SIRAS Phase Determination of Pressurized-Xe Protein Crystals with High-Energy X-Rays

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The Bio-Crystallography beamline (BL-41XU) was constructed for crystal structure analysis of biological macromolecules on the multiple isomorphous replacement method with optimized anomalous scattering (MIR-OAS). The energy range available with the first harmonic emission of undulator is from 7 keV to 17.5 keV, which is useful for anomalous data collections around L3 absorption edges of heavy atoms usually utilized in the MIR method. The energy range with the third harmonics is from 21 keV to 38 keV, which will be effective for non-dispersive data collection like a remote data collection in the multi-wavelength anomalous dispersion (MAD) technique. The ultra-high energy X-rays over 30 keV is expected to be useful for precise data collections with no absorption and damage effects on sample crystals. Further-more, K-edge of a rare gas Xe (34.6 keV) is in this energy range. The Xe atoms are generally introduced into macro-molecular crystals at a high pressure. Based on this fact, the 34.6 keV X-rays are remarkable to open a general protocol for resolving the phase problem in crystallography by the MAD technique on Xe.

In order to use freely the ultra-high energy X-rays, automatic beamline alignment is indispensable to change X-ray energy easily. Precise setting parameters of all beamline components were determine by our group at six points of X-ray energy between 21 keV and 37.6 keV. Using the parameters as a data base, automatic beamline alignment was realized for every X-ray energies selected by users. We pursued X-ray damage effect of a tetragonal lysozyme crystal with 37.6 keV X-rays, and measured K-absorption edge of Xe-pressurized myoglobin crystal prepared with a cryo-Xe siter. The comparison of the lysozyme data collected at the ultra-high energy with that collected at a conventional energy of 12.4 keV is in progress.