

Anisotropy and the optimal aspect ratio of a bent crystal

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Abstract. A thin bent rectangular crystal plate can be used as the second crystal in a double-crystal monochromator to focus sagittally a wide synchrotron X-ray beam. When bent in the sagittal direction, the plate also bends in the tangential direction (so-called anticlastic bending), which can adversely affect the diffracted beam. It is known that the undesirable anticlastic deformation can be minimized if the plate aspect ratio (length to width) is optimized. The present study investigates the influence of crystal material anisotropy and shows that ignoring it in the design of a sagittally bent crystal can lead to a significant underestimation of anticlastic deformation. For example, analysis shows that the optimal aspect ratio for a simply supported bent Si(220) plate ranges from 2.13 to 2.82 depending on the in-plane orientation of the cut rectangular plate. Treating silicon as isotropic with material properties in the literature leads to a plate design with an optimal aspect ratio of 2.36 and a plate with significant anticlastic bending.

1. Introduction

Most synchrotron X-ray experiments can benefit from higher photon intensity that is often achieved by focusing a beam. Wide beams, such as radiation from bending magnet sources, are typically focused by sagittal focusing.

There are two common techniques for sagittal focusing a wide X-ray beam. One involves the use of cylindrical (or mildly conical) mirrors. Such mirrors provide achromatic focusing for relatively narrower x-ray beams with photon energy not much in excess of about 30 keV. At higher energies, the required incident angle becomes very small (< 3 mrad), leading to an elongated beam footprint and a rather long mirror [1] unless the mirror is multilayer coated. The rather small sagittal radii that are required, however, limit the optical aperture and the size of the beam the mirror can accommodate.

The second technique uses a sagittally bent second crystal in a double-crystal monochromator system, in either Bragg or Laue geometry [2-14]. Diffraction angles are much larger (even for higher-energy photons) compared with reflection angles off mirrors, allowing focusing of wider X-ray beams.

Sagittal bending, however, is accompanied with anticlastic (tangential) bending stemming from the non-zero Poisson's ratio of materials, as illustrated in Figure 1. While it can be exploited in the Laue geometry [2-4], anticlastic bending is generally undesirable in Bragg geometry, for it introduces a slight deviation to the incident angle ("slope error") resulting in an increase in divergence and a possible decrease in the diffracted beam intensity. Minimization of the anticlastic deformations within the beam footprint is often necessary (with the exception of situations where anticlastic bending is exploited for focusing [15]).



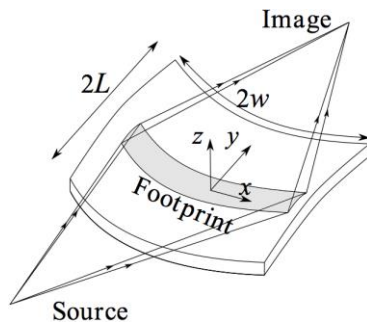


Figure 1. Schematic for a bent crystal plate. The filled area is the beam footprint. L and w are the half-length and half-width of the plate.

To reduce the anticlastic bending in diffracting crystals, several geometric remedies have been suggested, such as fabricating crystals with ribs [5,6] or with slots [7-10], or crystals in the form of thin, flat rectangular plates with an optimized length-to-width (aspect) ratio [11-14].

Crystals with ribs or slots can significantly reduce anticlastic curvature, rendering a large part of the crystal length usable. However, the crystals exhibit oscillations in the sagittal direction—due to the influence of ribs and slots—degrading focus quality [16]. These crystals are also costly to fabricate, are fragile, and cannot be generally bent to small sagittal radii without additional complexities [10].

Flat crystal plates, on the other hand, are not as fragile and are easy and inexpensive to fabricate. More importantly, their anticlastic bending can be minimized by an appropriate choice of crystal length-to-width ratio.

The dependence of anticlastic bending on the said aspect ratio was first realized by Kushnir et al. [11], who proposed a bent silicon crystal design based on the selection of an aspect ratio that results in a zero anticlastic curvature in the center of the bent plate. This optimal aspect ratio was shown to depend only on (1) the Poisson's ratio (silicon was assumed to be isotropic) and (2) how the plate was mounted. The optimal aspect ratio varies between 2 and 3.2 for simply supported isotropic plates and is less than 2 for clamped plates.

