Design of an XAFS beamline at the Photon Factory: possibilities of bent conical mirrors

NOMURA Masaharu * and KOYAMA Atsushi *

Photon Factory, Institute of Materials Structure Science, KEK, Oho, Tsukuba 305-0801, Japan. Email:masaharu.nomura@kek.jp

A new XAFS beamline which uses a pair of bent conical mirrors for collimation and focusing is under construction. A double crystal monochromator is placed between the two mirrors. This beamline is to provide high flux without sacrificing the energy resolution. Ray-trace results indicate that a bent conical mirror is not only a good approximation of a rotating paraboloidal, but also that of rotating ellipsoidal, mirror.

Keywords: XAFS, beamline, bent conical mirror, focus

1. Introduction

A small beam size as well as a high x-ray flux are required for XAFS experiments when the size and/or the concentration of a sample is limited. A beamline using a highly collimated x-ray beam from an undulator with a double-crystal monochromator and proper focusing mirrors could be a solution. However, since the Photon Factory is a 2.5 GeV second-generation storage ring, it is not practical to install an undulator which emits hard x-rays. Therefore, it is important to focus the beam from a bending magnet or a multi-pole wiggler efficiently.

A sagittal focusing double-crystal monochromator is a powerful method (Sparks & Borie, 1980) and is used at the Photon Factory (Nomura, Koyama & Sakurai, 1991). There are several merits to adopting this system: 1) it can focus a widely diverged beam; 2) the geometrical restriction of the beamline is not very strict and 3) the construction cost is not high. However, since the focusing condition is a function of the Bragg angle, it is required to adjust the sagittal radius of the crystal when the x-ray energy is changed. It usually requires also adjusting the parallelism between the two crystals. Furthermore the energy resolution and the throughput is sensitive to the alignment of the sagittal crystal (Koyama *et al.*, 1992). Thus, it is not easy to optimise the focusing condition for many XAFS experimenters. Another solution is to focus the beam by mirrors. A toroidal or a bent cylindrical mirror is often used (Howell & Horowitz, 1975; Nomura & Koyama, 1996) for such purposes, which realises a fixed focus independent of the x-ray energy. Thus, it is suited for XAFS experiments of small samples. However, the horizontal acceptance of a mirror is limited by its length, the incidence angle and the source-to-mirror distance (Heald, 1982). Although the optics provides good focus when its magnification is one, the aberration becomes significant when the magnification deviates from one. In such cases, a rotating ellipsoidal mirror can be used instead. Hereafter, the rotation axis of the monochromator is assumed to be horizontal.

In both cases, the vertical collimation of diverging synchrotron radiation (ca. 0.1 mrad) is important in order to increase the flux at the sample without loosing the energy resolution, since it is larger than the rocking curve width. We have arrived at a similar design as for UK-CRG beamline at ESRF (Paul *et al.*, 1995) and are constructing a beamline which uses a pair of bent conical mirrors for collimation and focusing purposes. The design and the expected performance of the beamline is discussed according to ray tracings. Also, another possibility of a bent conical mirror is discussed.

2. Design of the beamline BL-9A

It is well known that a rotating paraboloidal mirror collimates the beam from a point source. Since the beam divergence is very small, a double-crystal monochromator placed after the mirror can monochromatize the whole beam without loosing the energy resolution. Another rotating paraboloidal mirror focuses the monochromatized beam to a point. However, it is difficult to manufacture such rotating paraboloidal mirrors. Thus, bent conical mirrors are used in place of rotating paraboloidal ones.

Beamline BL-9A uses radiation from a bending magnet BM09, whose critical energy is 4 keV. Two other branch beamlines have been constructed, which also use the radiation from BM09. Thus, there were certain geometrical restrictions for the design of BL-9A. A schematic drawing of BL-9A is shown in Fig. 1 and the specifications of the source and optical elements are listed in Table 1. A bent conical mirror indirectly watercooled through an In-Ga alloy collimates the diverged beam both vertically and horizontally. The horizontal acceptance of the mirror is 3 mrad and the total heat load on the mirror is less than 100W. The x-rays of required energy are chosen by a Si(111) double crystal monochromator; the motion of the two crystals are guided by two cams (Matsushita *et al.*, 1986). The fist crystal is also indirectly water-cooled through an In-Ga alloy. Then,



Figure 1

Schematic drawing of BL-9A. The beam is collimated by a bent conical mirror, monochromatized by a double-crystal monochromator, then focussed by another bent conical mirror. Higher orders are rejected by a pair of parallel aligned flat mirrors.

