Adjustment of Golovchenko-Type Double Crystal Monochromator

Misaki Katayama[1] and Yasuhiro Inada[2]

1) *Research Organization of Science & Engineering, Ritsumeikan University, 1-1-1 Noji-Higashi, Kusatsu 525-8577, Japan*
2) *Department of Applied Chemistry, College of Life Sciences, Ritsumeikan University, 1-1-1 Noji-Higashi, Kusatsu 525-8577, Japan*

Three geometrical factors, a tilt angle of the first crystal, an offset distance of the crystal surface, and a tilt angle of the horizontal guide rail, cause the drift of the exit beam height of the monochromatic X-ray for the Golovchenko-type monochromator. We have formulated the geometrical factors and established the technique to adjust the alignment of the monochromator to restrain the beam drift.

1. Introduction

A most important component of the X-ray beamline is the monochromator for the X-ray absorption fine structure (XAFS) experiments, because the XAFS experiments generally require the scan of the X-ray energy. The crystal monochromators extract the monochromatic X-rays from white X-ray emitted from a light source by using the Bragg diffraction. Double crystal monochromators are widely used to obtain the exit X-ray at a fixed position, which is parallel to the incident white X-ray. One of such double-crystal monochromators, the Golovchenko-type monochromator [1], in which both crystals translate along the horizontal guide rail driven by the rotation of the main axis to change the Bragg angle, is used at the hard and tender X-ray XAFS beamlines, BL-3, BL-4, BL-10, and BL-13, in the SR Center of Ritsumeikan University. In this paper, some essential geometrical parameters are discussed for the alignment of this monochromator.

2. Beam Height of Monochromatic X-Ray

The Golovchenko-type double crystal monochromator (Fig. 1) gives monochromatic X-ray beam at a fixed position, only when it is adjusted on the proper alignment condition. First and second crystals are set on a L-shaped stage, which is rotated to change the energy of the diffracted X-ray. The angle of the crystal surface to the incident X-ray varies with the direction of

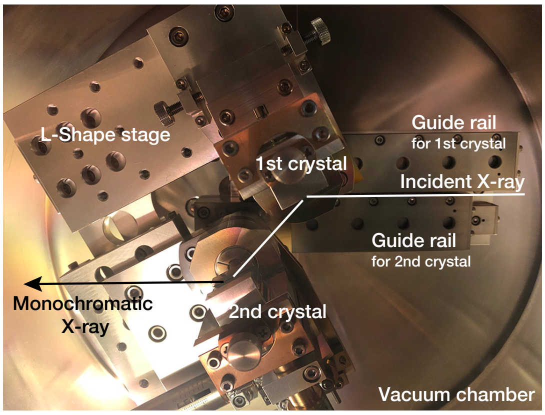

Fig. 1 Double crystal monochromator of BL-4.

