Mail-in Data Collection and Beamline Automation at SPring-8 Structural Biology Beamlines

The structural genomics projects progressing worldwide, including Protein 3000 project by MEXT of Japan, are aiming at accumulating the information on a significant number of three-dimensional protein structures and functions based on genetic sequencing analyses [1]. Such cyclopedic projects are supposed to drive the biological research to associate protein structures with their functions. Furthermore, those efforts are anticipated to originate new approaches to drug discovery based on genomics. In order to deal with a vast variety of protein crystals in the structural genomics project, development of a high-throughput beamline for protein crystallography was indispensable. RIKEN Structural Genomics Beamlines I & II (**BL26B1** & **BL26B2**) [2] have been constructed to address the requirement of rapid diffraction data collection for numbers of protein crystals. The demand of the more efficient use of the beam-time led to technical development of a beamline automation system.

The schematic diagram of device and control system of the RIKEN Structural Genomics Beamlines is shown in Fig. 1(a). The light source and optics adopted are the standard design for bending magnet beamlines at SPring-8 [3]. The beamline accommodates MAD (Multi-wavelength Anomalous Diffraction) experiments with heavy atoms typically used for protein structure determination. Equipments in the end station are designed for users to conduct the automatic operation without entering the experimental hutch. A sample auto-changer robot SPACE (SPring-8 Precise Automatic Cryo-sample Exchanger) [4] is installed to automate the sample handling procedure without human error. A goniometer head can be positioned by a remote translation stage for sample centering. Other devices are also mounted on the remote-controllable alignment stages, including two types of area detectors; a mosaic CCD (Charged Coupled Device) and a large IP (Imaging Plate), which are remotely switchable.

The control system of the beamline was developed based on the client and server architecture, on which each device is controlled by distributed server program. BSS (Beamline Scheduling Software) [5] is a graphical user interface (GUI) controlling entire beamline *via* the network. The BSS provides the whole utilities for users to operate the beamline, such as exchanging samples, collecting diffraction images, XAFS (X-ray Absorption Fine Structure) measurement, and so on. In particular, the most outstanding feature of the BSS is the scheduling function of successive data collections for multiple sample crystals, which makes the unattended beamline operation possible for a long term (Fig. 1(b)).

The SPACE handles the specially designed sample pin and tray, originally developed at SPring-8 (Fig. 2). The sample pin is equipped with screw threads to be attached to the goniometer, which ensures the high positional reproducibility (< 10μm) of protein crystals. Once the first centering is manually done at the beamline, the centering can be automatically reproduced on the second mounting, or later. This is the most outstanding feature of the SPACE, which makes the unattended beamline operation possible over a long period of time.

Samples and data management system covering laboratory and beamline, i.e. mail-in system, is supported by a networked database D-Cha (Database for Crystallography with Home-lab. Arrangement) (Fig. 3). The D-Cha manages the massive sample information by tray identification number, and provides the GUI to edit the experimental schedule of each tray *via* a web browser. Prior to experiments, users send sample trays to beamline with dry shipper *via* home delivery service. The individual crystal information and experimental schedule are uploaded to D-Cha from users laboratory. At the beamline, the experimental schedule is extracted from D-Cha, and registered to BSS. The SPACE installed at the

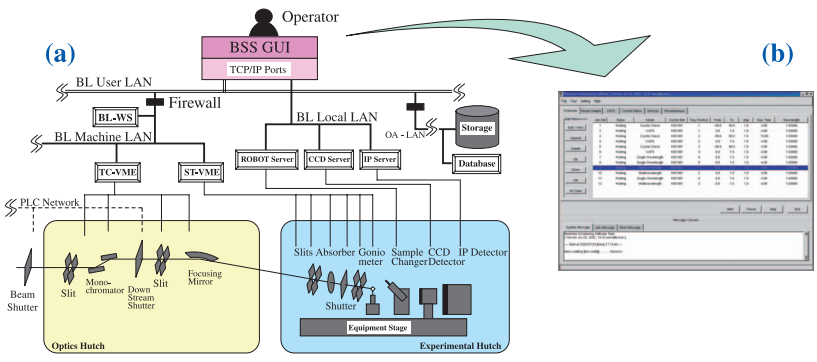

Fig. 1. **(a)** Schematic diagram of device and control system of RIKEN Structural Genomics Beamlines. **(b)** BSS main window. Schedule list of successive data collection is shown.

