Long Wavelength X-rays for Phasing and Redox Biology

Richard Strange, Michael Hough, Svetlana Antonyuk, and Samar Hasnain

Institute of Integrative Biology, University of Liverpool, Liverpool L69 7ZX, UK

Ten years ago, in the light of the high-throughput structural genomics initiatives being planned worldwide, it was expected that SAD phasing at long x-ray wavelengths, which exploit the presence of sulphur or an intrinsic metal atom, would become a standard method of automated structure determination on synchrotron beamlines. This has not come to pass, indeed the vast majority of current (and relatively recent) protein crystallography beamlines have been designed to operate optimally at a shorter wavelength, for exploiting recombinant Se-Met protein derivatives.

A snapshot will be shown of the current capabilities and limitations of several modern variable wavelength protein crystallography beamlines – I02 and I03 at the Diamond Light Source, X06SA at the Swiss Light Source, Proxima-I at SOLEIL, and 22-ID at the Advanced Photon Source – to perform S-SAD experiments using their longest accessible wavelengths, in practice covering the wavelength range 1.9 – 2.4 Å.

The accuracy of long wavelength datasets remains limited by a number of factors, including purity of x-ray beams, non-optimised source-monochromator-mirror combinations, the size, geometry and DQE of detectors, beamline air-paths and detector-windows, the speed of accurate data collection, the higher x-ray dose on crystals and the increased radiation damage. These limitations need to be overcome via dedicated long wavelength (1.5 – 4 Å) beamlines as being envisaged at a number of advanced synchrotron sources. The possibility of using a dedicated long wavelength beamline for performing controlled photo-induced metal-redox chemistry of systems containing transition metals (V, Mn etc) for capturing ‘reaction intermediates’ will also be discussed. Both of these require rapid data collection with accuracy so that capabilities for acquiring ‘maximum data for minimum-dose’ are catered for in these sophisticated beamlines. Thus, in addition to fast and accurate diffraction detectors, such beamlines need to consider high-quality XANES data collection capabilities and single crystal spectrophotometers for on-line optical and Raman measurements. Some examples of current research will be presented to highlight this potential development.