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Is diffraction limited by the crystal or beam? A comparison of FEL vrs Synchrotron protein diffraction data.

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The development of X-ray Free-Electron Lasers (XFELs) has created a range of novel crystallography experiments such as the use of liquid-jet injectors. The use of goniometer-based FEL experiments(1) allows the direct comparison of diffraction from the same or similar crystals at both sources.

The diffraction of a set of crystals tested on the MX2 beamline at the Australian Synchrotron and the XPP beamline at the Linear Coherent Light Source (LCLS) will be presented. The diffraction for most crystals was found to be similar with a small increase in observed resolution limit for some samples.

The cases where a significant increase in diffraction is expected to be seen when using an XFEL will be discussed along with other experiments that can only be done on an XFEL. Data collection at an XFEL poses a series of significant challenges. The samples are vaporised by the beam and the resulting diffraction image covers an extremely small rocking curve.

These data suggest that for most “standard”MX crystals the increase in resolution expected at an XFEL over a microfocus MX beamline is marginal. For the collection of samples presented, the intrinsic diffraction limit of the crystals and not the intensity of the source was the limiting factor. These data suggest the use of XFELs will be most effective for well-ordered micro crystals or systems where the radiation damage “free”nature of XFEL data is required for characterisation of states such as oxidised and reduced forms of metallo-enzymes.

Keywords

XFEL, Synchrotron, Protein, Crystallography, Diffraction, Crystal

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