It was also shown [11] that there is an asymptotic solution: if the crystal is long (aspect ratio > 7), the anticlastic curvature could be minimized. Nisawa et al. [14] later showed that clamped plates with an aspect ratio greater than 3 would do likewise.

In these analyses, the plate material was considered to be isotropic, yet the crystal materials used for sagittal focusing are often anisotropic and can only be treated as isotropic in special cases. Neglecting anisotropy could result in a design with significant anticlastic deformations.

Krisch et al. [17] and Li [18] later showed that the anticlastic curvature in bent anisotropic crystals strongly depends on the crystallographic orientation. Their analysis was based on *beam* theory, which is valid only for narrow crystal slabs. The present paper concentrates on general *flat* plates. The dependence of the optimal aspect ratio on the crystallographic orientation of a crystal plate is shown. It is demonstrated that ignoring anisotropy in design can introduce significant tangential slope.

2. Optimal aspect ratio of a bent crystal plate

Let us consider a thin rectangular crystal plate (Figure 1) $2L \times 2w$ in size with the aspect ratio defined as $\gamma = L / w$. Plate edges at $x = \pm w$ are simply supported while the other two edges are free. A constant bending moment is applied to the supported edges to bend the crystal into a cylinder. It is assumed that the plate thickness is much smaller than other dimensions (for the thin plate theory to apply), and the maximum deflection is less than a quarter of the thickness (so the lateral forces can be ignored). With these assumptions, linear deflections depend on the applied moment. The ratio of anticlastic K_a to sagittal K_s curvatures everywhere in the bent plate can be shown [19] to be independent of the applied moment and can thus be used as the criterion for determining the optimal aspect ratio.

The analytical series solutions for bent plate profile were derived in [11,18] for isotropic materials and in [18] for anisotropic materials in specific orientations. The series converge very rapidly in the center of the plate where the anticlastic curvature must be zero at the optimal aspect ratio. Thus, the optimal aspect ratio can be derived from the first term in the series. For isotropic materials, the optimal aspect ratio $\gamma_{\text{opt}} = 2(3-\nu)/\pi(1-\nu)$, where ν is Poisson's ratio.

For anisotropic materials, the optimal aspect ratio also depends on the crystallographic orientation of the rectangular plate's diffracting surface as well as the orientation of its sides. A rectangular Si(220) plate, for example, can be cut from a (220) wafer in an infinite number of ways, so to specify the in-plane orientation of a rectangular plate, we introduce a 'cut angle' ϕ defined as the angle the

long edge of the plate makes with a reference crystallographic orientation. Computation of the optimal aspect ratio is then carried out for various cut angles using the finite element (FE) method, because simple analytical solutions are only available for specific crystal lattice orientations [19].

The dependence of the optimal aspect ratio on a cut angle is illustrated through an example here. Consider a thin single-crystal Si(220) wafer from which a rectangular plate is cut such that its long side is parallel to the crystallographic direction $\langle 001 \rangle$. We denote this as having a cut angle $\varphi = 0$. The short side of the plate is thus parallel to the $\langle \bar{1}10 \rangle$ direction.

For this primary in-plane orientation we use a dimensionless analytical solution [18] that provides the anticlastic-to-sagittal curvature ratio as a function of the aspect ratio for a rectangular plate bent into a radius $1/K_s$ for Si(220) with a cut angle of zero (Figure 2). Also shown is the solution for Si(111), which is in-plane, isotropic [11], and for which a cut angle need not be specified. The optimal aspect ratio is at $K_a/K_s = 0$. Similar curves for plates with any arbitrary cut angle can be constructed (using FE analysis) and their optimal aspect ratios determined. The result can then be presented in terms of the optimal aspect ratio as a function of the cut angle as presented in Figure 3 for Si (220). Also sketched in Figure 3 are three representative rectangular plates at different cut angles with different optimal aspect ratios. This gives the user some design options. For example, if the available (220) wafer has a small diameter, one would choose a 35° cut angle, which has the minimum aspect ratio requiring minimum plate length.

