

# Structural Biology I (BL41XU)

## 1. Introduction

The beamline for structural biology at the station BL41XU has been open for public use from October 1997. This beamline has the following two goals:

- \* To realize routine analyses of macromolecular crystallography by the MIR-OAS method, which is the heavy atom multiple isomorphous replacement (MIR) method combined with the optimized anomalous scattering effect (OAS) for heavy atom derivatives.
- \* To expand the applicable range of macromolecular crystallography in molecular weight and crystal size by taking advantage of the high brilliance characteristics of the beamline.

## 2. Beamline

The light source of the Bio-Crystallography beamline is an in-vacuum-type undulator [1]. X-rays from the undulator are led to the monochromator after reducing unnecessary heat loads by the front end elements. X-rays are monochromatized with a rotated-inclined double crystal monochromator [2] using Si(111) crystals. Two mirrors are utilized in a Kirkpatrick-Baez configuration to focus the X-ray on the sample position. Detailed specifications of each component are summarized in tables at the end of this paper and reference [3].

All of the components in the beamline (undulator, slit at front end, monochromator, slits at transport channel and mirrors) are fully controlled by computer. A program for controlling them and a database for tuning energy and tracking beam-position are completely equipped. By just inputting X-ray energy, this program can arrange all components automatically to their optimal positions in several minutes.

In 1999, major changes in this beamline are: (i) the current of the storage ring increased to 100 mA. (ii) the design of the "pin-post" structure for monochromatizing the 1st silicon crystal was changed, in order to decrease the deformation of its surface flatness by water-flow. Therefore, the photon flux at the sample position was increased about double what it was before. The overall characteristics of the X-ray are summarized in a table at the end of this paper.

## 3. Experimental Station

The goniometer has been changed to a horizontally aligned partial  $\chi$ -circle type. This goniometer has a partial  $\chi$ -circle (0 - 30 deg.) and a  $\phi$ -axis ( $\pm 180$  deg.) for rearrangement of crystal orientation on the rotation  $\omega$ -axis ( $\pm 178$  deg.). The monitoring system for the sample was changed from an optical microscope to a CCD video-camera. This new system

has sufficient magnification (about  $\times 300$  on 15' monitor), and so very small crystals less than 100 microns can be centered against the goniometer easily.

A CCD X-ray detector (marCCD165, marresearch) was newly installed in the experimental hut. This detector has a phosphor screen of 165 mm diameter as its active area. The readout time for one frame is 3.5 sec., and the turnover time for one frame is about 15 sec. Using this CCD X-ray detector, the total time for full data collection is greatly reduced compared to that using an imaging plate detector. Other detectors (RIGAKU R-AXIS IV, flat-type large imaging plate cassette and automated Weissenberg camera) are also available.

## References

- [1] H. Kitamura, SPring-8 Annual Report 1994 (1994) 47.
- [2] T. Ishikawa, SPring-8 Annual Report 1996 (1996) 30.
- [3] SPring-8 Annual Report 1998 (1998) 71.

Light Source	
Type	In-vacuum
Undulator period	32 mm
Number of periods	140
Tunable range	> 6.5 keV
Peak brilliance	$2 \times 10^{19}$ photons/s/mrad <sup>2</sup> /mm <sup>2</sup> /0.1% b.w.
Total power	5 kW
Power density	300 kW / mrad <sup>2</sup>

X-rays at Sample	
Energy range	6.5-17.5, 19-37.5 keV
Energy resolution	$\Delta E/E \approx 2 \times 10^{-4}$ ( $\Delta E/E \approx 10^{-3}$ over 20 keV)
Photon flux	$5 \times 10^{12}$ ph/s
Beam divergence	$\approx 0.1$ mrad
Beam size	H 0.2 mm $\times$ V 0.3 mm

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Facilities in Experimental Station

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- Horizontal aligned goniometer
 

$\chi$ - axis	0 - 30 deg.
$\phi$ - axis	$\pm 180$ deg.
$\omega$ - axis	$\pm 178$ deg.
Accessories	Scintillation Counter Non-LN <sub>2</sub> type cryostream CCD video camera & LCD monitor
- CCD X-ray detector (marCCD165)
 

Adjustable distance	120 - 500 mm
Detective area	165 mm $\phi$
- On-line imaging plate detector (rigakuRAXIS IV)
 

Adjustable distance	260 - 780 mm
Detective area	300 $\times$ 300 mm <sup>2</sup>
- Automated Weissenberg camera
 

Adjustable distance	260 - 1500 mm
Detective area	400 $\times$ 500 mm <sup>2</sup>
- Flat-type large imaging plate cassette
 

Adjustable distance	260 - 1130 mm
Detective area	800 $\times$ 800 mm <sup>2</sup>