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Table 1

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Source property and the list of optical components		
Optical component	Position	Specifications
Source	0 m	bending magnet #09
		$\sigma_x = 0.33 \text{ mm}, \sigma_y = 0.07 \text{ mm},$
Callimatian	14.21	$\sigma_x = 0.21 \text{ mrad}, \sigma_y = 0.02 \text{ mrad}$
Commating	14.21 m	Dent conical mirror
mirror		r(in)=117.2mm, $r(out)=121.4$ mm,
		<i>r</i> (mer)=6767 m
		Rh coated Si, $100(w) \times 70(t) \times 1000(l)$
		indirect side cooling
Monochromator	16.1 m	Si(111) double crystal mono.
Focusing mirror	17.6 m	bent conical mirror
		r(in)=66.7 mm, r(out)=62.5 mm,
		r(mer)=3667 m, Rh coated ULE,
		$100(w) \times 70(t) \times 1000(l)$
Higher order	23.5 m	flat double mirror,
rejection mirror		stripe of Rh/Ni coated quarts,
		$100(w) \times 30(t) \times 300(1)$

another bent conical mirror focuses the beam. The mirrors are coated with rhodium and the angle of incidence is 4.2 mrad, which corresponds to a cut-off energy of 16 keV. A pair of parallel aligned flat mirrors are used for further higher order rejection, whose surface is coated with stripes of Rh and Ni. The material of the reflecting plane is selected by sliding the mirrors horizontally in the vacuum chamber. The number and thickness of the beryllium windows are reduced so as to minimise the lower energy limit; thus, the x-rays between 2.1 and 15 keV can be used at BL-9A. The flux is expected to be more than 2×10^{11} s⁻¹ at 9 keV with an energy resolution ($\Delta E/E$) of better than 2×10^{4} .

The reason why a bent conical mirror is a good approximation of a rotating paraboloidal one is discussed hereafter. A paraboloid around x_0 (the centre of the mirror) is expressed as

$$y = \sqrt{4px} \sim \sqrt{4px_0} (1 + \frac{\Delta x}{2x_0} - \frac{\Delta x^2}{8x_0^2}),$$
 (1)

where,

p.

$$- x_0 \theta^2. \tag{2}$$

Here, Δx indicates the displacement from the centre of the mirror and θ is the angle of incidence. If the higher order terms are neglected, a part of a paraboloid is approximated by a straight line, which indicates that the sagittal radius of a rotating paraboloid varies nearly linearly. Putting the parameters for the first mirror listed in Table 1, the difference between the paraboloid and the straight line is less than $\pm 10 \ \mu m$; which is smaller than the accuracy of the radius. This suggests that a rotating paraboloidal mirror can be approximated by a conical one. However, a conical mirror is not enough to approximate a rotating paraboloidal mirror, since it has little ability to focus the beam vertically. Thus, bending of the conical mirror is required. The sagittal (r_i ; *i* indicates both ends of the mirror) and meridional radius (r_m) can be expressed as,

$$r_{i} = 2\theta \sqrt{x_{0}x_{i}},$$

$$r_{m} = 2x_{0}/\theta,$$
(3)

where, x_i indicates the distance from the source to an end of the mirror. The source can be replaced by the focus when the mirror is used for focusing purposes.

