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APPLICATIONS:  
CALCULATION OF THE ENERGY BANDPASS**

DOUBLY BENT CRYSTALS FOR X-RAY MICROFOCUSING  
APPLICATIONS: CALCULATION OF THE ENERGY  
BANDPASS

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Abstract

Synchrotron radiation from third-generation, high-brilliance rings is an ideal source for X-ray microbeams. The aim of the present article is the discussion of bent crystals properties as focusing optical elements designed to obtain micron-size photon spots with high intensity and wide bandpass monochromatization. In particular, simple mathematical expressions are derived for the energy bandpass of a strongly demagnifying doubly bent crystal, where the contribution from the sagittal curvature is particularly important.

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GOULD BETA CHRYSTALS FOR X-RAY MICROGRAPHY  
APPLICATIONS CANNOT AFFORD THE EXPENSE  
BYPASS

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Abstract

beta-chrysolite, a natural mineral, is a promising material for x-ray micrography. It has a high refractive index and low absorption coefficient in the visible and near ultraviolet regions of the spectrum. The natural mineral is a single crystal of the orthorhombic system. The natural mineral is a single crystal of the orthorhombic system. The natural mineral is a single crystal of the orthorhombic system. The natural mineral is a single crystal of the orthorhombic system. The natural mineral is a single crystal of the orthorhombic system.

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## 1. Introduction

The advent of third-generation high-brilliance synchrotron radiation (SR) sources fitted with new insertion devices like wigglers and undulators has revived the interest in the field of hard X-rays microprobes [1]. SR induced X-ray emission (SRIXE), for example, is an ideal technique for trace-element microanalysis of biological samples. A recent survey of the SRIXE method is given in ref. [2].

The required features of the optical components in the hard X-rays energy range (3-20 keV) are high reflectivity, ultra-high vacuum stability, thermal stability and radiation endurance. An important parameter for a SRIXE microprobe is the degree of monochromatization. In most applications energy definition is not crucial, and optical elements with wide energy bandpass ( $\Delta E/E \sim 1 - 10\%$ ) are perfectly suited to enhance the signal-to-noise ratio and lower the minimum detection limit in absolute amount [3].

The ideal solution for these microprobes is the use of bent crystal monochromators [4,5]. Bent crystals provide wide bandpass monochromatization of the incoming beam and present additional advantages over conventional optical systems, such as high acceptance, good thermal stability and a reproducible surface figure.

In the following section simple formulas will be derived in order to calculate the energy bandpass of an X-ray microprobe for third-generation synchrotron radiation facilities such as ELETTRA, the high-brilliance ring under construction in Trieste (Italy).

## 2. Energy bandpass of a curved crystal

The focusing properties of bent crystals have already been examined (see for example ref. [6,7]), but the characteristics of the new high-brilliance, low-emittance SR sources require a completely new approach to the study of a micron-size microprobe.

One of the most powerful graphic methods used to determine the wavelength-position correlation in a focusing crystal is the reciprocal space diagram method (excellent reviews of this field were given by Freund [8,9]). The description of the crystal reflection width is physically adequate in reciprocal space, since the Darwin width is not a mere angular property of the crystal, but a broadened interference pattern extending parallel to the reciprocal lattice vector [10]. These diagrams are restricted to a single plane, so that the possible sagittal-to-meridional coupling cannot be shown adequately, and this method is not applicable in the important case of doubly bent crystals. Nevertheless, the focusing behaviour of a crystal (in both real and reciprocal space) can be fully understood only if the shape and orientation of the resolution function in reciprocal space are known.

The reciprocal space diagram method has already been used to describe the wavelength spread  $\Delta\lambda/\lambda$  of a cylindrical crystal [10] and we will extend the results to the calculation of the bandpass produced by a strongly demagnifying doubly bent crystal. This means that in the following calculations the entrance arm  $p$  of the focusing crystal will always be much greater than the exit arm  $q$ , *i.e.* the magnification  $M = q/p \ll 1$ . The total wavelength spread of a crystal will take into account different contributions, resulting

in

$$(\Delta\lambda/\lambda)_{tot} = \sqrt{\sum_i (\Delta\lambda/\lambda)_i^2}. \quad (1)$$

The terms  $(\Delta\lambda/\lambda)_i$  will be described in the following two subsections.

