### BL38B1 (Structural Biology III)

BL38B1 at SPring-8 is a bending magnet beamline suitable for high throughput macromolecular crystallography (MX) data collection at a cryogenic temperature (CT) using crystals larger than 100 µm. The optics of this beamline consist of the SPring-8 standard Si(111) double crystal monochromator (DCM) and a vertically bent cylindrical mirror. The available energy range is 6-17 keV, and the photon flux is  $8.6 \times 10^{10}$  photons/s at 12.4 keV. In addition to CT data collection, room temperature (RT) data collection using the humid air and glue coating (HAG) method <sup>[1, 2]</sup> is available. We also developed an X-ray topography measurement system as a tool for qualifying protein crystals. In FY2017, we upgraded the beamline optics to increase both the photon flux and photon density by installing asymmetrically cut Si(111) crystals in DCM, a capillary lens, and a beam-defining aperture-insert system composed of a tantalum plate with various sized pinholes. Lightweight and compact  $\kappa$  and  $\varphi$ goniometers were also developed for accurate diffraction data collection <sup>[3]</sup>.

In FY2018, we implemented the following upgrades and developments.

#### 1. Installation of a pixel array detector

The detector was replaced with a pixel array detector (PAD), Pilatus3 6M (Fig. 1). Pilatus3 6M can read out images with a maximum frame rate of 100 frames/s, which is much faster than that of the charge-coupled device detector that required a reading time of 1-2 s/frame. With Pilstus3 6M, more efficient measurements are possible in combination with an increased photon flux and

photon density due to the upgraded beamline optics.



Fig. 1. Overview of the diffractometer in BL38B1.

## 2. Development of beamline optics using asymmetrically cut Si(111) crystals

After introducing the asymmetric crystal of 6.33° in DCM, the photon flux increased from  $8.45 \times 10^{10}$ photons/s (at 13.78 keV) to  $2.22 \times 10^{11}$  photons/s (at 13.78 keV). However, the available energy was restricted below 14.59 keV due to the incident angle limitation. Therefore, we installed new asymmetrically cut Si(111) crystals whose asymmetric arrangement is decreased to 4.40° to enable the use of energy above 14.59 keV. The available energy range is extended up to 16.98 keV. It also increases the photon flux to  $1.46 \times 10^{11}$ photons/s at 13.78 keV (Fig. 2).

Furthermore, a new crystal holder for the 1<sup>st</sup> crystal was developed. In the former holder, several parts had to be assembled prior to use, which deteriorated the reproducibility of crystal positioning in DCM. To fix the problem, all parts are made of bronze and integrated into one in the new holder (Fig. 3).



Fig. 2. Comparison of the photon flux of symmetric (blue), asymmetric 4.40° (red), and asymmetric 6.33° (green) cut crystals in DCM.



Fig. 3. Crystals and new first folder of integrated type for asymmetric 4.40° Si(111) first crystal installed in DCM at the optics hutch.

# **3.** Development of beam monitor for automated alignment system.

Previously, a coaxial camera was used to adjust the X-ray beam path onto the sample position by observing the beam from the upper stream of the sample (Fig. 4(a)). However, the coaxial camera cannot be used to align the beam collimated by the capillary lens and the Ta pinholes. The capillary lens exclusively shares the position with the coaxial camera and the pinholes plate (Fig. 4, magenta), blocking the view of the coaxial camera (Fig. 4(b)). Therefore, we developed a new small beam monitor,

which can observe the beam form downstream of the sample position (Fig. 5). In the future, we will develop an automatic alignment system of X-rays to measure the sample position using this beam monitor.



Fig. 4. Overview of the sample position layout. (a)
Sample mounting environment in the sample-alignment mode. (b) Inserted to the Ta pinholes plate (magenta) for beam-defining and capillary lens (cyan) for capillary-focusing mode.



Fig. 5. New compact beam monitor. Outside YAG phosphor is used to adjust the X-ray position from the coaxial camera. Inside YAG phosphor is used to adjust the Ta pinholes plate and capillary lens.

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#### **References:**

[1] S. Baba et al., Acta. Cryst. D 69, 1839-1849

(2013).

- [2] S. Baba et al., J. Appl. Cryst. 52, 699-705 (2019).
- [3] S. Baba et al., AIP Conf. Proc. 2054, 060008 (2019).