Compact full-field hard x-ray microscope based on advanced Kirkpatrick-Baez mirrors: supplementary material

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1. Simulation study for designed objective mirrors

A. Abbe's sine condition

An important characteristic of developed advanced Kirkpatrick-Baez (AKB) mirrors is reducing the coma aberration, unlike the Kirkpatrick-Baez (KB) mirrors. Coma-free optics can be obtained when the Abbe’s sine condition [1] is satisfied at all ray in the optical system. The Abbe’s condition requires that the ratio of the sines of the angles between the optical axis and the incident ray (\(\phi\)), and the reflected ray (\(\theta\)) remain a magnification factor of optical system \((M = \sin \theta / \sin \phi = M \text{ (const.)})\). Figure S1 shows the magnification factors, calculated with 5000 rays, of designed AKB mirrors based on Wolter type I (AKB-I) and Wolter type III (AKB-III) optics. It was confirmed that the designed mirrors almost satisfy the Abbe's sine condition and eliminate the coma aberration.

B. Fields-of-view

Theoretical fields-of-view (FoVs) of designed AKB-I and AKB-III optics were investigated by wave-optical calculations. Point spread functions (PSFs) of the optics at a photon energy of 15 keV were calculated with varying positions on the image fields. The full-width at half-maximum (fwhm) values were evaluated. Figure S2 shows the results. We postulated a threshold of 43.65 nm fwhm, corresponding to 120% of \(0.44 \times \lambda/\text{NA}\), and determined the theoretical FoVs of 7.6 \(\mu m\) in AKB-I (vertical) and 12.44 \(\mu m\) in AKB-III (horizontal) optics, respectively. The FoVs correspond to angles-of-view of 180 \(\mu rad\) in AKB-I and 420 \(\mu rad\) in AKB-III optics, respectively. Note that these FoVs are limited by the field curvatures [3-5], which indicates that PSFs out of the field are mainly blurred by not the problematic aberrations, but the defocus effect.

![Fig. S1. Ray-tracing calculation results of magnification factors.](image-url)

The red line denotes the result for the AKB-I optics (left axis). The green line denotes the result for AKB-III optics (right axis). The maximum errors from designed magnification values are 0.0012 % in AKB-I and 0.0004 % in AKB-III optics, respectively.
2. Immobilization of mirror pairs of AKB-III optics

We assembled and bonded the elliptical concave and hyperbolic convex mirrors for AKB-III optics, as shown in Figure S3. The bonding experiment was performed with one-dimensional (horizontal) focusing setup in BL29XU at SPring-8, at a photon energy of 15 keV. First, the position of two mirrors was roughly adjusted using an optical microscope, tilt sensors combined with an optical parallel reference, and X-ray shadow-based measurements. Then, a wavefront sensing technique of a single-grating interferometer [6] was applied (Figure S3(a)). The utilized grating was made of 1.4-µm-thick tantalum with 2.5 µm period and gap/period ratio of 0.5 (NTT Advanced Technology Co.). A scintillator based X-ray camera (effective pixel size of 3.1 µm, image size of 6.3 × 6.3 mm², Orca-Flash 4.0 V2 and AA40, Hamamatsu Photonics K. K.) was employed for the detector. The grating and detector were placed 38.76 mm and 1.558 m downstream from the source, respectively, that corresponded to the Talbot order of 0.5 and 3. The wavefront errors were calculated by a 10 step fringe-scanning method and subtraction of a fitted 2nd order function. Based on the wavefront measurements, the relative positions between two mirrors were finely tuned while observing residual coma aberrations, as previously reported [2]. For the tuning, a relative angle between two mirrors (Figure S3(b)) was adjusted with microradian accuracy, resulting in gradual reduction of the coma aberration, corresponding to third-order functions in Figure S3(c). We confirmed the minimum condition of misalignments, and then, the mirrors were bonded to a Si substrate using an ultraviolet curing resin, as shown in Figure S3(d). The wavefront aberration after the bonding was as small as 1.1 rad (λ/6) in peak-to-valley (PV) and 0.37 rad (λ/17) in root-mean-square (rms) values, which did not exceed the Rayleigh’s rule (PV value < λ/4) and the Maréchal’s criterion (rms value < λ/14) [1].

