Optimization of monochromator crystal bending designs using computer simulations

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Sagittal focusing of a synchrotron radiation beam by cylindrically bending the second crystal in a double-crystal monochromator is an important way of increasing beam density at the sample posiion. In this paper we describe results obtained by finite element analysis of various optimized Si (111) crystal shapes. For the bending magnet and wiggler sources, we analyzed ribbed crystals and found conditions at which the sagittal curvature is cylindrical and the anticlastic effect is minimized. For the undulator-A source, we found that a single slot in the center of a thick plate would be sufficient to eliminate the anticlastic effect and ensure cylindrical sagittal bending. Autofocusing of the beam by means of a trapezoidal slot was investigated, and simulation results are discussed.

I. INTRODUCTION

Sagittal focusing of synchrotron beam is important for both bending magnet (BM) and insertion device (ID) beamlines as a means of increasing beam density at the sample position.[1-3] Designs for the second crystal of a double-crystal monochromator share the goals of producing a uniform sagittal radius and minimizing anticlastic bending[2,4] of the crystal. Most current designs use crystals with parallel stiffening ribs or slots. In practice it has been found that these designs may have a sagittal radius that varies across the surface due to the ribs or slots and thus deteriorates the focus.[5]

We describe results obtained by finite element analysis (FEA), using commercial software,[6] of various optimized crystal shapes. Crystal geometry and material properties (Young's modulus and Poisson ratio) were used to calculate crystal surface deflections and radii of curvature for different bending mechanisms simulated by appropriate boundary conditions. For the BM and wiggler sources, where the beam cross section is a few centimeters wide, we analyzed ribbed crystals and found conditions at which the sagittal curvature is cylindrical and anticlastic effect is minimized. For the undulator-A source, where the beam cross section is a few millimeters, we found that a single slot in the center of a thick Si (111) plate would be sufficient to eliminate the anticlastic effect and ensure cylindrical sagittal bending. Finally, we analyzed conditions for autofocusing of the beam during a scan employing a trapezoidal slot shape.

II. BEAM FOCUSING FOR BENDING MAGNET AND WIGGLER SOURCES

The focal spot size will be minimized if the sagittal radius R_s obeys the equation:

$$R_s = \frac{2 f_1 f_2}{f_1 + f_2} \sin\Theta , \tag{1}$$

where f_1, f_2 are the distances from the monochromator to the source and sample, respectively, and Θ is the diffraction angle. Sagittal bending of the second crystal is always accompanied by the anticlastic bending in the meridional plane due to the Poisson ratio ν (0.262 for Si (111) crystal[4]). The anticlastic effect reduces the intensity at the focal spot due to the spread in diffraction plane's positions. This negative effect becomes noticeable if the spread of diffraction angles, $\Delta\Theta$, at the second crystal becomes greater than some fraction of the rocking curve width. On the another hand, $\Delta\Theta$ is related to the anticlastic radius of curvature, R_a, by the equation: $\Delta\Theta = f_1\phi_\nu/2R_a \sin\Theta$, where ϕ_ν is the vertical divergence of the beam.[2] Therefore, knowledge of R_a is valuable information for crystal design and applications.

We have developed a simulation procedure employing FEA to calculate and optimize sagittal and anticlastic radii. Linear stress analysis was performed over the crystal of a predefined shape. To produce a bending moment, we considered the crystal to be supported by two parallel fixed rods in the direction of the beam (Fig. 1), which were simulated by applying appropriate boundary conditions to the

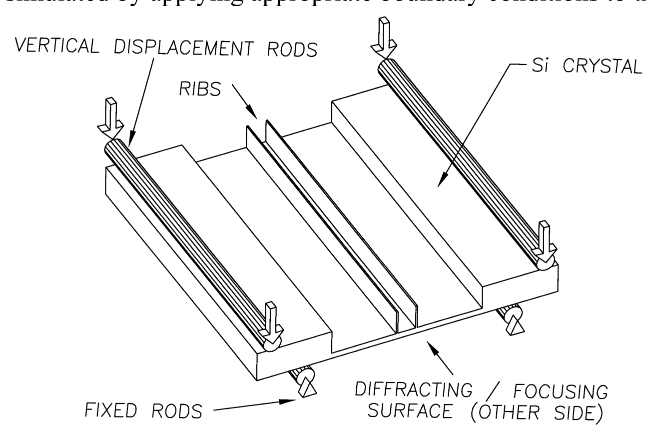

FIG. 1. Model of the crystal with stiffening ribs (for BM or wiggler sources).

model. Two more rods placed along the edges of the crystal, to be actuated by motors, were considered displacement boundary elements in the model. Displacements were chosen to produce the desired radius of curvature.