### *2.1. Contributions due to the meridional focusing*

If we ignore penetration depth effects, the X-ray beam vertical divergence  $\Omega$  (FWHM) is increased, after reflection from a crystal, to  $\Omega + 2\epsilon$ , where  $\epsilon = \theta_1 - \theta_2$  is the change of lattice plane orientation across the incident beam on the crystal surface and depends on the radius of curvature of the crystal and the beam width. The wavelength spread is related to the angle  $\Delta$  between the direction of the diffracted wavevector and the major axis of the volume where the reflected wavevectors are ending, which describes the angle-wavelength correlation of the resolution element in reciprocal space. The total wavelength spread reflected by a bent crystal is composed of two contributions. A first term

$$(\Delta\lambda/\lambda)_1 = \cot \theta_B \omega_0 \quad (2)$$

(where  $\theta_B$  is the Bragg angle) is due to the intrinsic angular width  $\omega_0$  of the Bragg reflection; a second term

$$(\Delta\lambda/\lambda)_2 = \cot \Delta (\Omega - 2\epsilon) \quad (3)$$

is due to the finite beam divergence and the variation of lattice plane orientation across the illuminated crystal. In the case of cylindrically bent

of the crystal itself. Two vectors  $\mathbf{SO}$  and  $\mathbf{R}_S\mathbf{O}$  are chosen as follows (see fig. 1):

$$\mathbf{SO} = (0, p \cos \theta_B, -p \sin \theta_B) \quad (14)$$

$$\mathbf{R}_S\mathbf{O} = (0, 0, -R_S), \quad (15)$$

where  $R_S$  is the sagittal radius of curvature.

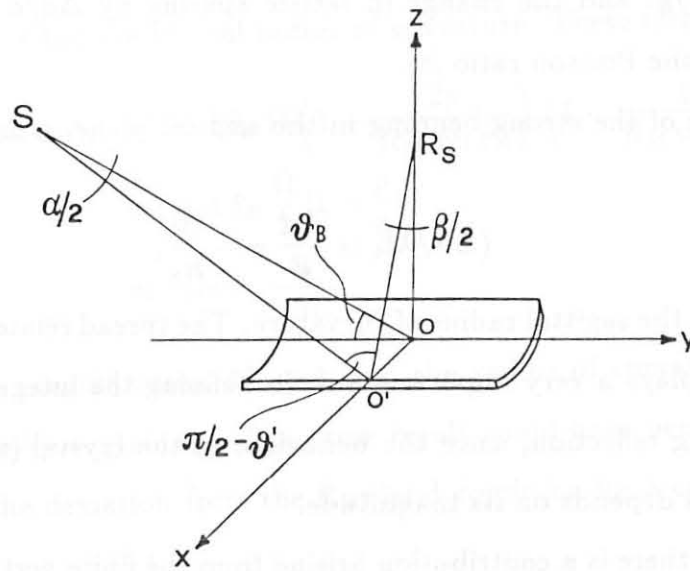


Fig. 1. Geometry of the curved crystal for the calculation of the  $\Delta\theta$  error resulting from the sagittal curvature.

