X-Ray Monochromator Geometry for Focusing Synchrotron

Radiation Above 10 keV*

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The relative merits of crystals versus mirrors for focusing synchrotron radiation at energies above 10 keV are explored. As mirrors have critical angles of reflection typically 1/20 of the Bragg scattering angles for crystals, large mirror surface areas are required. Sagittal focusing is weak for mirrors and limits the amount of radiation intercepted. We show that crystals bent to a simple cylindrical curvature will accept large divergences of radiation for sagittal focusing. At a magnification near 1/3, the cylindrically curved crystals are shown to make the proper Bragg angle for energies above 5 keV and for divergences larger than 10 mrad and to produce x-ray beams which are approximately focused.

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1. Introduction

Because of the large distances between the synchrotron radiation source and the experiment, condensing optics are useful to confine the beam to a reasonable size at the sample and to collect as much of the radiation as possible. The radiation is spread over 2π in the plane of orbit but is confined to small opening angles, ϕ , in a plane perpendicular to the plane of the storage ring. This angle is approximately given by the rest mass energy of the electron divided by the energy of the circulating electron, $m_0 c^2/E$, about 0.2 mrad for electron energies of 2.5 GeV. In the plane of orbit, the radiation spread available from typical bending magnets is from 20 to 50 mrad. Higher intensities and smaller beam areas are produced at the sample by collecting and focusing this large divergence.

Two methods for focusing photons are specular reflection from mirror surfaces and diffraction from crystallographic planes. Typical glancing angles for critical reflection of photons from mirror surfaces are about 1/20 of that for diffraction from crystallographic planes. For photon energies exceeding 10 keV, the small reflection angles require that mirrors be large if they are to intercept the divergence of the source^{1,2}. In addition, sagittal focusing (perpendicular to the plane of scattering) with mirrors requires very small bending radii, R_g , and, consequently, only small divergences, ψ , may be intercepted. Shown in Fig. 1 is a comparison of the divergence intercepted by a Ge(111) crystal and a platinum-coated mirror for different photon energies. The Ge crystal is limited to a practical dimension of 20 cm. At 10 m from the source, the crystal intercepts 20 mrad of radiation. The divergence intercepted by a crystal bent to a cylindrical radius for focusing at magnifications, M , of 1 or less is generally restricted to $\frac{1}{2} = R_g/F_1$ and cannot exceed $2R_g/F_1$. (See Fig. 2 for the geometry defining these terms.) Divergences

below 20 mrad shown by the dashed lines in Fig. 1 are limited by $\psi = R_g/F_1$ for the Ge(111) crystal. No physical size limitations were placed on the mirror, and the divergences intercepted, ψ , shown by the solid line are restricted only by the radius R_g . Above 10 keV, photon energies, crystals intercept from 3 to 15 times the divergence accepted by mirrors because crystals have larger scattering angles.

Table I gives the sizes of mirrors located 10 m from the synchrotron radiation source required to intercept the divergences ψ and ϕ . The parameters used in Table I are identified in Fig. 2. The radius R_g determines the divergence ψ intercepted by the mirror. Even for small divergences of $\psi = 2.1$ mrad, a doubly-curved mirror would need to be in excess of 2 m in length when set to reflect 40 keV photons. At energies near to and below 10 keV, mirrors may be preferable to crystals as focusing devices because of their simplicity of construction and increased capacity for intercepting larger divergences.

It is our purpose to assess the properties of crystals for focusing synchrotron radiation of photon energies above 5 keV. An approximation is made to the ideal focusing, doubly-curved surface with a simpler cylindrical bend. Such a curved crystal has been previously used for focusing synchrotron radiation³. At magnifications near 1/3, the error in the Bragg diffraction angle, θ , for sagittal rays can be eliminated independent of the divergence intercepted. Thus a singly-curved crystal will produce an approximately focused beam at this magnification while maintaining a narrow $\Delta E/E$.