A phase-space diagram at the monochromator position, 2 m from the centre of the first mirror, is shown in Fig. 2. Those for natural diverging beam and after a toroidal mirror whose focus is





Phase-space diagram in Z-Z' plane at the position of the monochromator. (a) after a bent conical mirror, (b) incoming synchrotron radiation without any optical element and (c) after a toroidal mirror. The parameters of the bent conical mirror are listed in Table 1. The ray trace was carried out by using a modified version of SRXRAY (Muramatsu *et al.*, 1987).

designed to be infinitely distant are compared. The vertical divergence of the beam from the bending magnet is about 0.1 mrad (21 arcsec), while that after the bent conical mirror is only 0.013 mrad (3 arcsec), which is small compared with the rockingcurve width of Si(111) crystal at 8 keV (8 arcsec). Therefore, the vertical slit, which is usually used to improve the energy resolution, is not required, and the flux at the sample position is expected to increase. Figure 3 also indicates that toroidal mirrors cannot be used for collimation.

The optics described above is compared with a conventional one using a toroidal mirror. Here, the distances between the source and the mirror (f_1) and that between the mirror and the focus (f_2) are set as 16.2 and 9.1 m in order to maintein the source-to-focus distance and the magnification. The effective horizontal acceptance of the beamline with a pair of bent conical mirrors is 3 mrad, which is larger than that with a toroidal mirror (1.7 mrad). This is due to the increase in the sagittal radius (Heald, 1982). The sagittal radius of a corresponding toroidal mirror is 4.9 cm, while that of the conical mirror is ca. 12 cm (see



Figure 3

Spot diagrams at the focus position with (a) a pair of bent conical mirrors and (b) a pair of rotating paraboloidal mirrors.

Table 1), which increases the effective horizontal acceptance.

Spot diagrams at the focus position obtained with bent conical and rotating paraboloidal mirrors are shown in Fig. 3. Bent conical mirrors give a similar focus shape and size as the rotating paraboloidal mirrors. This is a big merit of taking this optics compared with the conventional one using a toroidal mirror, since it trails under a given condition (see Fig. 4c).

3. Approximation of rotating ellipsoid by a bent conical mirror

Although the optics described above gives high energy resolution and high flux at the sample position, the beam collimation with this optics is not sufficient for XAFS experiments above 20 keV, even if the surface is polished ideally. This is due to the finite source size. Actually, the slope error of the mirror (usually 1 - 5arcsec.) will not be neglected compared with the rocking curve width at higher energies. Thus, focusing by a rotating ellipsoidal mirror placed after a monochromator is required in such cases. It is a good focusing element even when the magnification deviates from one. An ellipse is expressed as

$$x^{2} /_{a^{2}} + \frac{y^{2}}{b^{2}} = 1, \quad a = (f_{1} + f_{2})/2, \quad b = a\sqrt{1 - e^{2}}, \quad (4)$$

$$e = \sqrt{f_{1}^{2} + f_{2}^{2} - 2f_{1}f_{2}\cos 2\theta} / 2a,$$

where, f_1 and f_2 indicate the distance between the sorce and the mirror and that between the mirror and the focus, respectively. Similar to a paraboloid, a part of an ellipse can be approximated by a straight line as

$$y = \frac{b}{a}\sqrt{a^2 - x^2} \approx \frac{b}{a}\sqrt{a^2 - x_0^2}(1 + \frac{x_0\Delta x}{a^2 - x_0^2}),$$
 (5)

where the symbols have the same meanings as in eq. 1.

If a toroidal mirror is used instead of conical mirrors in this beamline, f_1 and f_2 become 16.2 and 9.1 m, respectively. The deviation of the ellipse from the straight line is within $\pm 25 \ \mu m$



Figure 4

Spot diagrams at the focus position with (a) a bent conical mirror, (b) a rotating ellipsoidal mirror and (c) a toroidal mirror.

under this condition, which can also be compensated by meridional bending. The spot diagrams at the focus position with a rotating ellipsoidal, a bent conical and a toroidal mirrors are compared in Fig. 4. The focus with the bent conical mirror is slightly larger than that with a rotating ellipsoidal mirror, but the difference is much smaller than the broadening due to slope error. These focuses are much smaller than that with a toroidal mirror. Thus, a bent conical mirror can also be used as an approximation of a rotating ellipsoidal mirror.

4. Conclusion

Bent conical mirror approximates rotating paraboloidal and rotating ellipsoidal mirrors. By using a pair of bent conical mirrors, both a small fixed focus and a high flux can be realised at the same time. However, the actual performance strongly depends on the finish of the mirror surface.

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