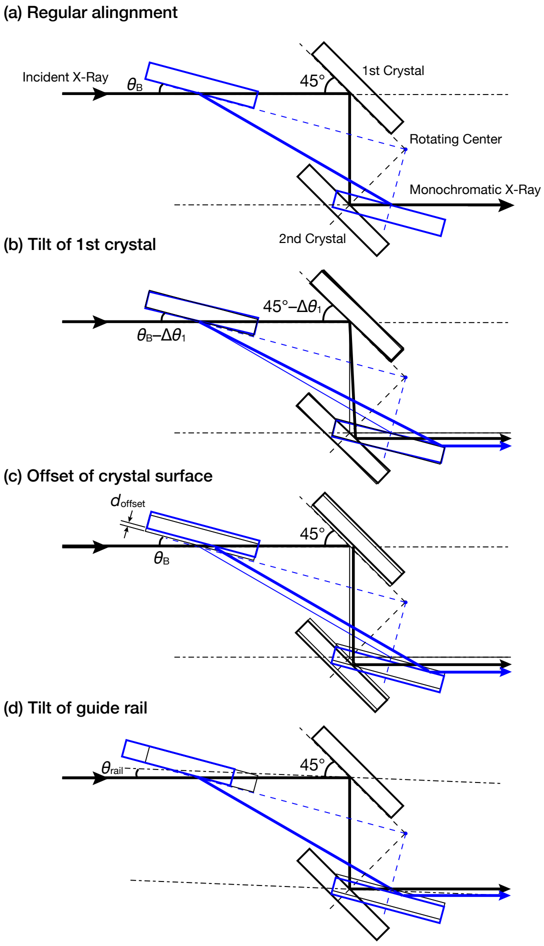

Fig. 2 X-Ray paths in the Golovchenko type monochromator under the regular alignment (a), with an additional tilting of crystals (b), with an offset of crystal surface (c), and with an additional tilting of the horizontal guide rails (d).

the rotating L-shape stage. The crystal units slide on arms of the L-shape stage and each horizontal guide rail, when the L-shape stage rotates. The schematic diagram is shown in Fig. 2(a), although the actual stage is more complicated (see Fig. 1). In Fig. 2, the arrows show each centerline of the X-ray beam without its divergence. The dashed lines mean the L-shaped stage, and dot-dashed lines show the horizontal guide rail. The crystal center keeps at the crossing point of them. Figure 2(a) shows the arrangement at $\theta_B = 45°$ (black) and 15° (blue), where θ_B means the Bragg angle (strictly the angle of L-shape stage). The X-ray beam diffracted from the first crystal reaches the center of the second crystal in both cases. As the result, the monochromatic X-ray beam keeps the fixed position during the energy scan by changing θ_B. In the original design by Golovchenko *et al.*, the rotation center was located on the center of the first crystal and the first crystal kept the position. On the other hand, the right angle part of the L-shape stage moved on the guide rail. In the design of our monochromators, both crystals are located on the horizontal guide rail with the same length, and the available θ_B range is from 15° to 75°.

For the Golovchenko-type monochromator, the horizontal guide rail must be parallel to the incident X-ray beam. Moreover, a distance between the center of crystals must become shortest when $\theta_B = 45°$. That is, the geometrical error of Bragg angle and the offset of the crystal surface are forbidden to achieve the fixed-position exit of the monochromatic X-ray during the energy scan. Such factors cause the drift of the position of monochromatic X-ray beam. Figures 2(b), (c), and (d) illustrates the effects of an additional tilt of the first crystal ($\Delta\theta_1$), an offset of crystal surface (d_{offset}), and an additional tilt of the guide rail (θ_{rail}). Here, we have defined that the positive $\Delta\theta_1$ increases θ_B. Similaly, the positive d_{offset} moves the crystal surface to the downstream direction, and the positive θ_{rail} rises the downstream side of the horizontal guide rails. When the diffraction surface of the first crystal is not parallel to the L-shape stage arm, $\Delta\theta_1 \neq 0$ as shown in Fig. 2(b). In such case, the beam diffracted by the first crystal reaches to the off-centered position of the second crystal at $\theta_B = 45°$. The diffraction angle at the second crystal ($\theta_B - \Delta\theta_2$) become equal to $\theta_B - \Delta\theta_1$ due to satisfy the diffraction condition. Therefore, $\Delta\theta_2 = \Delta\theta_1$ (= $\Delta\theta$) and the monochromatic X-ray beam is parallel to the incident beam. However, the diffraction center of the second crystal moves when θ_B is changed. As a result, the beam height drifts by the scan of X-ray energy.

In the cases of Figs. 2(c) and 2(d), the diffraction center of the first crystal also moves according to the change of θ_B, and thus the beam position at the second crystal changes. Although the monochromatic beam is parallel to the incident beam under the condition of $\Delta\theta_2 = \Delta\theta_1$, the beam height drifts as in the case of $\Delta\theta$.