3. Beamline BL29XU at SPring-8

A. Beamline parameters

All experiments were performed in a second experimental hutch (EH2) of the beamline BL29XU at SPring-8 [7]. The source is a SPring-8 standard in-vacuum undulator that has 32 mm magnetic period length and 140 period. A front-end (FE) slit is placed at 28.9 m from the source. The FE slit was opened to 1 × 1 mm² during our experiments. The X-ray beam from the undulator was monochromatized by a Si (111) double-crystal monochromator. The EH2 is located at 60.2 m from the source. In the EH2, the X-ray beam with a size of 0.8 V × 1.9 H mm² and a divergence of 12.5 (V) µrad × 32.2 (H) µrad is provided.

B. Photon flux in the experiment

We estimated the photon flux at the camera of 1 × 10¹³ photons/s at 15 keV with following parameters: incident flux of 4.5 × 10¹³ photons/s with Si(111) monochromator (beamline parameter), attenuator transmission of 0.5684 (calculated with Si thickness of 0.25 mm), diffuser transmission of 0.8882 (measured), slit transmission of 1.279 × 10⁻² (calculated with slit size of 70.96 × 273.98 µm²), mirror reflectivity of 0.454, and absorption due to remained 110-cm air path of 0.82684.

4. Experimental results

A. Absorption contrast in the obtained image

Figure S4(a) shows an image of the radial test pattern without enlargement, obtained at a photon energy of 15 keV. The change of resolution, which are described as the FoV in Sec. 1-B, were observed in the image especially in the vertical direction; the edge structures in the center region are sharper than those in upper region. Still, the rough structures were observed without a significant distortion in entire image size of approximately 15 × 15 µm². It was suggested that the FoVs were limited by the field curvatures.

Figure S4(b) shows a histogram of the image. Because the image of empty area on the Siemens star substrate was utilized for the flat-field correction, the line (space) structures had pixel values of approximately 1.0 (1.12). When we utilized image without the sample for the flat-field correction, the space structures had pixel values of 1.0. Using the peak values in the histogram, we calculated the averaged absorption contrast of the image, according to the formula \(\frac{I_{\text{max}} - I_{\text{min}}}{I_{\text{max}}}\). The calculated contrast was 10.33 % which was consistent with the theoretical absorption of tantalum 500 nm thickness of 10.23 %. Additionally, the same calculations in the images at 12 and 9 keV, shown in Figure 3(c) of the main text, returned the contrasts of 16.88 % and 9.51 % (cf. theoretical values of 17.12 % and 9.41 %), respectively.

The gray scale values in the X-ray images of the main text is listed in Table 1. The contrast values in Figure 4(b) of the main text were...
difficult to be determined, because the CT image was reconstructed from the individually normalized data sets, resulting in loss of the quantitative value.

Fig. S4. (a) X-ray image of the Siemens star without an enlargement. The image size is approximately 15 × 15 µm^2. (b) Histogram of (a).

| Table. S1. Gray scale values in figures of the main text. | Maximum value | Minimum value |
|---------------------------------------------------------|---------------|---------------|
| Figure 3(a)                                             | 0.92          | 1.20          |
| Figure 3(c) 15 keV                                      | 0.92          | 1.20          |
| Figure 3(c) 12 keV                                      | 0.85          | 1.40          |
| Figure 3(c) 9 keV                                       | 0.87          | 1.33          |
| Figure 4(a) left                                        | 0.164         | 0.183         |
| Figure 4(a) right                                       | 0.028         | 0.035         |

The images shown in Figure 3(c) of the main text, which were acquired with different photon energies of 15, 12, and 9 keV, were applied to the PSA. The Figure S5 shows the results. In this case, the profiles were averaged over 360 degree. The difference in profiles of 15, 12, and 9 keV at the spatial frequencies of from 8 to 13 lines/µm reflected the theoretical resolutions of the images.

B.  Power spectral analysis (PSA)

PSA is often used to estimate the smallest detectable features in the X-ray microscope [8, 9]. The PSA was performed as follows. The centered area of the image was multiplied by the Hanning window function. It was subjected to the Fourier transform, and then a power spectrum density (PSD) was calculated by a power of the Fourier transform divided by a 2-pixel spatial-frequency resolution, and averaged azimuthally. In Figure 3(b) of the main text, the horizontal profiles were given by the averages in range of -5-to-5 and 175-to-185 degrees. The vertical profiles were the averages in range of 85-to-95 and 265-to-275 degrees. The ratio profiles were given by the PSDs of the sample images divided by PSDs of empty images.

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