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Beamline Automation of RIKEN Structural Genomics Beamlines

Koh Ida, Masaki Yamamoto*, Takashi Kumasaka, Go Ueno, Hiroyuki Kanda
Masashi Miyano & Tetsuya Ishikawa
RIKEN Harima Institute, 1-1-1, Kouto, Mikazuki, Sayo, Hyogo, 679-5148, Japan

RIKEN Structural Genomics Beamlines have been constructed for the crystallographic analysis in the structural genomics research at synchrotron radiation facility SPring-8. Synchrotron radiation accelerates the crystallographic analysis of protein structure. The target of the research and development is focused on the automatic beamline operation to maximize beamline efficiency. We are developing the sample management system, which is composed of the sample auto-changer and the database system, for high-throughput data collection. The sample management system and the beamline operating system make it possible to execute automatic data collection without any operators. The beamlines will be ready for user operation in autumn 2002. The concept of automatic beamline operation and the present status of RIKEN Structural Genomics Beamlines will be presented.

Keywords : beamline automation, SPring-8, structural genomics, synchrotron radiation

INTRODUCTION

Recent many whole genomic DNA sequencing projects such as the Human Genome Project are producing a vast amount of the genetic codes, which control the wide variety of biological systems. In order to elucidate the nature of biological systems, detailed knowledge of the relationship between the genetic information and the structure/function of each protein is necessary. The function is tightly related to its three-dimensional structure. A main goal of Structural genomics study is to accumulate the 3D-structure of many proteins to elucidate protein function. Protein crystallography is an advantageous technique for studying the three-dimensional structure of biological macromolecule, and synchrotron radiation has been becoming the indispensable in it.

SPring-8 BL26B1& B2 were assigned to RIKEN Structural Genomics Beamline I & II. The function of RIKEN Structural Genomics Beamline is the high throughput data collection for a huge amount of protein crystals. The new concept and design for a simple and high efficient operation was developed. In the future, the beamlines put the routine analysis of macromolecular crystallography into a view.

*To whom correspondence should be addressed.
E-mail : yamamoto@postman.riken.go.jp

BEAMLINE DESIGN

The two Structural Genomics Beamlines have the identical beamline design from the source point to the end station (Figure 1). The SPring-8 standard optics design for the bending magnet was adopted for simple and easy operation. The beamline optics with a fix-exit Si double crystal monochromator followed by a two dimensional focusing-mirror can facilitate MAD (Multiple-wavelength anomalous diffraction) experiment with high-flux monochromatic X-rays.

The experimental station sets the high-efficient diffractometer with κ-goniostat that makes it possible to align the optimum crystal orientation for time-effective data collection. The sample auto-changer is mounted on the opposite position to κ-goniostat. Two different types of detectors, a mosaic CCD detector (RIGAKU/MSC Jupiter210) and a large-IP detector (RIGAKU RAXIS-V) [1] are installed to cope with a wide variety of the unit-cell and the intensity of samples. All axes of diffractometer and a high-speed shutter are controlled by the SPring-8 standard control system.

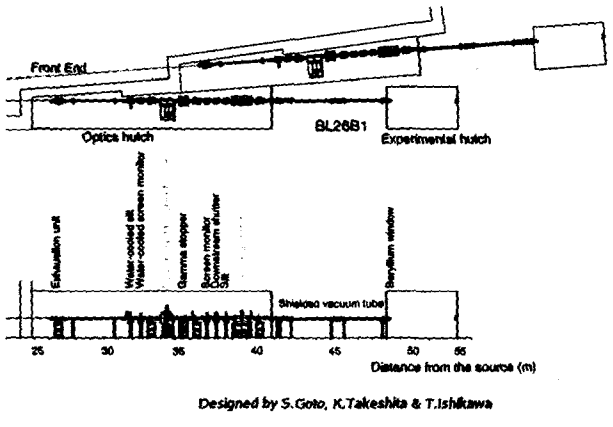

Figure 1. Schematic drawing of Bl26B1&B2

OPERATING SCHEDULE OF THE BEAMLINE

The high throughput data collection is realized to increase the speed of data collection and avoid the waste of beam time for inadequate data. The beamlines are operated with the fixed schedule (Figure 2), which is separated into the sample inspection and the automatic data collection. All samples, which are mounted on a sample tray and identified by the unique sample ID number, are brought into the beamline. The inspection of all samples is interactively executed by using the sample management system during the office hours. The all inspection data will be stored into the on-line database under the sample ID.

