Optimization of X-ray energy resolution from a horizontally focused single-crystal monochromator

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Abstract

A method has been developed to optimize the energy resolution of a horizontally focusing monochromator. The method consists of determining the optimum radius of curvature of the cylindrically bent monochromator crystal by minimizing the total diffracted X-ray flux measured through an X-ray absorption foil. When measured at an absorption edge a global minimum can be identified, which corresponds to the minimum energy band accepted along the entire length of the crystal. Experimental verification of this method has been validated by comparing X-ray fluorescent scans taken for a series of crystal curvatures and by directly measuring the X-ray beam profiles at the corresponding points. The actual optical configuration and asymmetric-cut parameter of the focusing monochromator on beamline X4C at the National Synchrotron Light Source are modeled and ray tracing simulations of the optical system are compared with direct beam profile measurements.

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1. Introduction

Since the discovery of synchrotron radiation, analytic techniques have been continually developed to exploit the intrinsic source parameters of electron storage rings. As many state-of-the-art methods pursue the advantages of high flux and polarization it should be noted that many methods would otherwise be impossible without good energy resolution. One such technique applied to macromolecular structure determination is multi-wavelength anomalous diffraction (MAD) [1] which takes advantage of differences in anomalous signals at carefully selected wavelengths to determine the phases of X-rays diffracted by protein crystals. Although energy resolution is not intrinsic to synchrotron radiation it is the contracted phase space resulting from relativistic effects that is the predominate reason why high energy resolution is achievable at synchrotron light sources. It is less complicated and therefore more common that the smallest phase plane be utilized in conjunction with a monochromator to achieve good energy resolution. Optimum energy resolution can be achieved by either matching or limiting the angular acceptance of the monochromator to the Darwin width of the monochromator crystal. One common monochromator geometry at synchrotron beamlines utilises a flat unbent crystal oriented to scatter in the vertical plane. The vertical plane is usually chosen because of its much smaller phase plane but still requires reduction of angular acceptance by utilizing limiting slits or a collimating mirror.

Given a bend magnet or wiggler source the horizontal phase planes are generally many times greater than their corresponding vertical phase planes. However, the monochromator geometry discussed and analyzed in this article utilizes a single crystal cylindrically bent [2,3] to accept and focus 2 mr of X-rays from the horizontal plane following a bend magnet at the National Synchrotron Light Source (NSLS). The main advantage of this geometry is the large horizontal acceptance that can be matched to the Bragg condition eliminating the need for a comparably large grazing incident mirror. The 2 mr of angular acceptance from the NSLS X4 bend magnet corresponds to a horizontal phase plane that is 35 times larger than the vertical phase plane. To achieve good energy resolution with this large angular acceptance the radius of curvature of the crystal must be set and maintained to satisfy the condition of diffraction along the entire length of the crystal. The X4C beamline at NSLS is dedicated to macromolecular crystallography and requires a practical method to maintain energy resolution that is satisfactory for MAD experiments. The optimization method discussed in this article demonstrates a simple method to set the radius of curvature of the crystal and achieve optimal energy resolution.

2. Description of optical geometry

The optical configuration associated with the X4C beamline is illustrated with the schematic shown in Fig. 1. For clarity only the
optical elements relevant to the geometry are shown where the conjugate points are labeled source and image, respectively. The optical layout utilizes two cylindrically bent optics in the Kirkpatrick–Baez [4] configuration were the tangential focusing planes are, respectively, separated by 90° about the optical axis. The convolution of these two cylindrical optics results in the formation of a two-dimensional image of the source. The first optic labeled OE1 in Fig. 1 is the vertical focusing mirror and the second optic label OE2 is a horizontally focusing crystal monochromator.

