A Sagittally Bent Crystal for the Short Pulse X-ray Beamline at the Advanced Photon Source

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Abstract. The Short Pulse X-ray Imaging and Microscopy (SPXIM) Beamline at the Advanced Photon Source (APS) is being designed to provide a short-pulse focused beam at the sample some 60 m from the source. The second crystal in the horizontally diffracting double-crystal monochromator system is sagittally bent to focus the full vertical fan of the beam, preserving the flux of a typical undulator beamline at the APS, while providing a time-angle correlated beam on the sample with a few-picosecond pulse duration. An energy scan using this system requires changing the bent radius of the second crystal. Undesirable distortions in the sagittally bent second crystal are due to anticlastic deformations. In this paper, the analysis and design of the bent crystal is presented including an examination of the mechanical interaction between the crystal and the two pairs of rollers used to bend it. Ray tracings including the anticlastic deformations obtained from an optimized finite element model show a minimal effect on the spot size at the sample position.

1. Introduction
The proposed SPXIM beamline for the APS upgrade [1] uses a horizontally diffracting double-crystal monochromator (DCM). The thermal load on the first crystal of the DCM can be handled using existing cryogenically cooled designs. The sagittally bent second crystal (see Fig. 1) will collect most of the photons generated when the chirped electron beam, which has a correlation between vertical divergence and time, traverses the undulator. The bent crystal focuses the beam along the vertical direction at the timing slits, which are 54 m downstream from the source. To maximize the throughput of the bent crystal, the optimal design must minimize deviations from the desired cylindrical shape. The focusing at the sample position is done with a Kirkpatrick-Baez (KB) mirror system in which a pair of in-tandem mirrors is used. One mirror focuses the beam vertically and the other horizontally, to the same spot [2]. The first KB element is a horizontally deflecting elliptical mirror downstream of the timing slits that focuses the beam along the horizontal direction. A vertically deflecting elliptical mirror images the time slit along the vertical direction.

Undesirable distortions in sagittally bent crystals are due to anticlastic deformations. As a plate is bent in the sagittal direction, the non-zero Poisson’s ratio of the material leads to bending in the tangential, or anticlastic, direction (see Fig. 2). Three common design approaches exist to decrease anticlastic bending: ribbed crystals [3], slotted crystals [4], and flat-plate geometries with an optimized aspect ratio of length to width [5].

Kushnir et al. [5] numerically determined the optimal aspect ratio for flat-plate crystals, assuming isotropic material. Their results revealed that the optimal aspect ratio for a sagittally
bent crystal depends only on Poisson’s ratio and how the crystal is held and bent. There are analytical solutions for idealized plate and boundary conditions; however, they do not always accurately reflect the behavior of an actual bent crystal. Here, we report on the preliminary design of the sagittally bent crystal for the SPXIM beamline, determined numerically using a finite element (FE) model and including the effects of the roller/crystal interface.

2. Preliminary analysis of the anticlastic deformation

The approach to optimizing the crystal to minimize anticlastic distortion involves calculating the appropriate sagittal bending radius based on the beamline parameters, selecting the initial crystal plate geometry based on the beam footprint, analytically calculating the necessary moment to bend the crystal to the desired radius, converting the bending moment to an equivalent force, applying the force using a simplified FE model, and then refining the model. The roller/crystal interface is added to the FE model in section 3.

The crystal plate material used is silicon (111). Although silicon is not an isotropic material, the stiffness and Poisson’s ratio are uniform in the (111) plane and thus in both the sagittal and tangential directions [5]. Idealized boundary conditions of simply supported edges and two lines of force were used to represent the crystal being bent by rollers (see Fig. 3). The crystal plate was assumed to have uniform thickness.

Based on the energy range to be covered by the Si (111) crystal (4.5 - 8.3 keV), the distance from the source to the bent crystal (36 m), and the distance to its focus (18 m), one finds that the sagittal radius needs to be changed between 6.8 m (at 8.3 keV) and 12.6 m (at 4.5 keV).

