

Oral presentations

MS1. Recent experimental developments in synchrotron macromolecular crystallography

Chairs: Gordon Leonard, Marjolein Thunnissen

MS1-O1 Serial synchrotron crystallography experiments at EMBL beamline P14 at PETRA III

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Beamline P14 on PETRA III (DESY, Hamburg) offers a high flux micro-focused beam for extracting diffraction data from crystals with linear dimensions of less than 10 μm . At an energy of 12 keV, the beamline can deliver on the order of 5×10^{12} photons/s into a $5 \times 5 \mu\text{m}^2$ focal spot corresponding to an X-ray dose of approximately 100 MGy deposited into a typical macromolecular crystal per second. At this dose-rate, the lifetime of a macromolecular crystal reduces to several hundred ms at cryo-genic temperatures and several ten ms at room temperature.

Being able to extract the entire diffraction information from a crystal on a sub-second time-scale allows applying the serial crystallography paradigm - originally developed for FEL-based experiments [Chapman et al. (2012) *Nature* 470:73] - to synchrotron data collection. In serial crystallography, a carrier containing many small crystals is systematically exposed to the X-rays. Irrespective of whether or not crystalline material is in the exposed sub-volume or not, each sub-volume of the carrier is sampled with an X-ray dose sufficient to extract a

maximum of diffraction data. All acquired frames are then filtered, integrated, and scaled using custom-made processing software such as CrystFEL [White et al. (2012) *J.Appl.Cryst* 45:335] resulting in the assembly of a set of structure factor amplitudes against which a crystallographic model can be refined.

On P14, we have performed Serial Synchrotron Crystallography 'SSX' experiments both at cryogenic and at ambient temperature. At cryogenic temperature, a cryo-cooled suspension of small ($1 \times 1 \times 10 \mu\text{m}^3$) crystals of Cathepsin B was mounted in a standard crystallographic loop [Gati et al. (2014), *IUCrJ* 1:87]. At ambient temperature, small (10-20 μm linear dimensions) crystals of Insulin were grown in low-background CrystalDirectTM crystallization plates [Cipriani et al. (2012) *Acta Cryst. D*68:1393] for *in situ* data collection from the crystallization drops. For both cases, diffraction data were collected from hundreds of crystals via a continuous series of parallel helical scans as implemented in the MD3 diffractometer resulting in data sets against which models were refined.

The SSX data collection strategy is available via the MxCuBE v2 user interface installed on P14.

We will present results obtained with the SSX strategy, discuss current possibilities for difficult to crystallize systems, and extrapolate to the future.

Keywords: serial crystallography, radiation damage