2.1. Source

The X4 beamlines utilize the synchrotron radiation emitted from the 2.8 GeV electrons in a bending magnet at the NSLS. These 2.7 m arcs formed by the 1.36 T dipole magnets emit at 12658 eV from the 2.8 GeV electrons in a bending magnet at the NSLS. These

2.2. Analytical theory for a tangentially reflecting surface of revolution

Because chromatic effects can confuse the interpretation of image size expected [5–8] from an asymmetric-cut monochromator design, we first explicitly discuss the basic geometric issues independently of the physics associated with diffraction. The focusing formula can be derived by first choosing three points on a circle to define the two chords \( f_s \) and \( f_i \). The lengths of these chords are defined from each optic pole to the two conjugate points associated, respectively, with the source-to-optic chord \( f_s \) and the optic-to-image chord \( f_i \). By expressing these chord lengths in terms of the circle radius \( R \) and the angles these chords make with the optic surface the following formula can be derived for a point source:

\[
\frac{1}{R} = \frac{\sin \theta_i}{f_i} + \frac{\sin \theta_s}{f_s}
\]

where \( \theta_i \) is the angle of incidence and \( \theta_s \) represents either the reflection or diffraction angle. Before proceeding to the oblique cases for grazing reflection and diffraction we examine the simple case for \( \theta_i = \theta_s = 90° \) in which the two conjugate points are on the principal optical axis. For this case (Eq. (1)) reduces to the familiar mirror formula

\[
\frac{1}{R} = \frac{1}{f_i} + \frac{1}{f_s}
\]

The conjugate points \( f_s, f_i \) and focal length \( R \) are distances along the optical axis to the pole of a spherical surface. By expressing this spherical section as a binomial series expansion [9,10] it can be shown that the first term in the series is identical to a conic section when \( R = \rho/2 \) where \( \rho \) is the radius of curvature of a spherical optic. Also worth noting is that the higher order terms in the series represent the deviation of a circular surface from an elliptical surface. Therefore the paraxial region is defined by the first term resulting in spherical surface that is nearly indistinguishable from an elliptical surface when \( R = \rho/2 \). This condition also applies to the oblique case where \( R \) defines the radius of the principal circle containing the two conjugate points. Ideal focusing will then exist for the paraxial region of a cylindrically bent optic with a spherical radius equal to two times the radius \( R \) of the principal circle. The radius of curvature for the optic is therefore constrained by the conjugate points that define chords on the focusing circle and by the angle these chords make with the optical surface.

2.3. Vertical tangential focusing mirror

The focusing formula for a tangentially focusing mirror can be derived by combining the law of reflections and the condition \( \rho_m = 2R \) to (Eq. (1)). Given specified grazing reflection angle

![Fig. 1. Top view of the optical configuration.](image-url)
\[ \theta = \theta_i = \theta r \text{ and } R = \rho/2, \text{ the tangential focusing formula is} \]
\[ \frac{1}{f_s} + \frac{1}{f_i} = \frac{2}{\rho_m \sin \theta} \]  
(3)

where \( \rho_m \) is the cylindrical radius of curvature. Given the actual X4C vertical mirror parameters
\[ f_s = 9.84 \text{ m} \]
\[ f_i = 4.01 \text{ m} \]

choosing \( \theta_i \leq \) critical reflection angle (\( \approx 0.278^\circ \)) reflectivity (\( \approx 84\% \)) for rhodium at 12.658 keV, the computed radius of curvature is \( \rho_m \approx 1173 \text{ m} \).

The source demagnification produced by a perfect mirror is defined as \( 1/m = f_s/f_i \), where \( m \approx 2.5 \) is associated with the actual vertical mirror parameters at beamline X4C.

### 2.4. Horizontal tangential focusing monochromator

When the above focusing condition is combined with a diffracting surface the principal focusing circle is historically referred to as a Rowland circle. Rowland [11] combined the condition for ideal focusing with the condition of diffraction from a grating of constant ruling to develop perfect spectrographic instruments. Johann [12] later extended these conditions to include a crystal as the diffracting element. The conditions are identical and therefore the historical reference to the “Rowland condition” and “Johann condition” are interchangeable. For a symmetric-cut crystal in which the diffraction angle \( \theta_d = \theta \), the focusing formula is identical to that of the mirror (Eq. (3)). The Rowland condition is defined as the radius of curvature that satisfies the condition of diffraction for the two conjugate points on the Rowland circle. The condition for asymmetric diffraction is restricted by Bragg's law expressed in terms of the asymmetric angle \( \alpha \)
\[ \sin \theta_i + \sin \theta_d = \frac{\lambda}{d} \cos \alpha \]  
(4)

where the incidence \( \theta_i \) and diffraction angles \( \theta_d \) are defined as
\[ \theta_i = \theta + \alpha \]  
(5)
\[ \theta_d = \theta - \alpha. \]  
(6)

