BL26B1
RIKEN Structural Genomics I

1. Introduction

RIKEN Structural Genomics Beamline I consists of SPring-8 standard bending magnet beamline components and an end station dedicated to high-throughput protein crystallography [1]. Diffraction data can be automatically collected from a vast amount of cryo-cooled protein crystals with the auto-sample exchanger SPACE and the user interface BSS [2,3]. Asymmetric diffraction crystals (asymmetric angle of 4.4°) for the double-crystal monochromator are adopted, and the capillary focusing lens (Hamamatsu J12432) upstream of the sample is optionally available by switching the configuration on the user interface program [4]. Also, optional devices for room-temperature crystallography are provided at the end station. The temperature-controllable humid air and glue coating mounting method (HAG) system [5] can control the temperature and relative humidity of the sample environment in the ranges from 2 to 20 °C and from 40 to 100%, respectively. The crystallization plate scanner, plate stocker, and exchanger apparatuses with a dedicated interface program for users to rapidly exchange and address a position in an SBS 96-well crystallization plate are also installed [6]. Eighty percent of the total beam time is assigned to public users and ten percent each is assigned to the Basis for Supporting Innovative Drug Discovery and Life Science Research by AMED (BINDS) project and RIKEN users.

2. Recent activities

For the HAG system, continuous developments to cover higher temperatures ranging from 20 to 70 °C have been conducted (Fig. 1). The new device is equipped with improved sheath gas piping with an insulation layer to avoid condensation caused by high-temperature humid gas. Moreover, the humid air generation system has been upgraded by replacing the bubbling humidifier with a spray humidification system. The relative humidity of around 98% at the sample has been achieved at 70 °C. By the end of the fiscal year, commissioning with a user group had started. Applications to studies of the structural dynamics of macromolecules derived from, for example, thermophilic bacteria, are expected.

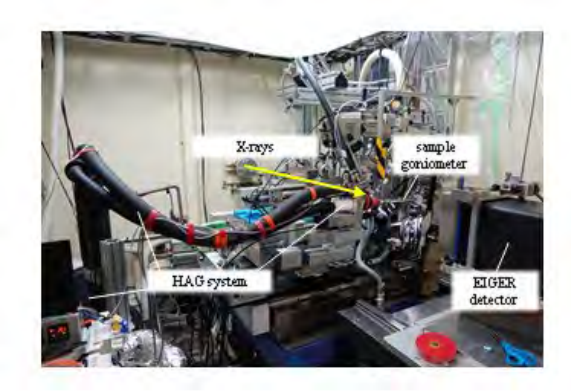

Fig. 1. Instruments for high-temperature HAG system installed at BL26B1 end station.

For the plate scanner system, research and development for further convenient and efficient use, such as the development of a new crystallization plate specialized for *in situ* data collection and automation of data collection with software upgrades, have been conducted. The

online device control software has been improved to import the predetermined positions of crystals in the plate, which are stored in an offline sample observation system. The positions of crystals are converted to goniometer coordinates at the beamline using reference points on each plate visualized with digital microscope images (Fig. 2). The coordinates are used to align crystals with an X-ray beam. In the current system, the positional error of crystals was within 100 μm. To ensure further precision and efficiency, the development of an automatic digital image processing system is in progress.

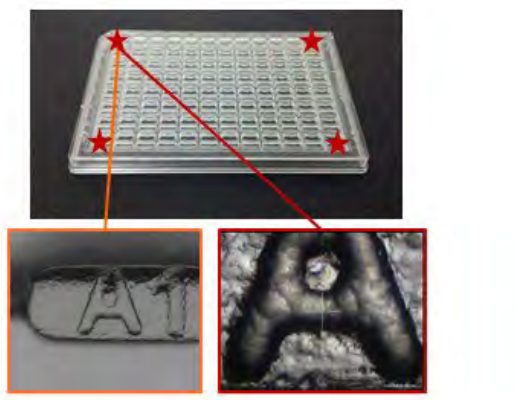

Fig. 2. Digital images of reference points on a crystallization plate. Plate orientation and position are corrected and converted between off-line and on-line observation systems using these coordinates.

UENO Go[*1] and OKUMURA Hideo[*1,*2]

[*1]SR Life Science Instrumentation Team, Life Science Research Infrastructure Group, Advanced Photon Technology Division, RIKEN SPring-8 Center

[*2]Experimental Instrumentation Team, Structural Biology Division, JASRI

References:

[1] Ueno, G. et al. (2006). *J. Struct. Funct. Genomics* **7**, 15–22.

[2] Murakami, H. et al. (2012). *J. Appl. Crystallogr.* **45**, 234–238.

[3] Ueno, G. et al. (2005). *J. Synchrotron Radiat.* **12**, 380–384.

[4] Baba, S. et al. (2019). *AIP Conf. Proc.* **2054**, 060008.

[5] Baba, S. et al. (2019). *J. Appl. Crystallogr.* **52**, 699–705.

[6] Okumura, H. et al. (2022). *Acta Crystallogr., Sect. F: Struct. Biol. Cryst. Commun.* **78**, 242–252.