2. Optical Geometry

The near ideal geometry for point-to-point focusing x-ray optics for Bragg reflecting crystals has been given by Berreman et al.⁴. This geometry is shown in Fig. 2. Bragg planes are curved to the two different radii-- R_1

(in the meridian or scattering plane (then ground to $R_m/2$)²) and R_s (in the sagittal plane perpendicular to the scattering plane). The following relationships are derived for this geometry:

$$\tan \gamma = [(F_1 - F_2)/(F_1 + F_2)] \tan \theta \quad (1a)$$

$$R_m = F_1 / \sin(\theta + \gamma) \quad (1b)$$

$$R_s = F_1 \sin(\theta - \gamma) \quad (1c)$$

$$\text{Magnification, } M = F_2/F_1 = \sin(\theta - \gamma)/\sin(\theta + \gamma) \quad (1d)$$

A source point at S will undergo a magnification of F_2/F_1 which is less than one for the geometry shown in Fig. 2. For typical source distances of 5 m or more for synchrotron radiation, the radius R_m is usually greater than 10 m for angles θ and γ of a few degrees. However, R_s (Eq. 1c) is a much smaller radius than R_m (Eq. 1b) so the better single curvature approximation to this doubly curved surface would be a cylinder of radius $N = R_s \cos \gamma$, as shown in Fig. 2. We investigate how closely this cylindrical curvature can match the ideal geometry.

Shown in Fig. 3 is the geometry of this singly-curved surface from which the following relations are derived (See Appendix A):

$$\sin \theta' = \sin \theta [(1 + \alpha \tan \theta / 2) / (1 + \tan \theta / 2)]^{1/2} \quad (2a)$$

where

$$\alpha = (2F_1/N \sin \theta) - (F_1/N)^2, \quad (2b)$$

and where

$$N = R_s \cos \gamma. \quad (2c)$$

If $\alpha = 1$, then $\theta' = \theta$. This occurs when values of F_1/N or F_1/R_s are chosen so that

$$\frac{F_1}{N} = \sin \theta / (1 \pm \cos \theta), \quad (3a)$$

or

$$\frac{F_1}{R_s} = \sin \theta / \cos \gamma (1 \pm \cos \theta). \quad (3b)$$

The solution with $(1-\cos\theta)$ is that which converges the radiation in the xy plane, Fig. 3, and is of most interest here. When $\alpha=1$, the values of $\theta'=\theta$ are independent of the divergence ψ . It is desirable to fix the magnification to obtain constant values of F_1 and F_2 so that the experiment does not need to be moved to track the horizontal focus which changes with the energy. Equating the ideal solution given by Eq. (1c) with that for the cylindrical approximation given by Eq. (3b), we have that

$$\sin(\theta-\gamma) = \cos\gamma (1-\cos\theta)/\sin\theta \quad (4a)$$

For photon energies above 10 keV where θ and γ are small angles,

$$\gamma \approx \theta/2 \quad (4b)$$

On substitution of this result in Eq. (1d), we find that for a magnification of:

$$M \approx 1/3 \quad (4c)$$

the error in $\theta'-\theta$ will be minimized for small values of θ .

The other solution of Eq. (3a) $(1+\cos\theta)$ results in a large radius of curvature which corrects the $\Delta\theta$ error arising from the diverging rays intercepting a flat crystal. In this case, the rays continue with the same divergence as before scattering from the crystal. This error is calculated from the relation $\sin\theta'' = \sin\theta\cos(\psi/2)$. The error is small, less than 0.5 sec of arc for $\psi = 10$ mrad and 2 sec of arc or less for $\psi = 20$ mrad for a Ge(111) crystal located 10 m from the source and when diffracting photon energies of 10 keV or more. It is important to know that this $\Delta\theta$ error is small since it follows that a flat crystal located either before or after the crystal curved for the solution $(1+\cos\theta)$ of Eq. (3) will intercept the horizontally diverging or converging radiation with a similarly small $\Delta\theta$ error.

In the following, we calculate the $\Delta\theta$ error for the solution $(1+\cos\theta)$ for various magnifications from 1 to 0.1 including $M = 1/3$.

3. $\Delta\theta$ Errors for a Cylindrically Bent Crystal.

A Ge(111) crystal is chosen for calculating the $\Delta\theta$ error introduced when curving the crystal for sagittal focusing, though crystals with similar d spacings give similar results. To keep the beam focus fixed at a constant distance from the curved crystal, the curvature N of the crystal is varied to maintain $F_1 \dots F_2$ fixed, as the photon energy varies from 5 to 40 keV. The $\Delta\theta$ errors ($\theta' - \theta$) plotted in Fig. 4 are calculated from Eq. (2a) for various magnifications and photon energies. For magnification near $1/3$, a cylindrically curved crystal intercepts divergences in the sagittal plane up to ~ 20 mrad with negligibly small $\Delta\theta$ errors for these rays in the midplane of the vertical distribution from the storage ring. If the experiment will tolerate the energy spread associated with the vertical opening angle of the synchrotron radiation [~ 0.2 mrad or 41.3 sec (FWHM) for photon energies of 10 keV or above, for the NSLS storage ring operating at 2.5 GeV^5], the error in $\Delta\theta$ for the horizontal opening need not be more restrictive. This matching of the vertical and horizontal $\Delta\theta$ errors permits the x-ray optical system to operate with $\Delta\theta$ errors in the horizontal plane between two vertical lines at ± 20 sec of arc in Fig. 4 without increasing the energy spread in the monochromated beam over that determined by the vertical opening angle. The dashed line, shown in Fig. 4, is the Darwin width of a symmetrically cut Ge(111) crystal. For a magnification of $1/3$, the $\Delta\theta$ errors are less than the Darwin width down to and below 5 keV. Magnifications which are larger than $1/3$ can be chosen for photon energies below 20 keV to eliminate the