The Rowland condition is conserved for asymmetric diffraction only when the Bragg condition is satisfied: therefore
\[ \frac{\sin \theta_i}{f_s} = \frac{\sin \theta_d}{f_i}. \]  
(7)

Using this formula to find the conjugate points associated with given diffraction angles, the following focusing formula is used to compute the radius of curvature:
\[ \frac{\sin \theta_i}{f_s} + \frac{\sin \theta_d}{f_i} = \frac{2}{\rho_c} \]  
(8)

where \( \rho_c = 2R \) is the radius of curvature of the diffracting crystal and \( R \) is the radius of Rowland circle. It follows directly that
\[ \rho_c = \frac{f_s}{\sin \theta_i} = \frac{f_i}{\sin \theta_d}. \]  
(9)

Given the actual X4C monochromator parameters
\[ 2d = 6.271 \text{Å for a silicon crystal with Miller indices (1 1 1)} \]
from Bragg’s law: \( n \lambda = 2d \sin \theta \)
then \( \theta = 8.988^\circ \) at 12.658 keV
given asymmetric angle \( \alpha = 4.8^\circ \) cut off the Si(1 1 1) scattering plane
given \( f_s = 10.6 \text{ m} \)

then conjugate point of focus on the Rowland circle is \( f_i = 3.249 \text{ m} \) and from the asymmetric focusing formula the radius of curvature \( \rho_c \approx 44.478 \text{ m} \).

#### 2.4.1. Energy dispersion analysis

The Rowland condition is highly constrained by the angular acceptance of the monochromator crystal as defined by the rocking width for a monochromatic source. Given a polychromatic source, a monochromatic beam is produced at the radius of curvature that satisfies the Rowland condition and will produce an energy band pass limited by the source size and crystal rocking width. It is worth mentioning that the symmetric-cut crystal will produce a focus without energy dispersion when observed at the conjugate point of the image on the Rowland circle. Contrary to the symmetrical case, the asymmetric-cut crystal will produce a focus with energy dispersion when observed at the conjugate point of the image. The energy dispersion associated with the asymmetric case results in a chromatic aberration in which different wavelengths within the crystal acceptance are smeared in the plane of diffraction. This spatial separation of wavelengths can be exploited to increase the energy resolution of the monochromator with the proper placement of slits. The energy dispersion for a crystal monochromator can be derived from the partial derivative of Bragg’s law with respect to the diffraction angle \( \theta \) which is
\[ \frac{\partial (n \lambda)}{\partial \theta} = \frac{d (2d \sin \theta)}{2d \cos \theta} \]  
(10)

dividing this derivative by Bragg’s law
\[ \frac{\partial (n \lambda)}{\partial E} = \frac{2d \cos \theta}{2d \sin \theta} = \cot \theta. \]  
(11)

Therefore the energy dispersion for a crystal monochromator is
\[ \frac{\partial E}{\partial \theta} = E \cot \theta \frac{\partial \theta}{\partial \theta}. \]  
(12)

Following directly from Bragg’s law this explicit definition of energy dispersion governs energy resolution. The convolution of any term of angular spread will result in an equivalent energy spread. As discussed in the above sections, we assume that the Rowland condition is consistent with the paraxial approximation where spherical aberrations are negligible. Therefore, given a point source, the Rowland condition matches the incident source divergence to the crystal acceptance and results in an energy resolution limited only by the Darwin width of the monochromator crystal. Finite source size spoils this limit and the actual energy resolution will be limited by the angular spread associated with the source extension and rocking curve associated with the monochromator crystal. One advantage of the asymmetric-cut crystal is that the width of angular acceptance directly follows the asymmetric angle \( \alpha \) as shown in Fig. 2. The three rocking curves in Fig. 2 are plotted at \( E_{hv} = 12658 \text{ eV} \) and the actual asymmetric angle \( \alpha = 4.8^\circ \) for beamline X4C. The incident rocking width \( \omega_d \) is reduced while the diffracted rocking width \( \omega_d \) is increased with respect to the rocking width of the symmetric case. The total angular acceptance and emergence can be determined by integrating the rocking curves along the length of the diffracting surface. This asymmetric condition is very unique in optics and therefore requires special attention in defining source demagnification.

