Automation in the Macromolecular Crystallography Beamlines and Construction of a New Micro-focus Beamline at the Photon Factory

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Structural Biology Research Center (SBRC) at the Photon Factory (PF) currently operates three macromolecular (MX) beamlines: insertion device (ID) beamlines AR-NW12A and BL-5A, and a bending magnet beamline BL-6A. The ID beamlines were recently constructed for high-throughput experiments, where a typical time required for collecting one dataset using crystals of normal (say 100 microns) size is 10 – 20 minutes due to fast read-out CCD detectors. However, to more optimize the use of synchrotron beam time, optimization of the other aspects in MX experiments should be required. On the other hand, to extend targets to macromolecules which are difficult to crystallize in the sufficient sizes, PF-SBRC is developing a new micro-focus beamline, BL-17A, dedicated to diffraction experiments with micron-size crystals.

Most of MX experiments are suitable to be automated because they are the repetitions of (i) exchanging sample on the goniometer, (ii) alignment of the mounted crystal, (iii) deciding measurement conditions and (iv) collecting a dataset with hundreds of images. Optimization of (iv) is mainly depends on the characteristic of beam and the performance of detectors, however, that of (i) - (iii) can be achieved by automating experimental steps as much as possible. Recent requirement to MX beamlines to be more stable and user-friendly will also be achieved by such automations. Increasing users unfamiliar with synchrotron facilities can perform experiments efficiently using well-organized beamline control system. Thus, recent development at currently operated MX beamlines of PF-SBRC was mainly focused on automations to bring out the capability of the beamlines through the aspects of (i) - (iii).

Sample changers were recently installed in the ID beamlines to reduce the considerable time wasted in the repetition in mounting and dismounting samples on the goniometer. The changers are the evolution of SAM system developed at Stanford Synchrotron Radiation Laboratory. The commission will be finished during the summer shutdown of FY2006, and will be available from the autumn. Beamline control software was modified to be more stable and functional with a common graphical user interface (GUI) at all the MX beamlines, through which users can execute all the operations required during experiments. The GUI was designed to provide a simple way to complete experiments with minimum steps of intervention, including automatic loop alignment, efficient energy scan with pre-defined parameters for MAD, and so on. Another control system based on a relational database is under development in parallel, which should allow secure remote access and automatic scheduled experiments together with the sample changer. The database is designed to contain information not only of beamline experiments but also from sample production to structure solution. All the information in the system should be easily tracked and managed due to the database feature.

The construction of BL-17A was finished in FY2005, which is now under commission to be commenced from the autumn of FY2006. The source of the beamline is a newly developed short-gap undulator installed in one of four short straight sections of PF 2.5GeV ring. The beamline was designed mainly for micro-crystal structure analysis, in addition, has the ability to deliver quite intense low energy beam around 2.0A which can be used for structure determination by SAD with light atoms such as sulfur. The measured focused beam size (FWHM) with the K-B mirror system was about 32.9 μm (V) x 234 μm (H). The photon flux at 12.4 keV collimated by 100 and 20 μm^2 were 8 x 10^{10} and 7 x 10^9 photons/sec, respectively. Although these preliminary results were encouraging, further optimization and stabilization of the optics will be required.