To verify FEA validity, we ran test simulations for simple, rectangular, uniformly thick crystals. We found the radii of sagittal and anticlastic curvature to be in good agreement with theoretical calculations,[4] for values at the plate center. Namely, the anticlastic effect was shown to be minimized at the aspect ratio (crystal's length to width ratio) of 2.4 for simple rectangular crystal shapes, in agreement with Ref. 4. With this information we went on to apply the method to more sophisticated cases, as described below.

The crystal shape for the ribbed design studied was a square, 100 mm × 100 mm in area, 10 mm thick with a 50-mm-wide, 2-mm-thick slot in the center (Fig. 1). We demonstrated that two parallel 0.5-mm-wide ribs, 6 mm apart, increase the anticlastic radius by a factor of two compared to the uniformly thick plate without ribs. Unlike our other models using plate elements, the abrupt and large thickness change of the ribbed model required the use of 3D brick elements. These computer resource intensive element types forced us to limit the model size to an insufficiently large aspect ratio of 2:1 for the slot region (100 mm long and 50 mm wide) and not attempt complete minimization of the anticlastic effect with a ratio much greater than 1.

Rib dimensions were obtained from the following considerations. Given the height of the rib (we used 8 mm), it is important to optimize its width, for it was shown[5] that the sagittal radius is increased in the region above the ribs, "underbending" the surface and producing strips in the intensity distribution. Different models were analyzed with rib widths of 3 mm, 1 mm, and 0.5 mm. The results (Fig. 2) show the underbending of the crystal in the rib region (sagittal radius is peaked in the center of the rib) for the 3-mm- and 1-mm-wide ribs, whereas, for the 0.5-mm-wide rib, the effect is minimal.

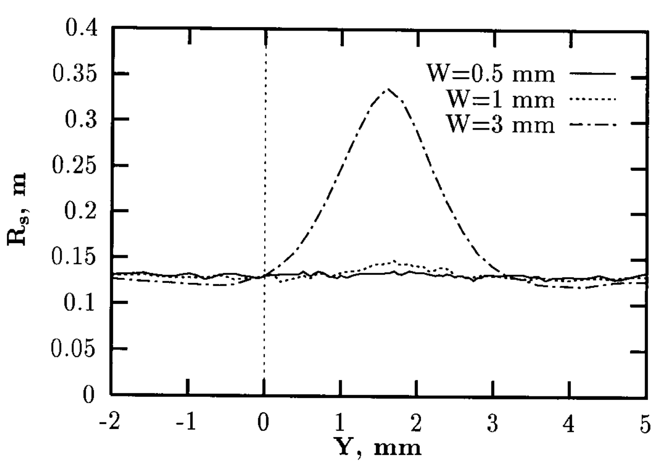

FIG. 2. FEA results for the sagittal radius in the region below the rib of three different widths W (3 mm, 1 mm, and 0.5 mm) vs. distance from the center of the crystal in the direction across the beam.

III. BEAM FOCUSING FOR UNDULATOR-A SOURCE

To sagitally focus the beam from the undulator-A source, we considered a model with a rectangular slot, narrow enough to diminish the anticlastic effect. We chose a crystal shape and dimensions to fit an existing crystal bender design by D. Adler.[7] Dimensions of the Si plate are 76 mm across and 66 mm along the beam. Figure 3 shows a sketch of the crystal in the bender. We took advantage of the four-fold symmetry of the model and analyzed a quarter-size part, applying appropriate boundary conditions at the edges. The width of the slot was 10 mm and its thickness 0.3 mm. Our results show that the sagittal radius is constant in the thin region of the slot, and this value is easily varied by applying different magnitudes of vertical displacements to the external rods.

The anticlastic effect was minimized by varying plate thickness and the minimum value of 5 mm was found, for the anticlastic effect to be neglible. The corresponding anticlastic radius of between 2500 m and 4200 m (Fig. 4) was obtained for the 20-mm-long, 5-mm-wide area in the center of the plate that is covered by the beam during the scan. In this range of variation of R_a, we consider the anticlastic effect neglible, given that the rocking curve width is greater than 10 μrad.