The divergence of the x-ray beam is 50 µrad (h) x 400 µrad (v), which gives a beam footprint size at the crystal of up to 7.6 mm horizontal and 14.4 mm vertical. Based on the size of the beam footprint and the optimal aspect ratio of 2.36 for simply supported plates [5], an initial set of crystal dimensions was selected as 236 mm long, 100 mm wide between the supporting edges, with a thickness of 1 mm.

With the above-mentioned crystal parameters, a sagittal radius of 6.8 m and the equation for the analytical solution given in Ref. [5], we obtained 0.2205 N-m for each of the two moments. These moments were implemented in the simplified FE model as two lines of 22.05 N force each simulating the rollers located at 10 mm from the pivot points. The lines of force had to be increased to 22.31 N to obtain the correct radius of curvature in the FE model.
The main result of the simplified FE model is illustrated in Fig. 4. The red trace in the figure shows that the tangential slope error along the middle of the crystal is very small over the illuminated crystal length. However, as shown in the next section, the realistic crystal/roller contact interface has a significant effect on the anticlastic deformation.

3. Roller/crystal interface in the FE model
To properly model the bent crystal, the crystal/roller interface must be addressed. Four cylindrical bodies were added in the FE model: two pairs of stainless steel rollers with a 10-mm diameter. The initial crystal dimensions were taken from the results of the previous FE model that used idealized boundary conditions. In the complete model (illustrated in Fig. 5), the length of the crystal is kept at 236 mm, the distance between the outer rollers is 100 mm, and they are located 5 mm from the ends of the 110-mm-wide crystal. To bend the crystal to the desired radius, forces are applied to the inner rollers, which are located 10 mm from the outer ones. The contact between the rollers and the crystal plate is assumed to be frictionless.

Figure 6 shows that with the optimized forces (22.31 N) obtained in section 2, the anticlastic bending given by the realistic model separates the rollers from the crystal over a large fraction of its length. This has a significant impact on the tangential slope error as demonstrated by the black trace in Fig. 4. This slope error translates to a tangential convex radius of curvature equal to 1.4 km, creating a virtual image of the horizontal source 6 m downstream of its original position.

Despite the separation between the rollers and the crystal, a significant reduction in the tangential slope error can be obtained by optimizing the crystal length while the other parameters in the model is kept unchanged. This is shown by the blue trace in Fig. 4, which was obtained by increasing the crystal length to 247 mm and by applying forces equal to 28.3 N to obtain a 6.8-m sagittal radius.

As mentioned in section 2 the monochromator energy range requires varying the sagittal radius between 6.8 and 12.6 m. The latter radius can be obtained by simply reducing the couple of forces to 15.2 N while all the other parameters in the FE model are unchanged. As expected, the slope errors along the tangential direction for 12.6 m, shown by the green trace in Fig. 4, are smaller than for the 6.8-m sagittal radius.

4. Ray tracings
The ray tracings were performed with the SHADOW code [6] with the timing slit set to 25 μm. The chirped source, a monochromator, and a KB mirror pair were included in the ray tracings. The KB set is assumed to have ideal figures so that the ray tracing reveals the result of aberrations in the bent crystal. Figure 7 shows the ray tracings at the sample position assuming the crystal is a perfect sagittal cylinder with a 6.8-m radius. Figure 8 shows the ray tracings including the deformation obtained from the FE model described in section 3. The captions
5. Conclusions
The proper modeling of the roller/crystal interface leads to non-uniform contact pressure and allows separation between the rollers and plate. Determining an optimal aspect ratio (other than the one predicted by the idealized model) can significantly reduce the anticlastic deformation. The optimized crystal geometry of the bendable crystal of the SPXIM beamline has dimensions of 247 mm long x 110 mm wide with a thickness of 1 mm. Ray tracings show that the optimized geometry and sagittal bending based on four rollers has a minimal effect on the focal spot.

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