$\Delta\theta$ error if that is more important than having a fixed focus position at $M = 1/3$. For example, at 10 keV the change in magnification required to eliminate the $\Delta\theta$ error would increase F_2 by 0.036 m in 3.34 m. Slits placed upstream from the monochromator crystals can be used to limit the vertical and horizontal divergences and control the energy spread in the diffracted beam. The curves in Fig. 4 are terminated by the 20 cm limit placed on the size of the crystal or by the restriction that $\psi < R_g/F_1$, whichever is smaller.

4. Size of Focus

A double crystal arrangement for synchrotron radiation which uses a cylindrically curved crystal is shown schematically in Fig. 5. This arrangement keeps the beam fixed in space. With crystals, both focusing and monochromation of the beam are accomplished. Focusing is not perfect and the general shape of the focal image of a point source photon beam is shown by the insert labeled "A-A" in Fig. 5. This is a section taken at A-A perpendicular to the beam direction. Similar images are obtained for cylindrically bent mirrors⁶. The horizontal width of the beam at the curved crystal labeled A is converted into a shape with the dimensions B and C. These dimensions are given in Table II for various photon energies and divergences. A comparison of the horizontal dimension A with B and C shows the extent to which the beam has been contracted in the horizontal and spread in the vertical plane. The external curvature of the crystal causes the vertical smearing, B, of the beam. If the crystal is shaped such that the crystallographic planes are curved and the external surface is flat, the focus would be nearly ideal except for the vertical divergence in the incident beam. However, this optical element would also need to be curved to compensate for changes in energy. For a vertical

angle of 0.2 mrad, a beam height of 2.7 mm would result at the distance $F_1 + F_2 = 13.34$ m. When the dimension B, Table II, is larger than 2.7 mm, there is no advantage in providing for a vertical focusing element before the cylindrically curved crystal unless the dimension of B is reduced as just described. If desirable, a mirror curved only in the meridian plane could be placed downstream of the curved monochromator crystal to reduce the vertical beam height, B, of the image. The reduction of the beam dimension A to the dimensions B and C, given in Table II, results in an acceptable beam size for many samples. By varying the position of the image plane, the shape of the focus can be configured for specific needs. Means to cylindrically bend the crystal to the radii N, given in Table II, may be similar to those used for mirrors⁷.

5. Conclusions

That the radius of cylindrically curved crystals can be chosen to eliminate the $\Delta\theta$ error introduced by the external shape of the crystal provides for both monochromatization and focusing from a single optical element. How well cylindrically bent crystals perform in terms of energy selection depends on the distortions introduced in bending. Results for bending radii above 300 mm indicates that the distortions in the meridian plane do not increase the Darwin width by more than a factor of two for the Ge(111) reflection⁸. Curved crystals intercept larger divergences for sagittal focusing than mirrors and may prove particularly useful for photon energies from 10 keV and above.

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Appendix A

We derive equations (2a) and (2b) from the construction of Figure 3.

The vector from S parallel to A, through the cylindrically bent crystal to the z axis has components $(F_1 \cos \theta, F_1 \sin \theta, F_1 \tan \psi/2)$. The vector $\vec{A}$ is that vector appropriately scaled so that it terminates on the monochromator and has components $(K \cos \theta, K \sin \theta, K \tan \psi/2)$. The parameter K is to be determined to satisfy that condition. It must be such that $y = -(F_1 - K) \sin \theta$ and $z = K \tan \psi/2$ satisfy the equation of the monochromator surface, $y^2 + 2yN + z^2 = 0$. With $\delta = F_1 \sin \theta - N$,

$$\delta = F_1 \sin \theta - N, \quad (A1)$$

there results

$$K = \{ \delta \sin \theta + [N^2(\sin^2 \theta + \tan^2 \psi/2) - \delta^2 \tan^2 \psi/2]^{1/2} \} / (\sin^2 \theta + \tan^2 \psi/2). \quad (A2)$$

The root for K causing K to equal F_1 when $\psi/2 = 0$ must be chosen.

