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Supporting information for article:

Optimal azimuthal orientation for Si(111) double-crystal monochromators to achieve the least amount of glitches in the hard X-ray region

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S1. General expression of glitch positions for one Si(111) crystal

As Van der laan's research reported (Van der laan & Thole, 1988), a coordinate system with zaxis along [111], x-axis along [11 $\overline{2}$], y-axis along [$\overline{1}10$] is set up. The schematic of the coordinate is in Fig. S1. After a series mathematical derivation, the general expression of glitch positions for one Si (111) crystal can be obtained:

$$E = \frac{h_0 c}{2d_0 n \sin \theta_0} \tag{S1}$$

$$\theta_{0} = \arctan \frac{(h+k-2l)\cos \varphi + \sqrt{3}(k-h)\sin \varphi}{\sqrt{2}(h^{2}+k^{2}+l^{2}-h-k-l)}$$
(S2)

Where $d_0 = 2\pi/|H_0|$, H_0 is the reciprocal lattice vector of the primary reflection (Weckert & Hummer, 1990). θ_0 is the Bragg angle. E presents the energy positions of the glitch. h_0 is plank constant and c is velocity of the light. h, k, l are the index of the operative reflection(Hummer & Weckert, 1995, Weckert & Hummer, 1997). n is the refractive index of silicon crystal. φ is the angle between the projection of incident beam to x-y plane with x-axis. i.e. the azimuthal angle.

S2. The influence of changing pitch, roll and azimuthal angle of the crystal

Generally, a crystal has three rotation axes correspond to the three adjustable angles. Firstly, considering the situation that the pitch angle change $\Delta \theta$, i.e. the crystal rotated $\Delta \theta$ around y-axis, while the roll and azimuthal angle keep constant. According to the coordinate transformation relations, the expressions as below can be obtained:

$$\begin{pmatrix} e_{x} \\ e_{y} \\ e_{z} \end{pmatrix} = \begin{pmatrix} \cos \Delta \theta & 0 & -\sin \Delta \theta \\ 0 & 1 & 0 \\ \sin \Delta \theta & 0 & \cos \Delta \theta \end{pmatrix} \begin{pmatrix} e_{x} \\ e_{y} \\ e_{z} \end{pmatrix}$$
(S3)

$$\sin\theta = \hat{k} \cdot e_z = \cos\theta_0 \sin\Delta\theta \cos\varphi + \cos\Delta\theta \sin\theta_0$$
 (S4)

In addition, for the situations that the roll angle change $\Delta\delta$, i.e. the crystal rotated $\Delta\delta$ around xaxis, while the pitch and azimuthal angle keep constant and the azimuthal angle change $\Delta\varphi$, i.e. the crystal rotated $\Delta\varphi$ around z-axis, while the pitch and roll angle keep constant, similar expressions as below also can be gotten:

$$\sin\theta = \hat{k} \cdot e_z = -\cos\theta_0 \sin\Delta\delta\sin\varphi + \cos\Delta\delta\sin\theta_0$$
 (S5)

$$\sin\theta = \hat{k} \cdot e_z = \sin\theta_0 \tag{S6}$$

Where θ_0 , θ present the Bragg angles of the incident beam before and after rotation respectively. e_i , e'_i (i = x, y, z) are the unit vectors of the corresponding coordinate system before and after rotation. \hat{k} is the unit vector of the incident beam.

From the expression (S4)-(S5), we can get that changing pitch and roll angles will cause Bragg angle variations of the incident beam, thus causing intensity variation of the output beam. Furthermore, varying the pitch and roll angle could also cause vertical and horizontal position shift of the output beam. Therefore, for the DCMs, it is difficult to reduce glitches by pitch and roll angle adjustment. However, from the expression (S6), varying the azimuthal angle will keep the Bragg angle of the incident beam fixed, so that it will have larger adjustment range. Therefore, it will be easy to get a proper azimuthal orientation of the crystals to achieve the least glitches.

Figure S1 The coordinate system that was chosen to calculate. \vec{k} presents the incident beam, φ is the azimuthal angle. $\vec{e}_i \ i = \{x, y, z\}$ are the unit vector of each axis respectively.



Reference

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