Beamline Developments for Lower Energy Phasing and Automation with Future Detector Development at the PF

Naohiro Matsugaki, Yusuke Yamada, Leonard Chavas, Masato Kawasaki, Ryuichi Kato, Masahiko Hiraki, Noriyuki Igarashi, and Soichi Wakatsuki

Structural Biology Research Center, Photon Factory, Institute of Materials Structure Science, High Energy Accelerator Research Organization (KEK), Tsukuba, Ibaraki 305-0801, Japan

SAD (single-wavelength anomalous dispersion) phasing with sulfurs or phosphors is currently one of the most attractive methods to solve macromolecular crystal structures. The method is particularly important for a range of macromolecules, which are difficult to prepare heavy atom or selenomethionine derivative crystals. The Structure Biology Research Center at the Photon Factory, Tsukuba, Japan, is developing a new beamline dedicated to sulfur SAD experiment as part of the national project "Targeted Proteins Research Program (TPRP)." It is a nationwide structural biology effort, which includes 35 target-oriented structural biology projects and 10 R&D projects in protein production, chemical library, structural analysis and bioinformatics. Two synchrotron radiation facilities, SPring-8 & Photon Factory, are building two complementary micro-focus beam lines and, together with Hokkaido Univ., Osaka Univ., and Kyoto Univ., developing techniques to facilitate user access and experiments at the two synchrotron sites. At SPring-8 a micro-beam beamline, BL32XU, has been constructed to provide highly intense 1-micron by 1-micron beam while the Photon Factory has built a micro-focus beam line, BL1A, optimized for low-energy SAD experiments. Each of the 35 target-oriented structural proteomics projects aims to solve structures of challenging targets in close collaboration with groups in cell biology, biochemistry, bioengineering, pharmacology, or medicine.

On PF BL1A beamline, an intense low-energy beam at around 4 KeV is provided using the first harmonic of an in-vacuum mini-gap undulator source to enhance anomalous signals from light atoms. For convenience, the same undulator produces x-ray beam suitable for Se-K edge MAD experiments at the same undulator gap. A cryo freezing device designed by Isao Tanaka's group of Hokkaido University is available for loop-less mounting of cryocooled crystals on site. The beamline consists of a cryo-cooled channel-cut monochromator and bimorph KB mirrors. In parallel, we have developed a system with an associated GUI, UGUI, for complete automation of data acquisition and initial data analysis, which is now implemented in all the beamlines at the PF, including the Astellas Pharma beamline AR-NE3A.

For low-energy SAD experiments a detector covering large solid angle will be useful. To build up such a detector system, a new project has been initiated to develop a pixel detector system based on DEPFET (DEpleted P-channel Field Effect Transistor) sensor in collaboration with Max Planck Institute, Munchen and Institute of Particle and Nuclear Studies Institute of KEK. The design concept of the detector system will be presented.