#### 2.4.2. Phase space analysis

The focusing properties of an asymmetric-cut crystal have been described within the constraints of the Rowland condition but mention of the expected demagnification has been postponed.
until now. The expected demagnification will be derived using the Liouville theorem which asserts an invariance in the evolution of a density distribution function defined in this case as flux per phase-space volume unit. This approach is especially useful in avoiding confusion when considering the asymmetric rocking curves shown in Fig. 2. For clarity Fig. 3 explicitly calls attention to the angular widths that are used to define the horizontal phase planes incident and diffracted. Referring to the illustration in Fig. 3 the incident angular width is $\sigma_{i}$ and diffracted angular width is $\sigma_{d}$. Consistent with the Liouville theorem the incident density function $D_{i}$ must equal the diffracted density function $D_{d}$:

$$D_{i} = D_{d} = \frac{n_{i}}{A_{i}} = \frac{n_{d}}{A_{d}}$$  (13)

$$2\sigma_{i} = \frac{L \sin \theta_{i}}{f_{i}}$$  (16)

$$2\sigma_{d} = \frac{L \sin \theta_{d}}{f_{d}}$$  (17)

Therefore optical magnification is identically defined as

$$m = \frac{L \sin \theta_{d}}{f_{d}} \frac{f_{i}}{L \sin \theta_{i}}$$  (18)

We are only concerned with the case in which Bragg’s law is satisfied along the entire length of the crystal; therefore, $L = L_{i} = L_{d}$. This case is limited to the radius of curvature that conserves the Rowland condition, where

$$\frac{\sigma_{i}}{\sigma_{d}} = 1 = m$$  (20)

where $n_{i}$ = incident flux and $n_{d}$ = diffracted flux, and where the incident and diffracted phase plane areas are, respectively, $A_{i}$ and $A_{d}$. For this analysis we can normalize the flux $n_{i} = n_{d}$ and given Gaussian distributions the horizontal phase planes are phase ellipse with the area

$$A_{\text{ellipse}} = \pi \sigma_{i} \sigma_{d}$$  (14)

Optical magnification $m$ is defined as the ratio of source dimension $2\sigma_{i}$ to image dimension $2\sigma_{d}$,

$$m = \frac{2\sigma_{i}}{2\sigma_{d}} = \frac{2\pi \sigma_{i} \sigma_{d}}{2\pi \sigma_{i} \sigma_{d}} = \frac{\sigma_{i} \sigma_{d}}{\sigma_{i} \sigma_{d}}$$  (15)

Given a crystal length $= L$ the incident angular width and diffracted angular width are, respectively,

$$\frac{2\sigma_{i}}{f_{s}} = \frac{L \sin \theta_{i}}{f_{i}}$$

$$\frac{2\sigma_{d}}{f_{d}} = \frac{L \sin \theta_{d}}{f_{d}}$$

Therefore optical magnification is identically defined as

$$m = \frac{L \sin \theta_{d}}{f_{d}} \frac{f_{i}}{L \sin \theta_{i}}$$

$$\frac{\sigma_{i}}{\sigma_{d}} = 1 = m$$  (20)
It is worth noting that for the symmetric case $\theta_1 = \theta_2$ we get the magnification consistent with the ratio of conjugate distances. Given this result does not exclude the possibility of the image increasing or decreasing relative to the original horizontal source extension. It is obvious to expect that the image will in fact increase due to aberrations. Neglecting spherical aberrations, the dominant reason for an increase in horizontal extension is due to the smearing of the image as a result of chromatic aberration. Less obvious is the reason for the image to decrease, which can easily be confused with a demagnification. By examination of the incident reflectivity curve in Fig. 2 for the asymmetric-cut crystal we find an incident Darwin width $\omega_{\text{inc}} = 11.65 \mu\text{rad}$. This angular acceptance highly limits the field of view of the optic and at $f_s = 10.6\,\text{m}$ the horizontal extension of the source viewable is

$$2\sigma_{12658\,\text{eV}} = 2f_s \tan \omega_{\text{inc}} = 247 \mu\text{m}. \quad (21)$$

Compared to the actual source extension $2\sigma_{\text{horz}} = 584 \mu\text{m}$ then only the central half of the source can be imaged. This effect should not be confused with demagnification. It is worth mentioning the complications associated with an extended source by pointing out the existence of a viewable distribution of shorter and longer wavelengths outside the given estimate of 247 $\mu$m at 12658 eV. Therefore a more complete imaging analysis should include the chromatically distributed acceptance of the crystal from an extended source and these details are studied better by ray tracing with a computer [5–8,13].

