum error in the Bragg angle is one-fifth the Bragg reflection width of the crystal. Si (111) crystal 10 m from a source of ϕ_V divergence with 0.5 mm wide ribs spaced on 2.5 mm centers and a Poisson's ratio of 0.25

Energy (keV)	ϕ_V (mrad)	θ_B (deg)	$\Delta\theta_B$ (mrad)	N_S (m)	R_m^a (m)	$\Delta\theta_E$ (mrad)	R_m^b (m)	h (mm)
5	0.34	23.24	0.055	3.94	15.78	0.273	391.7	2.5
10	0.21	11.38	0.031	1.97	7.89	0.674	872.4	4.2
20	0.15	5.66	0.015	0.99	3.95	1.928	2534.9	7.5
30	0.12	3.77	0.010	0.66	2.63	3.470	4562.6	10.5
40	0.10	2.83	0.008	0.49	1.98	5.128	6409.5	12.9

^aAnticlastic radius for an unconstrained crystal bent to the sagittal radius N_S .

^bAnticlastic radius permitted for a Bragg angle error of $1/5 \Delta\theta_B$.

Table 2

Bragg diffraction width and diffraction efficiency of a ribbed Si (111) crystal intercepting 3 mrad of horizontal divergence and bent to the radius, N_S , for various energies and magnifications, M .

Energy (keV)	θ_B (deg)	$\Delta\theta$ Unbent (arc sec)	M	N_S (m)	$\Delta\theta$ Bent (arc sec)	Diffraction Efficiency (%)
10	11.38	8.9	0.9	2.1	8.9	95 ± 3
10	11.38	8.9	0.3	1.1	8.9	95 ± 3
20	5.66	4.4	0.9	1.0	5.6	80 ± 10
30	3.77	2.9	0.9	0.7	4.7	50 ± 10

Figure Captions

- Fig. 1. Focusing geometry of a doubly curved optical element which identifies the parameters used in the text.
- Fig. 2. An anticlastic curvature, $\overline{R_m}$, is generated when a thin plate is bent to the radius N_S and results in a Bragg angle error, $\Delta\theta_E$, for meridian rays divergent from the central ray.
- Fig. 3. Schematic for a crystal with ribs cut parallel to the bending rods and which identifies the variables used in calculating the resistance to anticlastic bending imparted by the ribs.
- Fig. 4. Placement of the curved ribbed crystal in a two-crystal monochromator, (1,-1), with pinhole mask used to determine focusing aberrations.
- Fig. 5. A, B and C are pinhole images separated by 1 mrad horizontally of the source size at CHESS after passing through the focusing optics. ABC is a superposition of these images showing that the aberrations in the focus are no larger than the source size. The unfocused horizontal width of the 3 mrad beam is shown in comparison to the focused result.

Fig. 1. Focusing geometry of a doubly curved optical element which identifies the parameters used in the text.

Fig. 2. An anticlastic curvature, R_m^- , is generated when a thin plate is bent to the radius N_s and results in a Bragg angle error, $\Delta\theta_E$, for meridian rays divergent from the central ray.

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Fig. 3. Schematic for a crystal with ribs cut parallel to the bending rods and which identifies the variables used in calculating the resistance to anticlassic bending imparted by the ribs.

HORIZONTALLY FOCUSING TWO CRYSTAL MONOCHROMATOR

Fig. 4. Placement of the curved ribbed crystal in a two-crystal monochromator, (1,-1), with pinhole mask used to determine focusing aberrations.

20 KeV FOCUSING

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