The Bragg angle is defined by

$$\sin \theta_B = \frac{\mathbf{SO} \cdot \mathbf{R}_S\mathbf{O}}{|\mathbf{SO}| |\mathbf{R}_S\mathbf{O}|}, \quad (16)$$

while the new Bragg angle in the limit point  $O'$  along the sagittal direction will be defined by

$$\sin \theta' = \frac{\mathbf{SO}' \cdot \mathbf{R}_S\mathbf{O}'}{|\mathbf{SO}'| |\mathbf{R}_S\mathbf{O}'|}. \quad (17)$$

Considering

$$\mathbf{OO}' = [R_S \sin(\beta/2), 0, R_S(1 - \cos(\beta/2))] \quad (18)$$

we have that

$$\mathbf{SO}' = [R_S \sin(\beta/2), p \cos \theta_B, R_S(1 - \cos(\beta/2)) - p \sin \theta_B]. \quad (19)$$

Since

$$\mathbf{R}_S \mathbf{O}' = [R_S \sin(\beta/2), 0, -R_S \cos(\beta/2)] \quad (20)$$

it follows that

$$\mathbf{SO}' \cdot \mathbf{R}_S \mathbf{O}' = |\mathbf{SO}'| |\mathbf{R}_S \mathbf{O}'| \sin \theta' \quad (21)$$

from which

$$\begin{aligned} R_S |\mathbf{SO}'| \sin \theta' &= R_S^2 \sin^2(\beta/2) - R_S^2 \cos(\beta/2)(1 - \cos(\beta/2)) + \\ &+ p R_S \sin \theta_B \cos(\beta/2). \end{aligned} \quad (22)$$

Since the entrance arm  $p$  is much greater than the crystal dimensions, we have that  $|\mathbf{SO}'| \approx p$ , so that

$$\sin \theta' \approx \sin \theta_B \cos(\beta/2) + \frac{R_S}{p} \sin^2(\beta/2) - \frac{R_S}{p} \cos(\beta/2)(1 - \cos(\beta/2)). \quad (23)$$

The angle  $\beta$  is defined by

$$\sin(\beta/2) = \frac{p}{R_S} \tan(\alpha/2), \quad (24)$$

where  $\alpha$  is the horizontal angular divergence of the incoming beam. We will now consider

$$\cos(\beta/2) = \sqrt{1 - \frac{p^2}{R_S^2} \tan^2(\alpha/2)} = \sqrt{\delta}, \quad (25)$$



so we can write

$$\sin \theta' = \sin \theta_B \sqrt{\delta} + \frac{p}{R_S} \tan^2(\alpha/2) - \frac{R_S}{p} \sqrt{\delta}(1 - \sqrt{\delta}) \quad (26)$$

$$\sin \theta' = \sin \theta_B \sqrt{\delta} + \frac{R_S}{p}(1 - \delta) + \frac{R_S}{p} \delta \left(1 - \frac{1}{\sqrt{\delta}}\right) \quad (27)$$

$$\sin \theta' = \sin \theta_B \sqrt{\delta} + \frac{R_S}{p}(1 - \sqrt{\delta}). \quad (28)$$

By series expansion of  $\sin \theta'$  around  $\theta_B$  we obtain:

$$\Delta \theta \cos \theta_B \approx \sin \theta_B (\sqrt{\delta} - 1) + \frac{R_S}{p}(1 - \sqrt{\delta}) \quad (29)$$

$$\Delta \theta \approx (\sqrt{\delta} - 1) \left( \tan \theta_B - \frac{R_S}{p \cos \theta_B} \right). \quad (30)$$

Since  $R_S = \sin \theta_B (2pq)/(p + q)$  the second term in brackets becomes

$$\tan \theta_B - \frac{R_S}{p \cos \theta_B} = \tan \theta_B \frac{1 - q/p}{1 + q/p} \approx \tan \theta_B \quad (31)$$

in the case of strong demagnification. So equation (30) reduces to

$$\Delta \theta = \tan \theta_B (\sqrt{\delta} - 1) \quad (32)$$

which gives, since  $\Delta \lambda / \lambda = \Delta \theta / \tan \theta_B$  and  $\tan \alpha \approx \alpha$ ,

$$(\Delta \lambda / \lambda)_{Sag} = \left| \sqrt{1 - \frac{\alpha^2 p^2}{4R_S^2}} - 1 \right|. \quad (33)$$

As stated previously, there is also a contribution arising from the finite horizontal size of the source, but again in our case it can be considered negligible.

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