BL41XU
Structural Biology I

1. Introduction

BL41XU is a public macromolecular crystallography (MX) beamline using an undulator as a light source, and it has been contributing to various structural biology studies since it started operation in 1997. It provides two operation modes: the normal mode (NM) and high-energy mode (HM). NM is set up in experimental hutch 2 (EH2), and the X-ray energy range is 6.5–17.7 keV. It has been mainly used for the structural determination of challenging targets such as membrane proteins and macromolecular complexes using a high-flux beam of $2.3 \times 10^{12} – 1.1 \times 10^{13}$ (photons/s at 12.4 keV), which is one of the highest fluxes in MX beamlines in the world. The wide range of beam sizes from 5 × 5 μm to 20 μm (H) × 45 μm (V) enables data collection from microcrystals of a few micrometers as well as crystals larger than several hundred micrometers. On the other hand, HM allows data collection using high-energy X-rays from 20 keV to 35 keV in experimental hutch 1 (EH1). It is uncommon for an MX beamline to operate at such a high energy of X-rays. Therefore, HM provides unique opportunities, such as ultrahigh resolution data collection and the use of anomalous dispersion of atoms having absorption edges in this energy range.

After the start of operation of BL45XU in 2019, which has almost the same beam specification as BL41XU and specializes in the automatic data collection using the ZOO system [1], we decided to develop BL41XU so that it can also contribute to structural dynamics studies; i.e., time-resolved (TR) crystallography and room-temperature (RT) crystallography. However, the wide spread of COVID-19 in FY2020 limited users' access to SPring-8. Therefore, we partly supported automatic data collection. Moreover, a new remote access system was installed to cope with this difficult situation.

Here, we report our activities in FY2020.

2. Upgrade of diffractometer

The diffractometer for NM was upgraded to enlarge the space around the sample position so that the apparatus used for TR crystallography and RT data collection can be installed (Fig. 1). The major modifications are as follows: (1) the collimator stage was moved toward the goniometer, and the evacuation direction was changed from vertical to diagonally downward, (2) the evacuation direction of the beam stop was changed from vertical to

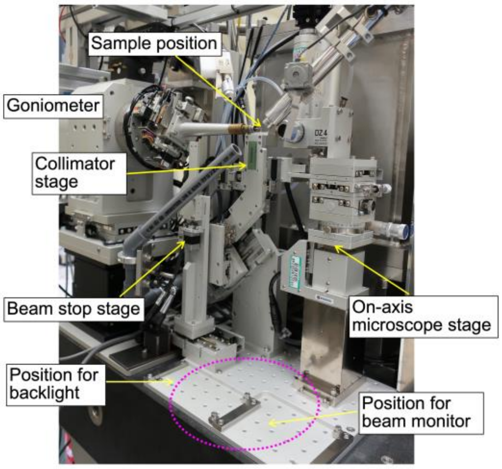

Fig. 1. Upgraded diffractometer for NM.
The dotted ellipse in magenta indicates the large space for the installation of various apparatuses. The backlight and beam monitor stages were removed to make this large space.

horizontal to prevent interference by the newly installed apparatus, (3) the stage of the on-axis microscope was modified to minimize its size, (4) the beam monitor and backlight stages were equipped with sliding bases, which can be easily detached from the diffractometer to enlarge the space beneath the sample.

3. Installation of excitation laser

A nanosecond tunable laser, NT230-30 (EKSPLA), was installed for use as a trigger light for TR crystallography (Fig. 2). It covers wavelength range of 210–2600 nm with a repetition of 30 Hz, a duration of 4 ns, and a pulse energy of 15 mJ at 500 nm. Since the laser is categorized as class 4, a safety interlock system was implemented in the experimental hutches, which immediately close the beam shutter located just in front of the emission port when safety condition is not fulfilled. It is going to be used in an injector-based serial crystallography (SX) experiment as well as fixed-target SX.

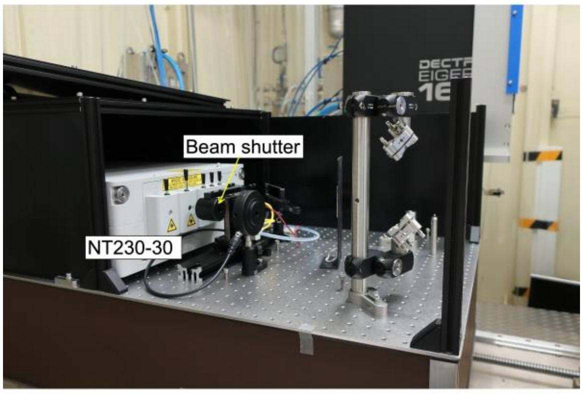

Fig. 2. Nanosecond tunable laser.

4. Installation of a new detector

A new detector, EIGER2 X CdTe 4M, has been installed as a detector for HM (Fig. 3). One of the problems in using high-energy X-rays in MX data collection had been the sensitivity of the detector because of the large transmission of high-energy X-rays. However, the appearance of a pixel array detector (PAD) equipped with a cadmium telluride (CdTe) sensor has solved this problem. The higher sensitivity as well as wide dynamic range of the detector is suitable for the ultrahigh resolution data collection using high-energy X-rays. Before the installation of EIGER2 X CdTe 4M, HM was operated using PILATUS3 X CdTe 1M borrowed from BL02B1 once every six months, which limits the availability of HM at BL41XU. We expect that the new detector could increase the users' utlization of HM.

Fig. 3. EIGER2 X CdTe 4M installed in experimental hutch1.

5. New remote access system

A new remote access data collection system using a remote desktop has been installed for NM with support from JASRI Information-technology Promotion Division. The original remote access system required the installation of designated client software (*SP8Remote*) in users' PC, which had the advantage that it could limit what users can do remotely [2]. However, it had the drawback that we had to modify the software whenever the on-site data collection software *BSS* [3] was updated. It also prohibited the use of other types of software such as automatic data processing software *SHIKA* [4]. In the new remote system, users can conduct experiments in an environment similar to that on-site by using the remote desktop software *NoMachine* (https://www.nomachine.com). Moreover, the safety at the beamline is kept at similar levels as before, because remote connection is established via the Remote Experimental Interlock Unit as with the previous system, which prohibits operations when a hutch door is opened. The new remote system offers users an alternative access to SPring-8 in addition to the automatic data collection.

Kazuya Hasegawa*1, Hironori Murakami*1, Takuya Masunaga*1, Tomoki Fukui*2, Seiki Baba*1, Nobuhiro Mizuno*1, Hideo Okumura*1, Yuki Nakamura*1, Takashi Kawamura*1, and Takashi Kumasaka*1

*1 Protein Crystal Analysis Division, JASRI
*2 Engineering Support Group, JASRI

References:

[1] Hirata, K. Yamashita, K. Ueno, G. Kawano, Y. Hasegawa, K. Kumasaka, T. & Yamamoto, M. (2019). *Acta Cryst*. D**75**, 138–150.

[2] Ueno, G. Hikima, T. Yamashita, K. Hirata, K. Hasegawa, K. Murakami, H. Furukawa, Y. Mizuno, N. Kumasaka, T. & Yamamoto, M. (2016). *AIP Conference Proceedings* **1741**, 050021.

[3] Ueno, G. Kanda, H. Kumasaka, T. & Yamamoto, M. (2005). *J Synchrotron Radiat*. **12**, 380–384.

[4] Yamashita, K. Hirata, K. & Yamamoto, M. (2018). *Acta Cryst*. D**74**, 441–449.