3. Simulation of Beam Drift

We have derived the theoretical expressions of the height of the monochromatic X-ray beam in considering the geometrical factors given in Fig. 2. The Bragg angle is denoted by θ_B, the distance between the two horizontal guide rails by d_{rail}, and the relative drift of the X-ray beam height to that at the correct alignment by Z. In the case of the monochromator at BL-3 and BL-4, d_{rail} is designed to be 40 mm.

The effect of an additional tilt of the first crystal can be formulated by eq. (1).

$$Z = \frac{d_{\text{rail}} \sin 2\Delta\theta}{\sin 2\theta_{\text{B}}} \qquad (1)$$

When both crystals have the same offset on the diffraction surface, the effect is described by eq. (2) using d_{offset}.

$$Z = 4 d_{\text{offset}} \cos\theta_{\text{B}} \qquad (2)$$

Although the beam drift caused by the additional tilt of the guide rail is complicated, we can derive the following equation in considering the difference from the ideal arrangement.

$$Z = \frac{d_{\text{rail}}(1 - \tan\theta_{\text{B}}) \sin\theta_{\text{rail}} \cos\theta_{\text{B}}}{\cos(\theta_{\text{B}} + \theta_{\text{rail}})} \qquad (3)$$

Figure 3 shows the simulated beam height drifts as a function of θ_B calculated by assuming some typical values for the three factors. In all cases, the beam height apparently changes versus θ_B, and it should be noted that the dependence on θ_B is different for the three cases. The curves for $\Delta\theta$ are symmetric with the center at $\theta_B = 45°$, and the drift becomes large when θ_B is far from 45°. The drift caused by d_{offset} is not very large at large θ_B, but the effect becomes serious at small θ_B. The curves for θ_{rail} cross at $\theta_B = 45°$, and its influence exponentially increased at large θ_B.

In addition, the drift of the monochromatic X-ray beams is also caused by the rotation of the crystal around the beam axis ϕ_1. The ϕ_1 rotation of the crystal mainly contributes to the drift of the horizontal beam position. Figure 4 shows the horizontal beam drift at the typical cases. For this calculation, the rotation of the second crystal, ϕ_2,

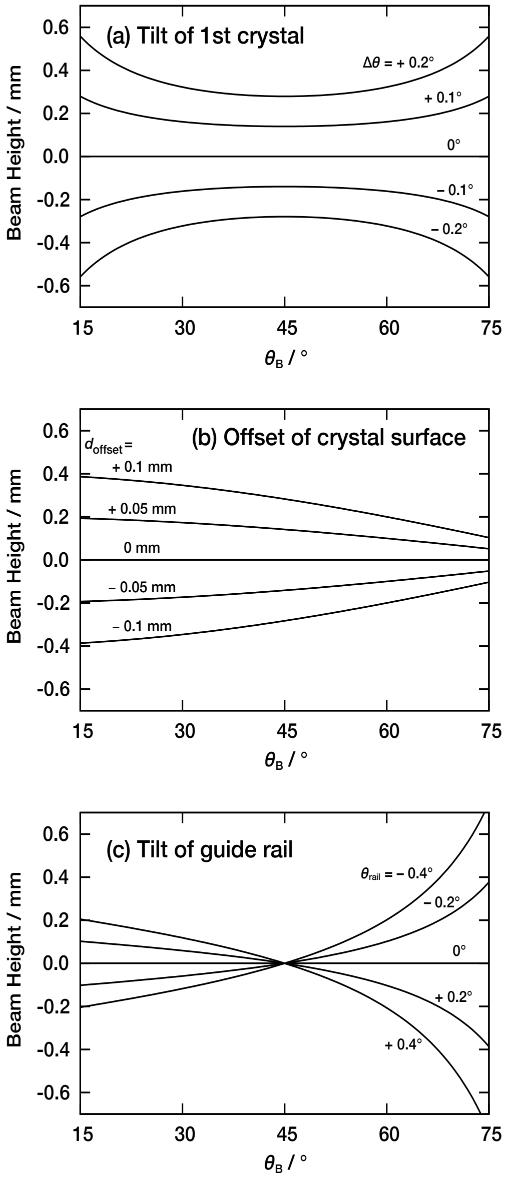

Fig. 3 Beam drifts calculated by using eqs. (1)–(3) with some typical values of $\Delta\theta$ (a), d_{offset} (b), and θ_{rail} (c).