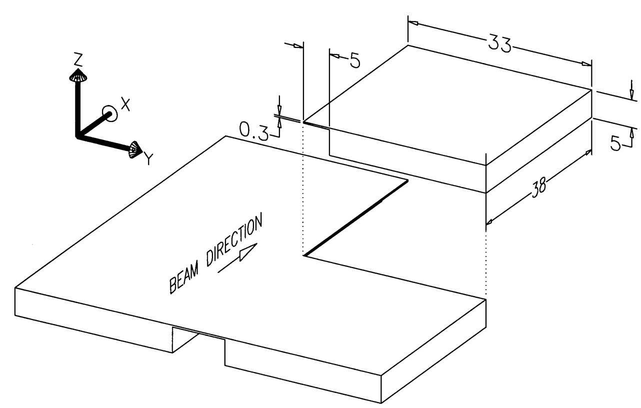

FIG. 3. Model of the crystal with a rectangular slot (for undulator-A source).

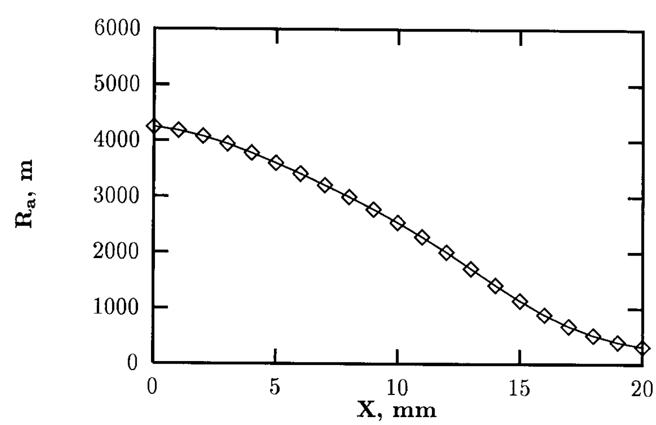

FIG. 4. FEA results for the anticlastic radius vs. distance from the center of the crystal in the direction along the beam.

IV. AUTOFOCUSING

An alternative way to sagittally focus the beam is autofocusing.[8] Optimal conditions for autofocusing were obtained using the construction parameters of an APS undulator-A PNC-CAT beamline: with f_1 = 32.7 m, f_2 = 21.3 m, $\sin\Theta = 12.4/2dE = 1.98/E$, where d = 3.136 Å is the lattice parameter for Si (111) and E is photon energy (in keV). Hence, $R_s = 51.1/E$ (where R_a is measured in meters). Thus the sagittal radius varies within 10.22 m < R_a < 2.04 m for the energy range available with Si (111): 5 keV < E < 25 keV. While a scan is in progress (the typical energy range is 1 keV), the separation S = 17.5 mm between the two Si crystals is kept fixed, for the purpose of avoiding error caused by any possible movement of the second crystal. For the same reason, it is advantageous to avoid dynamic bending of the crystal during the scan, so that R_s satisfies Eq. (1) providing for autofocusing.

Autofocusing can be achieved by having the beam "walk" across a surface with an appropriately varying sagittal curvature. To produce this curvature, the slot in the crystal is made trapezoidal (bases A and B, Fig. 5) rather than rectangular. Thus, R_s decreases through the walking distance ΔL of the beam. Equation $L = S \cot\Theta$, where L is the distance along the second crystal to the point where the beam was reflected, implies that $\Delta L \approx$ 9-9.5 mm for the 1 keV scan. Thus, the variations ΔR_s are to be as large as 1.7 m for E_0=5 keV and as small as 0.08 m for E_0=25 keV. To optimize the shape of the slot for the sagittal radius to vary in accordance with Eq. (1) and for the anticlastic radius to remain large enough throughout the whole energy range, one therefore has to reproduce the desired variation of $R_s(E)$ in the crystal shape, which is not practical or necessary. Fortunately, only lower energies are sensitive to an imprecise focusing radius. To parametrize the problem, we considered a perfectly cylindrical shape of the crystal with the radius kept fixed throughout the scan and chosen to satisfy Eq. (1) at $E = E_0$+0.5 keV, i.e., in the middle of the scan energy range. Then we calculated the focal spot size magnifications at the ends of the scan range, E_0 and E_0+1 keV, for all E_0 (5 keV < E_0 < 25 keV), and found that the defocusing is four times larger at lower energies (20% increase of the focal spot size) than at higher energies (5%). Thus, special care was taken to reproduce the functional dependence of $R_s(E)$ in the energy range of about 5-12 keV in the design (as our analyses have shown, a trapezoidal slot provides a good agreement of the sagittal radius with theory for larger energies as well).