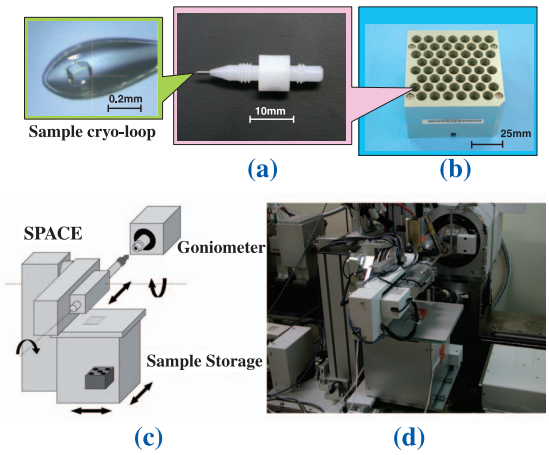

Fig. 2. **(a)** Sample pin. **(b)** Sample tray. A tray can store fifty-one samples at once. **(c)** Schematic view and **(d)** photograph of SPACE.

beamline sequentially changes the crystals according to the experimental schedule. The acquired data is uploaded to D-Cha, and the diffraction images can be browsed or downloaded by users *via* the Internet. Users need not to visit the beamline to obtain the diffraction data.

At the beamline, all crystals in the tray are successively mounted on the gonoimeter to collect the screening data, which is used to evaluate the crystal quality. Beamline operators assure the centering of each crystal at first. The diffraction data and the record of the goniometer translation are registered to D-Cha. Since the screening data for a crystal can be obtained within ten minutes, the screening experiment for a sample tray finishes within daytime. Users qualify the crystals referring diffraction image browser of D-Cha, and make the data collection schedule for selected crystals. By following the screening process, users can definitely select the best crystal to collect the data set, and also can make an efficient experimental schedule. A full-automatic overnight data collection is conducted according to the registered schedule. Samples are automatically mounted and centered utilizing the record of the goniometer translation, taking advantage of the screw-type sample pin with SPACE.

BL26B2 has been continuously operated with the automation system since 2003. In 2006, more than twenty-five crystals a day have been constantly delivered and screened, and eight data sets in daily average have been constantly collected. Examples of newly determined three-dimensional protein structures based on diffraction data collected at BL26B2 are shown in Fig. 4. Presently, technical developments such as BSS and SPACE are similarly implemented to other structural biology beamlines at SPring-8, providing users a common look and feel at all beamlines.

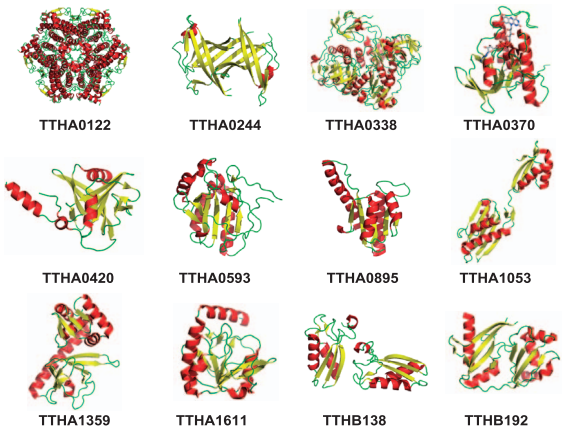

Fig. 4. Protein structures newly determined by diffraction data collected at BL26B2, SPring-8. All structures have been deposited into PDB. Provided by Akio Ebihara and Seiki Kuramitsu at SR System Biology Research Group, RIKEN SPring-8 Center.

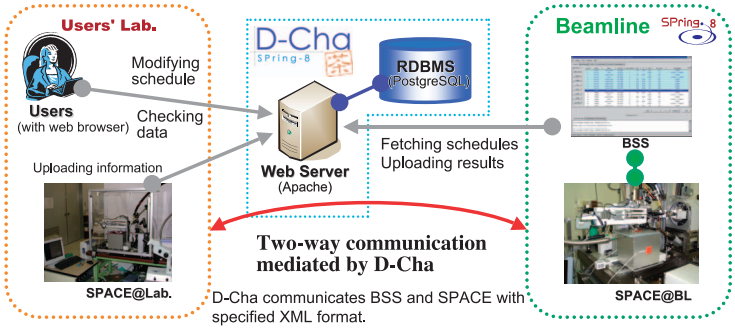

Fig. 3. Networked database D-Cha developed for mail-in data collection at SPring-8.

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