

*Exploiting wavelength longer than 3 Å for native SAD phasing*Naohiro Matsugaki¹, Yusuke Yamada¹, Ayaka Harada¹, Masahiko Hiraki¹, Miki Senda¹, Toshiya Senda¹¹High Energy Accelerator Research Organization, Tsukuba, Japan

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Native SAD (Single-wavelength anomalous dispersion) is a crystallographic phasing method which utilizes anomalous signals from naturally-included light atoms in macromolecules. It has been known as an attractive method because no derivative crystals are required for de-novo structural solutions. The method appeared more than 30 years ago [1], however, it is still uncommon even at the latest synchrotron MX beamlines due to experimental difficulties in using long wavelength X-ray required to enhance weak anomalous signals [2]. Using longer wavelength is preferred to efficiently detect anomalous signals from light atoms, on the other hand, causes severe beam absorption by the sample or air on the X-ray beam path. In addition, the large diffracting angle makes it difficult to obtain high resolution data with a flat area detector.

We have implemented a dedicated data collection environment for native SAD phasing at the long-wavelength MX beamline BL-1A at the Photon Factory. The diffractometer is equipped with a standing chamber enclosing both the goniometer and the X-ray detector, a helium cold stream recycling system, and a specially designed sample changer. The beam path is completely covered by helium allowing data collection with low background. Under such optimized experimental environment we showed using the wavelength longer than 2.7 Å was advantageous in native SAD phasing against using the wavelength of 1.9 Å, by which most native SAD data collection has been performed so far [3].

In exploiting further longer wavelength than 3 Å, two flat area detectors (Eiger X4M, Dectris Ltd.) were installed which can be configured in V-shape in the helium chamber. The problem of large diffracting angle was mitigated by the V-shape configuration: the data obtained with the V-shape configuration was superior in terms of not only the availability of higher resolution but also the data statistics at high resolution range when compared with the normal (single) detector configuration of very short sample-to-detector distance. One drawback of the V-shape configuration is the lower completeness of data which can be recovered by the mini-kappa goniometer installed at the beamline. We will present the feasibility of using the wavelength longer than 3 Å for native SAD phasing based on the systematic data collections and analyses with different conditions such as wavelength, detector configuration and sample size.

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Keywords: [native SAD phasing](#), [long wavelength](#), [macromolecular crystallography beamline](#)