**Focusing X-Ray Monochromator for EXAFS Studies in the
Energy Range 4-30 keV**

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The design and operating principles of a focusing x-ray monochromator are described. Consistent with EXAFS applications it allows rapid tuning while maintaining high energy resolution and a fixed focus at the sample. The basic instrument consists of two opposing two crystal monochromators with the second and third crystals operating as a dispersive monochromator. This provides the intrinsic resolution of the crystals independent of slit settings or source size effects. Focusing is achieved by a sagittally bent fourth crystal. To maintain a fixed focus two options are available. In the first, the second crystal pair is translated while the radius of the fourth crystal is held fixed. Thus, the focus remains at the sample even though the angle of incidence on the bent crystal is changing. In the second option the radius of the bent crystal is changed dynamically as the scan is carried out. These techniques are compared and a crystal bender designed for rapid tuning is described.

1. Introduction

The development of sagittally focusing crystals [1,2] has opened new possibilities in monochromator design. Crystals operate efficiently above 10 keV, energies which are difficult to handle with grazing incidence mirrors. In this paper the design of a monochromator is described which is meant specifically for EXAFS and XANES studies in the 4-30 keV energy range. Focusing and monochromatization are combined in a fixed input-fixed output design. Since a complete checkout of the monochromator awaits the operation of the

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NSLS x-ray ring the following discussion will concentrate on the principles underlying its design. A description of the beam line in which the monochromator will be used has been given previously [3].

2. Basic Design

An EXAFS monochromator has several fundamental requirements. Foremost is rapid tunability since a single absorption measurement only requires ~ 1 sec. The energy resolution should be better than or comparable to the lifetime broadening of the absorption edge which implies $\Delta E/E \sim 1-2 \times 10^{-4}$ for $E \sim 4-30$ keV. This is close to the intrinsic resolution of available Si crystals which is 5×10^{-5} and 1.3×10^{-4} for Si(220) and Si(111) reflections, respectively. In addition the beam line has up to 10 mrad available which should be concentrated to a focus of a few mm^2 .

Figure 1 shows a schematic of a monochromator designed for these requirements. It contains four crystals arranged in two double crystal stages. These stages rotate in opposite directions in a fashion first described by Beaumont and Hart [4]. This results in a fixed input-fixed output beam device. The second and third crystals are in a dispersive arrangement, the implications of which are described in the next section. The fourth crystal is sagittally bent to concentrate the horizontal radiation. To maintain a fixed focal position either the bent crystal radius must be changed or its position changed as the energy is scanned. Both options are available in this instrument and are described in detail in later sections.

The instrument is housed in a vacuum tank allowing operation at 10^{-4} - 10^{-5} torr. A photograph of the complete instrument with four flat crystals installed is given in Fig. 2. Not shown in either figure are Pb collimators which block the transmission of any line of sight radiation.

3. Dispersive and Nondispersive Monochromators

To quantitatively compare the present design with a nondispersive two crystal design, extensive raytracing calculations were carried out. These were done by modifying an existing program for treating geometrical optics [5] to include perfect crystal diffraction theory and calculating the monochromator throughputs for various Si crystals. Some results are shown in Fig. 3. Here the throughput versus energy is plotted for various cases. In 3(a) an ideal vertically collimating mirror is assumed to be positioned at 10 m from the NSLS source.

Since in the nondispersive case, the source size induced divergence is added to the intrinsic crystal diffraction width it was necessary to use Si(220) crystals to match the resolution of the Si(111) four crystal monochromator. Then the intensities and resolutions are essentially the same with the nondispersive case having slightly longer tails. In both cases the resolution is about 10^{-4} which is appropriate for most near edge and EXAFS studies in the 5-15 keV range. The dispersive monochromator does have an important advantage. If the source size is increased or the mirror is not ideal, the resolution remains the same with only the intensity being reduced. This is illustrated in 3(b) where the mirror has been removed. The dispersive monochromator curve is essentially the same (differences are caused only by the finite statistics of the raytracing calculation) with the intensity reduced by about 7. For the nondispersive case it is necessary to include slits to maintain the resolution. It is seen that for the same resolution the slit cuts the throughput to about half of the dispersive case.

Thus if resolutions comparable to the intrinsic Si diffraction width are desired a dispersive monochromator is superior or equal to a nondispersive

monochromator in terms of intensity. In addition it has a distinct advantage in having a well defined resolution independent of the source or preceding optical elements. If such resolutions are not required a nondispersive monochromator may be better since resolution can be sacrificed to gain intensity. For this reason the monochromator is designed to be operated in the two crystal mode by removing the first two crystals.