### 3. Computer simulation

The popular synchrotron optics code SHADOW [14] has been used extensively to simulate the performance of beamline X4C along with the general monochromator design issues associated with utilizing asymmetric-cut crystals. Since SHADOW precisely implements the ray tracing method and a dynamical theory of diffraction, it has been possible to study optical details that would otherwise be impossible to study. A detailed optical model of the beamline was constructed using SHADOW and it includes the actual asymmetric crystal parameters.

#### 3.1. Validation measurements

The computer model is validated by comparing scatter plots generated from SHADOW output with actual beam profile measurements made with a custom X-ray video camera (XVC). All beam profiles are shown with axes (actual camera pixels) and were measured with the XVC placed at the conjugate point corresponding to the image plane defined for 12658 eV X-rays. The beam profile shown in Fig. 4a was measured for the best observed focus. In comparison the corresponding beam profile computed with SHADOW for the optimum crystal radius is shown Fig. 4b. Since SHADOW keeps track of all rays including those highly attenuated by optic elements, the SHADOW output must be post-processed before scatter plots are generated and compared with measurements. In reference to the scatter plots presented here, only the rays with corresponding electric field vector amplitudes $\geq 32\%$ are plotted. Amplitudes $\geq 32\%$ were chosen to agree with the histogram analysis presented in Section 3.3.

#### 3.2. Correlation of bend units and curvature radius

Beam profiles measured for conditions of over and under focus at $\pm 10\%$ change in ideal radius of curvature are shown in Figs. 5 and 6 in comparison with the corresponding scatter plots computed with SHADOW. Scatter plots were computed over a range of crystal curvature radii and matched to actual beam profile measurements at the extrema of the bend scan shown in Fig. 10 of the following section. The ray trace analysis modeled a cylindrically bent monochromator crystal and the resulting correlation was used as a calibration of arbitrary bend units to actual crystal curvature radii. The bend units correspond to rotation in degrees of a cam that is used to apply a deflecting force to the monochromator crystal, which is a cantilever mounted elongated triangle. This mechanical deflection results in the cylindrical bending of the crystal and the cam rotation is therefore used to control the radius of curvature.

#### 3.3. Comparison of measured and computed profiles

By visual comparison of the measured and computed beam profiles in Figs. 4–6, there is a good agreement between observed and expected characteristics. A more precise analysis was done using the histogram utility to process all traced rays and generate the line profiles shown in Fig. 7a and b. Also shown in Fig. 7a and b are line profiles extracted from the actual beam measurements and comparison demonstrates agreement between measured and computed results. A modulation transfer function was defined for

![Fig. 4. Best focus with bend unit = 216.85 = R_i = 44.478 m. (a) Measured beam profile (6.35 μm/horizontal pixel). (b) Computed scatter plot.](image-url)
the XVC and identified a 100 μm resolution limit which is believed to be the predominant reason for the discrepancy seen in Fig. 7b.

### 3.4. Computed energy band pass

The analysis of the beam cross-section with the conditions of optimal focus shows good agreement between measurements and simulations, which validates the optical model and its use to study the energy dispersion and resolution of the cylindrically bent, asymmetric-cut crystal. The computed energy band pass of the diffracted beam is shown in Fig. 8 for the condition of optimal radius of curvature. The two curves shown in Fig. 8 are energy band passes computed for the full beam cross-section and the case where a horizontal limiting slit is positioned between the monochromator and the focal point. The similarity seen in these two curves is expected when the Rowland condition is satisfied. The effects associated with the limiting slits will be discussed in detail in Section 6.1 of this article.

### 4. X-ray absorption measurements

The following optimization technique consists of determining the optimum radius of curvature of the cylindrically bent monochromator crystal by minimizing the total diffracted X-ray flux measured through an X-ray absorption foil. Key features of this technique are that the position of the absorption foil is not critical and that it globally optimizes the average energy band pass of the entire beam. A 0.01683 g/cm² selenium foil (37.4 μm equivalent thickness) was positioned upstream of the ionization chamber as shown in Fig. 1. The following measurements presented were actually done with this foil positioned near the monochromator chamber exit port several meters upstream of the point of focus. Since end station instruments are positioned near the point of focus this eliminates potential interference with the experiments.