was treated so as two crystals to become parallel. Similar to the case of θ_{rail}, the beam drift becomes serious when θ_B is large, and the deviation is exponentially increased with the increase in θ_B.

The last parameter described in this section is related to the thermal expansion of the monochromator crystal. In the double crystal monochromator, the heat load of the first crystal is larger than that of second one. When the temperature of the first crystal differs from that of the second crystal, two crystals have different lattice parameters. This phenomenon is treated as the ratio of the lattice spacing (d_1/d_2), where d_1 and d_2 denote lattice spacings of the first crystal and the second crystal, respectively. The X-ray path from the monochromator with the different lattice spacing for two crystals is not parallel to the incident one, because the maximum X-ray intensity is achieved under the condition of $\Delta\theta_1 \neq \Delta\theta_2$. Figure 5 shows the beam height at 1.0 m downstream from the monochromator center in the cases of d_1 is by 0.01% and 0.02% larger than d_2. Because the calculated change in beam height presented in Fig. 5 is clearly different from the effects of $\Delta\theta$, d_{offset}, and θ_{rail} shown in Fig. 3, they are experimentally distinguished.

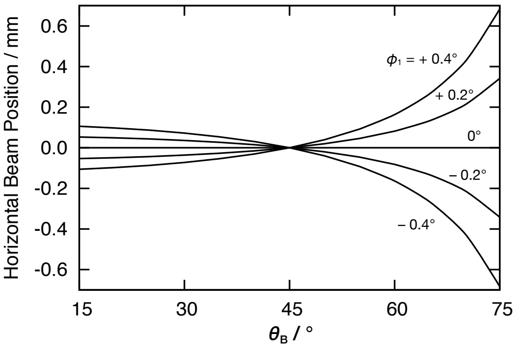

Fig. 4 Horizontal beam drift caused by ϕ_1.

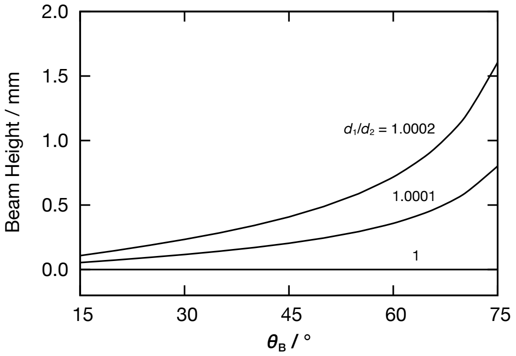

Fig. 5 Beam height drift caused by the difference of the lattice parameter of the first and second crystal.