4. Sagittal Focusing

4.1 General principles

A ray striking two flat crystals in a nondispersive arrangement makes the same angle on each giving $\Delta\theta = \theta_2 - \theta_1 = 0$. If the second crystal is bent to a radius R in the sagittal direction then to lowest order,

$$\Delta\theta = \frac{\omega_h^2 F_1}{R} - \frac{\omega_h^2 F_1^2 \sin\theta_0}{2R^2} \quad (1)$$

where ω_h is the horizontal divergence of the ray measured from the central axis, F_1 is the distance to the source and θ_0 is the incident angle of the central ray. Setting $\Delta\theta = 0$ gives $R = (F_1 \sin\theta_0)/2$ which if inserted into the lens equation gives the distance to the focus as $F_2 = F_1/3$. Ignoring aberrations this would give a horizontal width of the focus of $1/3$ that of the source. A cylinder provides no vertical focusing which means the vertical extent of the focus essentially that of an unfocused beam. In reality the aberrations defocus the image by an amount

$$\Delta x = \frac{8 \omega_h^3 F_1}{3 \sin^2\theta} \quad (2)$$

$$\Delta y = \frac{4 \omega_h^2 F_1}{3 \sin\theta}$$

For a fixed F_1 the radius of the crystal must vary as the energy is changed. A crystal bender designed for this purpose is described in section 5. The alternative is to hold R fixed and vary F_1 . This is described in the next section.

4.2 Fixed R Scan

If the radius R is held fixed then the focus will remain fixed if F_1 is varied such that

$$F_1 = \frac{L}{2} + \frac{L}{2} \left(1 - \frac{3E}{4E_0} \right)^{1/2} \quad (3)$$

where L is the source to focus distance, E is the desired energy and E_0 is the energy for which R is ideal. Since the ideal radius is not used, $\Delta\theta$ is no longer negligible and there will be some loss in efficiency. Combining eqs. (1) and (3) gives to lowest order

$$\Delta\theta = \frac{3\omega_h^2}{4 \sin\theta_0} \frac{\Delta E}{E_0} \quad (4)$$

where $\Delta E = E - E_0$. For the present monochromator $L=16$ m and the translation length is 1 m. This allows energy scans of 1 keV for $E_0=6$ keV increasing to 3.3 keV at 20 keV. Figure 4 shows some actual raytracing results for various cases assuming that 10 mrad are collected. Over a typical EXAFS scan range of ~1 keV it is seen that the intensity variations are $\leq 20\%$ which should be tolerable for most cases. From eq. (4) it is seen that the intensity is lost first from the outermost rays, which implies that as ω_h is reduced the variation is quickly eliminated.

5. Crystal Bender

In an EXAFS scan the energy is typically changed at intervals of ~1 sec. Thus a bender capable of dynamic bending must respond in a fraction of a second. This includes not only changing the crystal radius, but any translations

required to keep the crystal centered in the beam. Clearly it is desirable to minimize the number of adjustments needed which leads to a bender based on a cantilevered triangular crystal [6]. The radius is changed by a single motion of pushing on the tip. If the crystal is positioned such that the optic axis is along the base of the triangle then no vertical translation of the crystal is required as its radius is changed.

A prototype bender designed applying these principles is currently being assembled and tested. It employs a triangular crystal with a base 65 mm wide and a length of 85 mm. Bending is accomplished using an "Inchworm" piezoelectric pusher [7] which can be computer controlled and has an encoder accurate to $\pm 1 \mu\text{m}$. One problem with a triangular crystal is that for optimum efficiency the crystal should be translated horizontally as the angle is changed. This is illustrated in Fig. 5 which shows the footprints of the beam for $\theta=7^\circ$ and $\theta=30^\circ$. The necessary motion of 15 mm is accomplished automatically in the present design by positioning the crystal slightly off the rotation axis, which causes the beam to "walk" an appropriate amount as the angle is changed. As seen this prototype crystal will collect ~ 6 mrad over an angular range of $7-30^\circ$ with only one axis of adjustment. This corresponds to an energy range $E=4-16$ keV for Si(111) and $E=6-26$ keV for Si(220).

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Figure Captions

Fig. 1. Schematic of the monochromator: CB, crystal bender; CT, crystal translation stage; EN, encoder; GC, goniometer carriage for 1 m translation; GM, gimbal mounts for prealigning crystal; H, Huber model 421 goniometers; MM, motorized micrometer for coarse crystal alignment; PZ, piezoelectric translator for fine crystal alignment; SM, stepping motor; WC, water cooled crystal.

Fig. 2. Photograph of the monochromator mounted in its vacuum enclosure. A flat crystal is mounted in place of the crystal bender.

Fig. 3. Raytracing comparison of the throughput of dispersive and nondispersive monochromators. The solid curves are for a Si(111) four crystal dispersive case and the dashed curves for a Si(220) two crystal nondispersive case. E_{Bragg} is 10 keV in all cases. In (a) a collimating mirror precedes the monochromator while in (b) the mirror is removed. The throughputs include losses at slits but not those due to the collimating mirror.

Fig. 4. Intensity variations with scanning for a fixed radius bent crystal collecting 10 mrad. The curves are for 5, 10, 15, and 20 keV. The solid lines are for Si(111) and the dashed line for Si(220) crystals.

Fig. 5. Footprint of the beams striking a bent triangular crystal. The solid curves outline the one for $\theta=7^\circ$ and the dashed curves are for $\theta=30^\circ$. The $\theta=7$ curve is positioned in the optimum position.