

## BL41XU Structural Biology I

### 1. Introduction

BL41XU, which uses an undulator as a light source, is dedicated to public macromolecular crystallography (MX). To meet a wide range of needs in structural biology research, the beamline offers two operation modes: the normal mode (NM) and the high-energy mode (HM).

NM can perform experiments using an X-ray energy range of 6.5–17.7 keV in experimental hutch 2 (EH2). NM is 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-flux in MX beamlines in the world. Since the beam size can be changed from  $5 \mu\text{m}$  (H)  $\times$   $5 \mu\text{m}$  (V) to  $20 \mu\text{m}$  (H)  $\times$   $45 \mu\text{m}$  (V), it can handle various samples with sizes ranging from a few micrometers to several hundred micrometers.

HM allows for data collection using high-energy X-rays from 20 keV to 35 keV in experimental hutch 1 (EH1). Here, we report our activities in FY2019.

### 2. Installation of sample changer SPACE for HM

NM can exchange samples in 16 s using the sample changer SPACE-II<sup>[1]</sup>. However, samples had to be manually changed at HM, which led to experimental inefficiency. Moreover, since the sample preparation table is located downstream of EH2, the manual sample exchange requires a 10-m walk, which causes further inefficiency. To address this, a conventional SPACE system was installed at HM (Fig. 1). Although it takes 1 min to exchange

samples and accommodates a maximum of four Uni-Pucks, which corresponds to 64 samples, the throughput and capacity of SPACE are sufficient for ultrahigh-resolution data collection, which is the main purpose of HM. Liquid nitrogen is automatically supplied to SPACE from a 100-L liquid-nitrogen tank, which allows for successive operations for three days. Since 2019B, SPACE has been available to users.

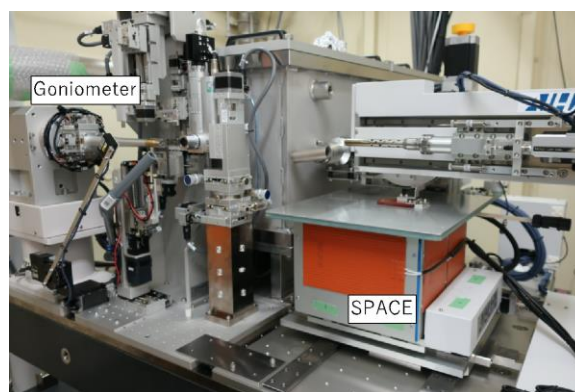


Fig. 1 SPACE for HE.

### 3. Development of a new sample viewing system

The sample viewing system for positional alignment was upgraded. Previously, microscope images were captured and displayed on a PC display using software, videosrv. However, videosrv is not compatible with the latest digital camera because it can only accommodate analog CCD or CMOS cameras, which are now obsolete. Therefore, videosrv was upgraded using the OpenCV library, and GigE digital cameras were installed for both HM and NM. In addition, an application was developed to set up the digital camera, tune white balance, etc. The new software was designed to have a high variability so that it can accept any kind

of digital camera with a USB, GigE, or Camera Link interface. This new viewing system will also be installed on the other MX beamlines.

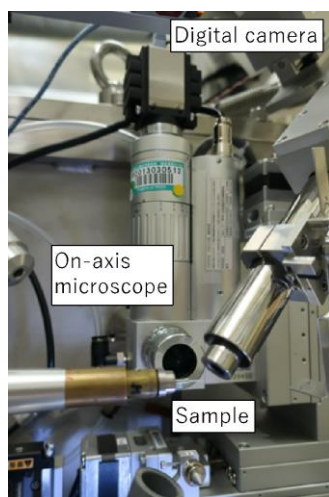


Fig. 2. Newly installed digital CMOS camera.

#### 4. Upgrade of data collection software BSS

All MX beamlines at SPring-8 use software, BSS, for data collection. To adapt to different hardware installed at various beamlines (e.g., detector), the source codes of BSS are becoming large. Currently, BSS has more than 100,000 lines of code. This large source code written in C programming language deteriorates the maintainability and scalability, making it difficult to add new functionality.

To improve the situation, the source code was rewritten in the C++ programming language, which enables object-oriented style coding. This upgrade also allows the latest open source libraries such as ZeroMQ to be used, which not only enables robust inter-process communication but also enhances the stability of BSS. Another upgrade to decouple the GUI from the main part of BSS is currently underway in an effort to further improve the scalability.

#### 5. Miscellaneous

Software to control the temperature of the cryo-stream system on the data collection PC was developed. When helium gas is used for sample cooling, the temperature of cryo gas is frequently changed because it must be warmed up at 100 K prior to sample exchange to avoid freezing of the liquid nitrogen. The new software has a web-based GUI (Fig. 3), which makes it easy to change the temperature. It also records the temperature in a log file, allowing the temperature to be traced during an operation.

For future increases in data, a 25-Gbps high-speed network that connects the beamline to the storage room was implemented.



Fig. 3. GUI for the cryo-stream control software.

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#### Reference:

- [1] Murakami et al., (2020). *Acta Cryst.*, **D76**, 155–165.