4. Fine Adjustment of Monochromator

We have tried to use eqs. (1)–(3) to stabilize the vertical beam position for the monochromators of BL-3 and BL-4. The change in the beam height measured by the slit scan at each θ_B from 20° to 70° are shown in Fig. 6. The plotted beam height is a center of the exit beam, and they are independent from a size of the light source and a beam divergence. The $\Delta\theta_2$ was tuned to obtain the maximum X-ray intensity before the measurement at each θ_B. This operation is necessary to adjust a mechanical perturbation of $\Delta\theta_2$ with a large movement of θ_B. The relative beam height to that at $\theta_B = 45°$ is plotted as a function of θ_B. The beam height before the adjustment of the monochromator given in Fig. 6(a) falls at both sides of the Bragg angle. In the case of Fig. 6(b), the beam oppositely rises at lower and higher Bragg angle regions. These plots show that the monochromatic X-ray beam moves several hundred micrometers during the energy scan for the XAFS measurement. When the monochromatic X-ray is masked using a slit before the I_0 detector, such the vertical movement of the X-ray beam leads the drop of the X-ray intensity. The measured beam heights were well reproduced by the summation function of eqs. (1) and (3) by optimizing the parameters of $\Delta\theta$ and θ_{rail}. For the Si(220) monochromator, the effect for the offset of crystal surface (eq. (2) and Fig. 3(b)) was not found at BL-3 and BL-4. The solid curves in Fig. 6 were depicted using eqs. (1) and (3) with $\Delta\theta = -0.72°$ and $\theta_{\mathrm{rail}} = -0.17°$ for BL-4 and $\Delta\theta = 0.63°$ and $\theta_{\mathrm{rail}} = 0.28°$ for BL-3, respectively.

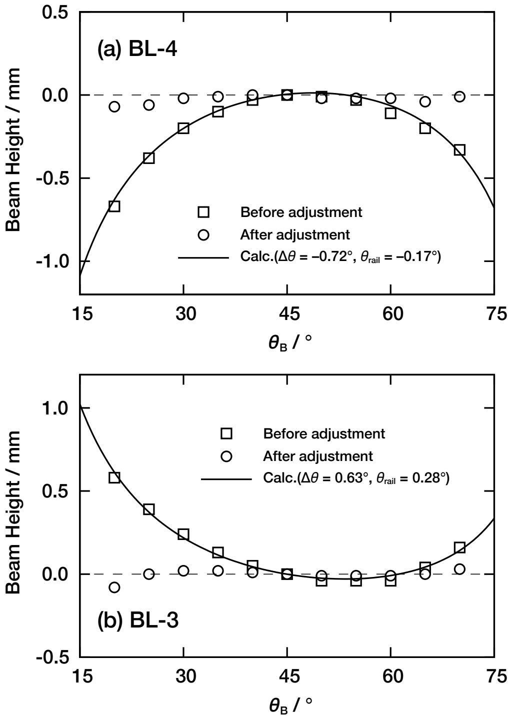

Fig. 6 Experimentally measured beam height before (square) and after (circle) the adjustment of the monochromator of BL-4 (a) and BL-3 (b). The solid line shows the curve calculated using eqs. (1) and (3).

The adjustment of the monochromators was performed based on the obtained parameters. Because the guide rails in the monochromator are fixed on the wall of the vacuum chamber, the tilt of the guide rail was adjusted by rotating the overall vacuum chamber. These monochromators have only a manual adjustment mechanism of the screw for the $\Delta\theta_1$ axis in the vacuum chamber. The estimated value for $\Delta\theta_1$ obtained by the analysis of Fig. 6 is thus very helpful for the fine adjustment. After the adjustment of the $\Delta\theta_1$ and θ_{rail} axes, the vertical beam drift decreased within 100 µm in the wide range of θ_B between 20° and 70° as shown by the circle plots given in Fig. 6. This is a permissive drift, because the scan angle of the monochromator for one XAFS measurement is typically a few degrees of θ_B.

5. Conclusion

We have extracted the geometrical parameters for the adjustment of the Golovchenko-type double crystal monochromators. Mainly three factors, $\Delta\theta$, d_{offset}, and θ_{rail}, drift the vertical position of the monochromatic X-ray during the scan of θ_B for the XAFS measurement. Similarly, the ϕ_1 angle changes the beam position in the horizontal direction. The present study clearly demonstrated how to adjust precisely the Golovchenko-type monochromator to diminish the vertical drift of the exit beam to keep the X-ray intensity during the XAFS scan.

Reference

[1] J. A. Golovchenko, R. A. Levesque, and P. L. Cowan, *Rev. Sci. Instrum.*, **1981**, *52*, 509.