#### 4.1. Crystal rotation Ω versus absorption scan

Before the optimal crystal radius of curvature can be determined the scattering vector of the monochromator crystals
must match the Bragg condition for the energy of interest. In general, matching of the crystal scattering vector is iterative with matching of the radius of curvature, but can also be set with the crystal unbent (flat) provided that the horizontal acceptance is highly limited to the central portion of the crystal. If the radius of curvature is within \( \pm 10\% \) the ideal bend, then crystal rotation \( \Omega \) can be determined with a simple absorption scan as shown in Fig. 9. The scan shown is X-ray transmission as measured while the monochromator crystal (scattering vector) is rotated. The rotation angle \( \Omega \) is plotted as X-ray energy, and then the angle corresponding to 10\% transmission is selected. Also shown in this plot is the theoretical transmission for a 0.01683 g/cm\(^2\) selenium foil. The theoretical transmission is plotted as a discontinuous step function at the K-edge and does not include the actual intrinsic broadening dominated by transitions to continuum states. With regard to the measured transmission plotted in Fig. 9 the edge features seen include broadening due to both instrumental and intrinsic effects. The intrinsic broadening is determined by the finite lifetime of the core-hole which partially decay by radiative recombination resulting in the emission of a fluorescent X-ray. As a rule of thumb [15], the intrinsic width for the K-edge is \( \approx 10^{-4} \) times the edge energy. Given the K-edge of 12658 eV then the intrinsic width would be \( \approx 1.3 \) eV for isolated atomic selenium. Therefore the broadening observed beyond \( \approx 1.3 \) eV in the actual transmission measurement plotted in Fig. 9 is due to instrumental effects which include the finite energy band pass of the monochromator crystal.

4.2. Crystal bend radius \( R_c \) versus absorption scan

Once the crystal rotation angle is set to the absorption edge the total reflected X-ray flux is again measured through the same selenium absorption foil while the curvature of the cylindrically bent monochromator crystal is varied. The radius of curvature is varied \( \pm 10\% \) about the ideal radius of 44.478 m. The bend scan in Fig. 10 is plotted from 39.891 m (left side) to 48.755 m (right side) versus the total reflected flux measured through a selenium foil at the absorption foil K-edge. The minimum seen at 10\% transmission in the plot shown in Fig. 10 corresponds to the global minimum in the energy band pass of the monochromator crystal at the selenium K-edge. Since this measurement is independent from the observation point along the Rowland circle it represents the curvature that satisfies Bragg’s condition along the entire length of the crystal. The Rowland condition is met at this radius of curvature when observed at the corresponding conjugate point on the Rowland circle. This conjugate point is easily computed with (Eq. (9)) and defines the location of optimal focus and therefore optimum energy resolution.
5. Beam profiles and fluorescent scans measurements

The series of measurements shown in Figs. 11–17 were made at the corresponding crystal curvatures plotted in Fig. 10 and the minimum transmission was verified as the point of optimal focus as indicated in Figs. 4a and 14a. Additionally, a series of selenium fluorescence scans were also made at the corresponding curvatures. The fluorescence scans were used as a metric to track energy resolution at the various crystal curvatures and are presented with corresponding profiles. All fluorescence measurements were made in the typical configuration used for actual crystallographic experiments. Referring to Fig. 1 the sample is located 618 mm upstream of the image point with 200 μm slits situated 155 mm upstream of the sample. Measurements were made with a custom scintillation detector oriented optimally along the polarization axis of the synchrotron radiation. For additional rejection of Thomson scatter noise, the detector was limited to 96 mr of angular acceptance along the polarization axis. The over plot shown in Fig. 18 is a comparison of the scans made with selenium and clearly reveals a sharpening in the fluorescent peak as the radius of curvature is increased. This observation indicates a decrease in the energy band pass incident on the fluorescent sample. The comparison in Fig. 18a shows the effect on energy resolution for the under focused and over focused cases relative to the ideal focus plotted in the middle. The same scans were normalized and are shown in Fig. 18 on an expanded scale that has been energy shifted to reveal the edge to peak features. For the comparison (right) the data were energy shifted to align the point of 50% maximum to the binding energy of selenium. It is important to point out that the observed increase in energy resolution is not intrinsic to monochromator energy acceptance and in fact for both the under and over focused cases the energy band pass diffracted by the monochromator crystal is broadened relative to the ideal energy band pass shown in Fig. 8. The actual reason for the increase in energy resolution is due to the 200 μm slits combined with the under focused mismatched case which can further reduce the energy band pass of the monochromator. This effect is due to energy dispersion associated with the asymmetric-cut crystal and will be discussed in detail in the following section.