If we take the monochromator radius N to be the vector shown in Figure 3, its components are $(0, N - [F_1 - K] \sin \theta, K \tan \psi/2)$, or $(0, K \sin \theta - \delta, K \tan \psi/2)$. The vectors $\vec{A}$ and $\vec{N}$ and the diffracted beam must lie in a plane such that $\vec{N}$ bisects the angle $\pi - 2\theta'$ between the diffracted beam and $\vec{A}$. Hence

$$\vec{A} \cdot \vec{N} = AN \sin \theta' = K \sin \theta (K \sin \theta - \delta) + K^2 \tan^2 \psi/2 = K^2 (\sin^2 \theta + \tan^2 \psi/2) - K \delta \sin \theta.$$

Since the length A must be $A = K(1 + \tan^2 \psi/2)^{1/2}$, we have

$$\sin \theta' = \{ K(\sin^2 \theta + \tan^2 \psi/2) - \delta \sin \theta \} / \{ N(1 + \tan^2 \psi/2)^{1/2} \},$$

or with K eliminated by equation (A2),

$$\sin \theta' = [N^2(\sin^2 \theta + \tan^2 \psi/2) - \delta^2 \tan^2 \psi/2]^{1/2} / [N(1 + \tan^2 \psi/2)^{1/2}]$$

or

$$\sin \theta' = \sin \theta [1 + \tan^2 \psi/2 (1/\sin^2 \theta - \delta^2/N^2 \sin^2 \theta)]^{1/2} / (1 + \tan^2 \psi/2)^{1/2} \quad (A3)$$

If we define $\alpha = 1/\sin^2 \theta - \delta^2/N^2 \sin^2 \theta$ or with (A1), $\alpha = (2F_1/N \sin \theta) - (F_1/N)^2$,

which is equation (2b), equation (A3) reduces to equation (2a). If we choose

$\alpha = 1$, which results in relation (3a), then $\theta' = \theta$ and the radiation fan of arbitrary divergence angle ψ satisfies the Bragg condition exactly at all points of its intersection with the cylindrical monochromator.

Table I. Width (L_s), length(L_m) and Divergences Intercepted by a Doubly Curved Platinum-Coated Mirror Located 10 m From the Synchrotron Radiation Source.

M	E keV	θ mrad	R_s mm	ψ mrad	R_m m	ϕ mrad	$L_s \leq R_s$ mm	L_m $L_1^a + L_2^b$ m
1/10	40	2.1	3.8	0.38	866	0.2	3.8	0.95 +0.23
1	40	2.1	21	2.1	4762	0.2	21	0.95 +1.25
1/10	10	8.4	15.3	1.53	216	0.2	15.3	0.24 +0.23
1	10	8.4	84	8.4	1190	0.2	84	0.24 +1.25
1/10	5	16.8	31	3.1	108	0.2	31	0.12 +0.23
1/10	1	84	153	15.3	22	0.2	153	0.024+0.23

^aLength of mirror to intercept a vertical divergence (ϕ) of 0.2 mrad for the reflecting angle θ .

^bAdditional length of mirror needed to intercept ψ with the curvature R_s .

Table II. Calculated dimensions of the focus from a point source obtained with a cylindrical curved Ge(111) crystal for $F_1 = 10$ m and $\theta' = \theta$.

Energy keV	ψ mrad	A* mm	B* mm	C* mm	N mm
40	10	100	3.2	2.9	237
30	10	100	2.5	1.6	317
20	5	50	0.44	0.092	476
20	10	100	1.72	0.73	
20	20	200	6.64	5.71	
10	5	50	0.86	0.022	957
10	10	100	1.93	0.18	
10	20	200	3.40	1.41	
5	5	50	0.10	0.005	1,972
5	10	100	0.41	0.039	
5	20	200	1.64	0.31	

* See Fig. 5 for a definition of these dimensions.

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- Figure 1 Comparison of the horizontal divergence intercepted with sagittal focusing by a Ge(111) crystal and platinum-coated mirror located 10 m from the radiation source as a function of photon energy and magnification, M . The crystal dimension is limited to 20 cm with no size restriction placed on the mirror.
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