The final order of the over night data collection will be fixed base on the inspection data in the on-line database by the scientist. The final order is instructed with the measurement conditions (wavelength, oscillation range and camera distance etc.) of each sample, and the beamline operating system will automatically translate the order into the action of data collection. The automatic data collections compose of sample changing, auto-centering, and tuning of the beamline and automatic data collection.

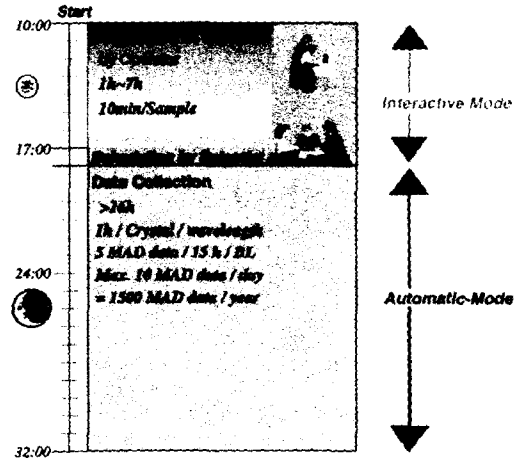

Figure 2. Time table of the beamline

SAMPLE AUTO-CHANGER AND SAMPLE MANAGEMENT SYSTEM

The sample management system is introduced to manage a huge number of samples and automatic data collection. A sample auto-changer (Figure 3) is the main component of the sample management system. The sample auto-changer has the simple design for the special pin, which has the turnbuckle like structure for simple operation. The sample pin has right and left handed screws at both ends and can be mounted or dismounted on the goniostat by simple rotation. During sample exchanging, the sample crystal is kept inside the screw hole of the changer at liquid nitrogen temperature. The sample auto-changer mounts the sample crystal from the sample tray to the gonistat according to the sample ID. The sample tray of this system can store 52 cryo samples, and has individual tray ID. An operator just once sets the sample tray at the start of the experiment and never touches the sample directly.

The auto-mounted sample is roughly located at the center position by a newly developed auto-centering system. After that, the operator does the precise centering of crystal by remote control system with a microscope (field of view 0.5 X 0.5 mm) coaxial with direct beam and XYZ stage on the goniostat. After centering, the beamline operating system starts to collect diffraction image for the crystal sample inspection. For a MAD sample, the system also manages an automatic-measurement of XANES (X-ray Absorption Near Edge Structure).

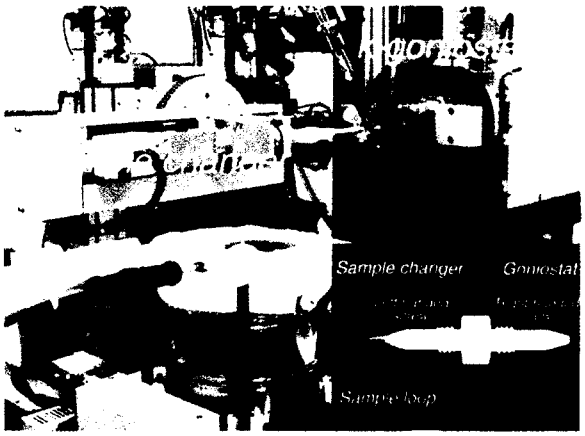

Figure 3. Sample changer & sample pin

PRSENT STATUS THE BEAMLINE

The RIKEN high throughput beamline project for the structural genomics research was started at the end of 2000. The construction was started in August 2001, and had been progressed satisfactorily by the end of March 2002. The commissioning of the beamline with synchrotron radiation has been started from April 2002. Now the tuning of the beamline optics and the experimental station are in progress.

ACKNOWLEDGMENT

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REFERENCES

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