BL45XU
Structural Biology III

1. Introduction

BL45XU is a macromolecular crystallography (MX) beamline dedicated to providing an experimental environment suitable for high-throughput diffraction data collection using high-flux X-rays from synchrotron. BL45XU was recently reborn as a high-throughput automatic MX beamline. Previously, it was operated as a SAXS beamline.

2. Beamline optics

The design of the new BL45XU is based on the time-proven undulator MX beamlines BL41XU and BL32XU, which can produce micrometer-order high-flux beams devoted to data collection from low-diffractivity crystals, including micro-crystals [1,2]. In FY2019, the in-vacuum tandem vertical undulator and diamond double crystal monochromator were replaced with SPring-8 standards (Fig. 1). The available energy range is 6.5–16 keV. The beam size irradiated at the sample position can be varied from 5 μm (H) × 5 μm (V) to 50 μm (H) × 50 μm (V) with a photon flux of 5.70 × 10^{12} – 1.75 × 10^{13} photons/s at 12.4 keV by adjusting the aperture of the virtual source slit and glancing angles of the vertical and horizontal focusing mirrors [3] (Fig. 1 and Table 1).

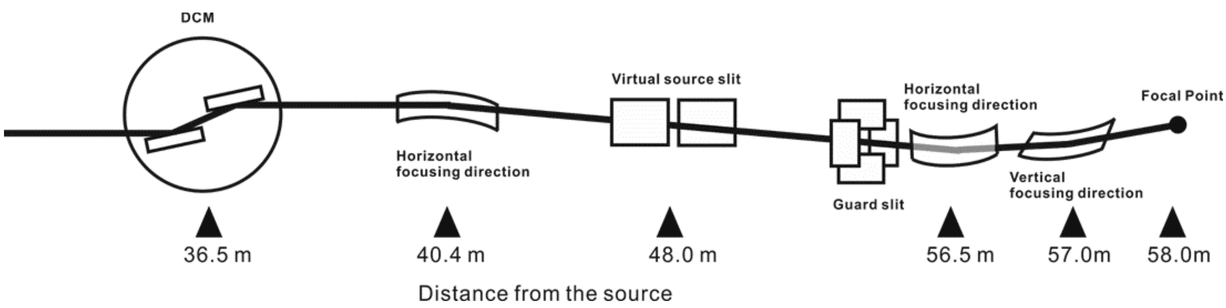
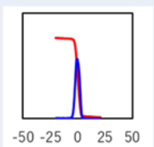
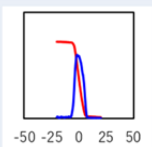
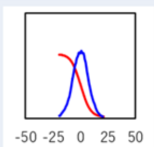
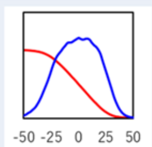


Fig. 1. Optics layout at BL45XU

Table 1. Photon flux and beam profile at the sample position

Beamsize @sample position (FWHM : H x V)	5 x 5	10 x 10	16 x 20	50 x 50
Photon flux (photons/sec)	5.70 x 10^{12}	1.03 x 10^{13}	1.73 x 10^{13}	1.75 x 10^{13}
Horizontal Beam profile (Blue) & Wire scan profile (Red) @sample position				

3. Automatic measurement system

To achieve fully automated data collection, a computer-controlled diffractometer and its supporting devices such as a high-speed sample changer SPACE-II [4] and a large-area pixel array detector were installed in the experimental hutch (Fig. 2). Device control for diffraction experiments, adjustment of the optics, beam size change, and beam position adjustment of the X-ray are all performed with the SPring-8 MX beamline control software BSS [5]. Moreover, the fully automated data collection system ZOO [6] is available at BL45XU, realizing unmanned collection of diffraction images while optimizing the absorbed dose in various experimental schemes such as the normal rotation, the multiple small-wedge, the helical and the SSROX schemes [7]. The measured diffraction images are automatically processed by the KAMO system [8]. Because these systems enable unattended automatic measurements, users can obtain diffraction data by sending crystals. This automatic measurement service at BL45XU began in late May 2019. From 2019A to 2019B, the number of users using automatic measurements has increased (Table 2).

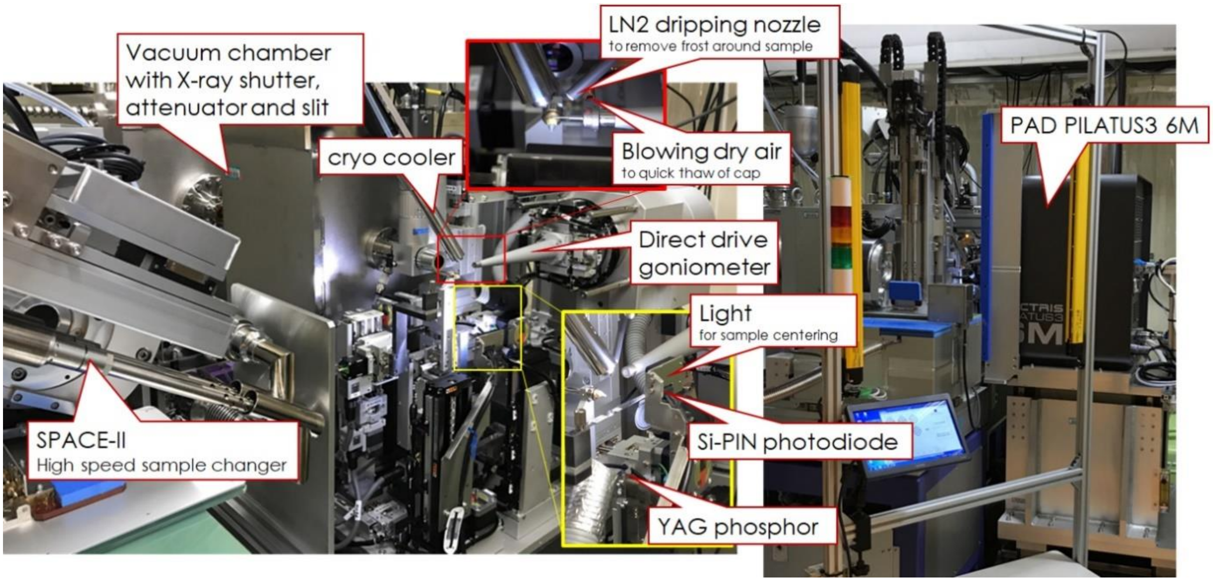


Fig. 2. Diffractometer components in the experimental hutch.

Table 2. Results of user time in BL45XU

Measurement type	2019A (shifts)	2019B (shifts)
Manual	84.0	51.5
Automatic	17.0	85.0

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