Fig. 10. X-ray transmission versus crystal bend.

Fig. 11. Over focused with bend unit = 216.76 ≈ Rc = 39.891 m. (a) Beam profile (6.35 μm/horizontal pixel). (b) Fluorescence scan.

Fig. 12. Over focused with bend unit = 216.79. (a) Beam profile (6.35 μm/horizontal pixel). (b) Fluorescence scan.
6. Discussion of energy resolution

6.1. Energy dispersion

Given an asymmetric-cut crystal two important features need to be considered in optimizing energy resolution. The energy acceptance of the crystal, which is globally minimized when the Rowland condition is satisfied, and the energy dispersion associated with an asymmetric-cut crystal, which can be exploited to spatially filter the energy by locating slits in the dispersive region. To examine the effects of spatially filtering energy with slits, the SHADOW beamline model was used to generate scatter plots of energy dispersion in the horizontal plane at the corresponding crystal curvatures plotted in Fig. 10. The plots generated are shown in Figs. 19–21 for the ideal curvature and the two extreme radii. X-ray energy (eV) is plotted versus horizontal dispersion (m) as observed at the image and slit position. The image position is fixed at $f_i = 3.249$ m for the ideal conjugate and the slit position is 618 mm upstream of the image position. Starting with the case for ideal radius of curvature shown in Fig. 20, we observe no energy dispersion at the slit position (Fig. 20a) along with dispersion at the image position (Fig. 20b). Because no energy dispersion is seen for this case at the slit position, the slit will have no effect in reducing the energy band.
pass. This result is verified with the computed energy band pass plot shown in Fig. 8 which is an over plot with and without the 200 μm slit. Examination of the over focused case shown in Fig. 19 reveals expanded energy dispersion at the image position (Fig. 19b) and a reduced dispersion at the slit position (Fig. 19a). Because of the reduced dispersion in the slit position, more off-energy X-rays are focused through the slits resulting in an increased energy band pass. Finally we call attention to the under focused case shown in Fig. 21 where we see an expanded energy dispersion at the slit position (Fig. 21a) which allows for the spatial selection of energy. These energy dispersion plots clearly illustrate the changing distribution of energy at the various radii of curvature and offer an explanation for the observed peak sharpening observed in the series of fluorescence scans.

6.2. Computed energy band pass

The SHADOW histogram utility was additionally used to compute the energy band pass plot for the three case examined in the previous section. These plots are shown in Fig. 22 and are in overall agreement with the previously examined trends but reveal an insensitivity in the under focused case where the fluorescence peak sharpening is strongly observed. Referring to Fig. 22, we see
Fig. 19. Horizontal energy dispersion at over focus, $R_c = 39.891$ m. (a) Slit position. (b) Image position.

Fig. 20. Horizontal energy dispersion at best focus, $R_c = 44.478$ m. (a) Slit position. (b) Image position.

Fig. 21. Horizontal energy dispersion at under focus, $R_c = 48.755$ m. (a) Slit position. (b) Image position.
that the energy band pass is greatly increased for the over focused case, consistent with the fluorescent scans, but for the under focused case we see only a slight decrease in energy band pass compared with the "best" focus, which is puzzling in light of the fluorescence scans.

7. Conclusion

We have reviewed the basic issues in utilizing a horizontally focusing monochromator and have demonstrated a simple method to optimize the crystal radius of curvature that is useful in maintaining the energy resolution. Our SHADOW ray-tracing model has been validated and has proven to be invaluable in studying the details of energy dispersion associated with an asymmetric-cut crystal monochromator. We also demonstrate that the expected magnification associated with the asymmetric-cut crystal is constrained when the Rowland condition is satisfied.

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