Our result (Fig. 6) shows that the slot with dimensions A = 5 mm and B = 15 mm produces a varying sagittal radius in fairly good agreement with theory (Eq. (1)). Six different bending displacements D were applied in simulations to cover six test scans, starting at E_0 from 5 to 8 keV and also two values at higher energies. The anticlastic radius was also monitored and was always larger than 3000 m, thus the corresponding spread of diffraction angles would be less than a half of the rocking curve width.

It is important to note that there exists an additional source of defocusing due to the finite vertical size of the beam. The footprint of the beam at the second crystal is being reflected ideally correctly (Eq. (1)) only in the center of the footprint, while the rest of it is being reflected under wrong angles since the sagittal radius varies along the surface. For the vertical beam size of 0.8 mm and vertical divergence of 14 μrad (for the undulator-A), we obtained only a 2% increase in the focal spot size due to these effects for the 5 keV-25 keV energy range. This is, therefore, a small negative effect compared to the positive effect of autofocusing and can be neglected.

V. CONCLUSIONS

We performed finite element analysis of second crystal sagittal focusing of a double-crystal monochromator and optimized parameters of several crystal designs for both bending magnet and insertion device beamlines. The results suggest the use of parallel ribs to reduce anticlastic bending of the crystal for the bending magnet and wiggler beamlines. An undulator-A beam will be well focused and unaffected by

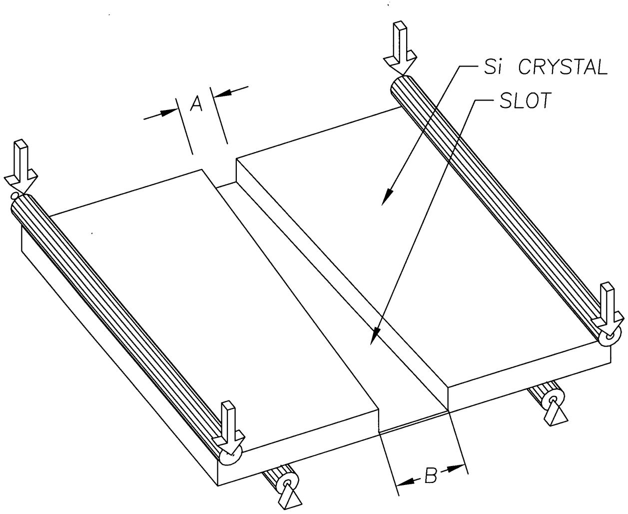

FIG. 5. Model of the autofocusing crystal (for undulator-A source).

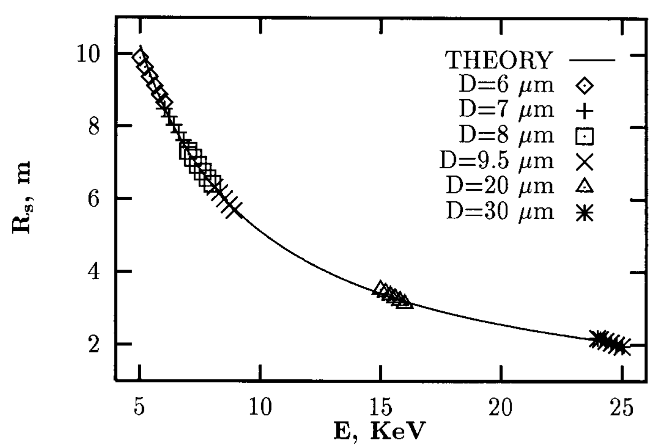

FIG. 6. FEA results (symbols) for the autofocusing crystal vs. theory (solid line) of the variation of the sagittal radius with energy.

anticlastic curvature with a slotted crystal with a large length-to-width slot aspect ratio. For autofocusing, a variation of the slot design employing a trapezoidal shaped slot was modeled. We found design parameters of the slot optimal for performance in the low energy range, where the correct focusing is most necessary.

ACKNOWLEDGMENT

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