To demonstrate the impact of neglecting anisotropy, consider plate C in Figure 3. Let us assume that the crystal plate is 1 mm thick, 40 mm wide (thus, 112.8 mm long), and bent to a sagittal radius of 1 m. Figure 4 shows the computed slope of the anticlastic deformation in the central 20 mm of the plate (a reasonable value of a typical beam footprint) along the line that passes through the center ($x=0$ in Figure 1) of the plate. This slope is rather modest, as shown. However, if anisotropy is neglected and the plate is designed with an aspect ratio of 2.36 for isotropic silicon [11], the slope is increased more than 10 times.

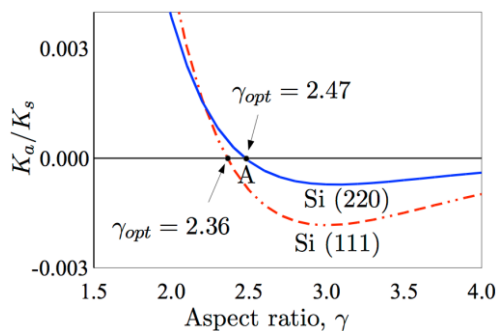


Figure 2. Ratio of anticlastic K_a to sagittal K_s curvatures versus aspect ratio for Si(111), which is in-plane isotropic and invariant in cut angle, and for Si(220) with a cut angle of zero (described in the text.)

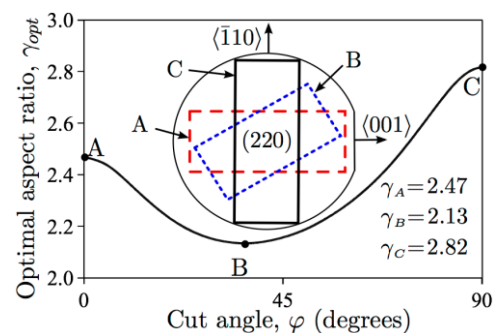


Figure 3. Dependence of optimal aspect ratio on the cut angle. A: initial in-plane orientation, $\varphi = 0^\circ$; B: cut angle $\varphi = 35^\circ$; C: cut angle $\varphi = 90^\circ$.

3. Conclusions

Sagittally bent crystals with minimized anticlastic deformation provide an attractive option for x-ray focusing. The minimization is accomplished by incorporating stiffening structures in the crystal plate or by simply choosing rectangular plates with optimal aspect ratios that can be determined analytically or by finite element modeling. Since the crystals are anisotropic, in this paper the impact of material anisotropy on anticlastic bending and the determination of optimal aspect ratio were discussed, demonstrating the strong dependence of optimal aspect ratio (e.g., geometry of the crystal) on crystallographic orientation. The recipe for design consists of a few steps. First, based on the desired energy range and resolution, a crystal plane (and material) is selected. Then through finite element

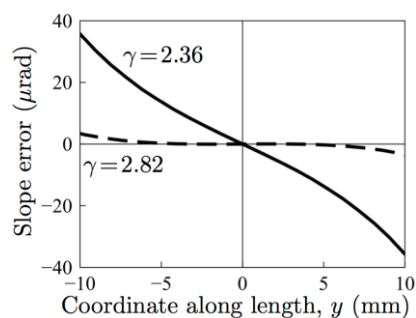


Figure 4. Tangential slope in the central part of a Si (220) plate (see text) with a cut angle of 90° (point C in Figure 3, $\gamma_{\text{opt}} = 2.82$). The slope for a non-optimal aspect ratio of 2.36 is also shown.

analysis (or analytical formulation, in certain cases), the variation of anticlastic-to-sagittal curvature ratio is computed and plotted against the plate aspect ratio. The aspect ratio at which the anticlastic curvature is zero is selected, and the process is repeated for a range of cut angles (as needed, based on the in-plane symmetry). A cut angle is then selected based on design considerations such as beam footprint size, available crystal size, etc., and the crystal is fabricated. The cut angle with the largest aspect ratio, for example, ensures both zero anticlastic curvature at the crystal center and the largest span of the crystal length with insignificant slope.

This analysis can be extended to asymmetric cut crystals where beam compression or expansion can be tailored to crystal tangential deformation.

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