# Present Status of RIKEN Beamline II for Structural Biology (BL44B2)

Shin-ichi ADACHI, Takuyo OGUCHI, and Tatzuo UEKI

RIKEN Structural Biology Group
SPring-8, Kamigori, Ako-gun, Hyogo 678-12, Japan

## 1. Summary

This beamline is dedicated to macromolecular crystallography in white (Laue) and monochromatic X-ray mode, and XAFS of diluted biological systems. White X-rays from the standard "B2" type bending magnet are focused with a 1m-long platinum-coated bent-cylinder mirror (white X-ray mode), or monochromatized with a fixed-exit double crystal monochromator (DXM) then focused with the same mirror (monochromatic X-ray mode). The first crystal of the DXM is moved in or out depending on the experimental mode. The grancing angle (2-5mrad), the radius of curvature (3000-7000m), and the vertical position (±15mm) of the mirror are adjusted for the optimum focusing at the sample position. The photon ux at the sample position ($1 \times 1mm^2$) is estimated to be $10^{15}$photons/sec (7-30 keV, white mode), and $10^{12}$photons/sec in 0.1% b.w. (@20 keV, monochromatic mode). The white X-ray mode is suitable for time-resolved Laue crystallography, and a typical exposure time using an Imaging Plate detector is likely to be 100 microseconds. XAFS experiments and routine macromolecular crystallography are performed with monochromatic X-rays, and the energy resolution ($\Delta$/E) is in the order of $10^{-4}$. XAFS experiments in fluorescence and transmission mode are feasible in the energy range of 6-30 keV.

The construction of hutches for the optics and experiments will be finished by March 1997. Installation of the front end, optics, beamline interlock and controll systems, and other experimental equipment are planned to be completed in the near future. Hopefully, we will be able to start the user run at BL44B2 from April 1998. This beamline is supposed to be used mainly by RIKEN users, while it is also planned that some part of beamtime is used by general users.

## 2. Light Source

The light source of BL44B2 is a standard bending magnet, at which magnetic field of 0.679T, total power of 0.15kW, power density of 1.5kW/mrad, and horizontal acceptance of 1.5 mrad. The peak brilliance is $3\times10^{15}$photons/sec/mm$^2$/mrad$^2$ in 0.1%b.w: at 28.9keV, which corresponds to the criticalwavelength of 0.429 A.

## 3. Front End

The front end of BL44B2 will be the SPring-8 standard type for a bending magnet beamline. Front end components consist of a fixed mask, a heat absorber, graphite filters, variable slits, Be windows, beam position monitors, a beam shutter, and pumping units.

## 4. Optics

A double crystal monochromator (DCM) is the first optical element of our beamline, which is located at 27.8 m from the source. When we use white X-rays for time-resolved experiments, the first crystal of the DCM is moved out from the light path and the white X-rays go through the DCM, then are focused by the second optical element, the toroidal mirror. The DCM is used for check of sample crystals before time-resolved experiment, for a monochromatic data collection of routine protein crystallography, and for a multi-wavelength anomalous diffraction (MAD) experiment. The energy resolution ($\Delta$E/E) will be in the order of $10^{-4}$, which gives enough energy resolution even for MAD experiments. The photon flux at the sample position is estimated to be $10^{12}$ photons/sec in 0.1%b.w. at 20 keV. The heat-load on the first crystal of the monochromator is expected to be about 0:1W/mm$^2$, and the heat load can be removed by indirect cooling with water.

A 1m-long toroidal mirror is the second optics for both horizontal and vertical beam focusing. The toroidal shape is obtained by vertical bending of a cylinder which makes it possible to vary demagnification factor M over the range 0.2 - 1.0. A typical demagni cation factor M is 0.46 and the grancing angle is 3.0 mrad. The mirror is coated by a layer of platinum with a surface roughness of 5 Årms. The longitudal gure error of the mirror is 9.0 µrad (rms) over the full lenghth. The size of the focal point is a competition between spherical aberrations and mirror inperfections, and the focal size at the sample position is estimated to be 0.3mm(H) 0.2mm (V) in FWHM. The cutoff energy is 30 keV, and the integrated photon ux at the sample position is $10^{15}$photons/sec (7-30 keV). A typical exposure time with an Imaging Plate detector is likely to be 100 microseconds per one image. The center of the mirror is located 32.3 m from the source point, and indirect cooling of the edge of the mirror with water will be applied.

## 5. Experimental Stations

*5-1 Diraction Station*

An oscillation camera with on-line Imaging Plate (IP) detector and one-axis goniometer is installed. The detector is at, and the size of the IP is 300 x 300 $mm^2$. Four IP's are installed in the detector, with which exposure and read-out can be repeated automatically. Although the total read-out time for one IP is about 4 minutes at the moment, the time will be shortened to be 2 minutes. The crystal-to-IP distance can be adjusted from 70 to 400 mm. Adjustable helium path between the crystal and IP can be used to aviod air scattering. A diraction pattern is read out as pixel data, the size of the pixel being 0.1mm  0.1mm or 0.05mm  0.05mm.

A cryostat using gas from liquid nitrogen and dry air can be used to contrtol the temperature of sample. The range of temperature control is 80-375K, and stability of the control is ±0.1K.

A pulse Nd:YAG laser and a YAG-pumped dye laser is used for initiation of relatively fast reaction. The pulse width of the laser is 8 nanosecond, and the maximum power of the 2nd (532nm) and 3rd (355nm) harmonics of the YAG laser is 700mJ and 400mJ, respectively. The wavelength of the laser is tunable by using the YAG-pumped dye laser, and the laser power varies from 20 to 150 mJ depending on the dye used. A Xe ashlamp is also useful to initiate relatively slow reaction like a cleavage of caged compounds. We are planning to install a Xe ashlamp, of which pulse width of 0.1 millisecond, total power of 300J and repetetion rate of 1Hz.

A flow-cell is also planed to use to control and change the pH and the concentration of the ionic species, or soak the substrate in the solution around the crystal.

An on-line microspectrophotometer with UV and visible wavelength region will be installed to monitor reactions in sample. A photomultiplier or a multi- senser head with an image intensier will be utilized to monitor time- dependent spectral changes during reaction. XAFS measurement equipment is used to select suitable X-ray wavelength to observe largest effects of anomalous scattering. The experimental station will be air-conditioned.

*5-2 XAFS Station*

In the XAFS Station, XAFS experiment of diluted biological systems which contain metal atoms can be performed. XAFS experiments in fluorescence and transmission mode are feasible in the energy range of 6-30 keV. Ge 19-element solid state detector and gas ow type ion chamber are planned to be used as detectors.

## 6. Items in Preparation Rooms

The following items are planned to be installed in the preparation rooms (Lab-M and Lab-S).

- O-line microspectrophotometer
- O-line Imaging Plate scanner
- Microscope
- Crystal mounting tools
- pH meter
- Electric balance
- Freezer and refrigerator
- Micro and large volume centrifuger
- Incubator