

**MS02-P02****3-D analysis of X-ray mesh scans and data collection strategies for macromolecular crystallography**Alexander Popov<sup>1</sup>, Igor Melnikov<sup>1</sup>, Gleb Bourenkov<sup>2</sup>

1. ESRF, Grenoble, France

2. EMBL, Hamburg Outstation, Hamburg, Germany

**email:** [apopov@esrf.fr](mailto:apopov@esrf.fr)

Data collection procedures at a modern macromolecular crystallography beamlines rely heavily on automated preliminary experiments and data collection strategy software. The standard methods commonly implement a classical beam bathed single-crystal experiment [1, 2]. Further developments of these methods are aiming in automating the design of optimal data collection strategies for complex multi-crystal experiments, sub-crystal diffraction and multi-positional data collection. Three-dimensional information about positions, dimension and relative diffraction strengths of crystals mounted in the sample holder is obtained via several low-dose two-dimensional raster scans at various orientations of the sample holder. Automated preliminary analysis of diffraction images is carried out in real time by the program *Dozor*, which identifies the presence of a diffraction pattern from a macromolecular crystal, estimates the diffraction signal and produces the list of candidate diffraction spot positions. Based on the *Dozor* output, the program *MeshBest* [3] automatically determines the areas which belong to individual crystals as well as the areas of crystal overlap. Latest version of *MeshBest* analyses multiple mesh scans simultaneously and provides 3D information on the dimensions, centroid positions and integral diffraction quality of each crystal resolved on the holder. The best achievable result of data collection for each individual crystal is estimated by the program *BEST* [2], which now uses empirical 3D model of crystal shape delivered by *MeshBest*. The strategy-optimization method has been extended to take into account the variations in irradiated crystal volume with a spindle rotation. *BEST* predicts the diffraction intensity at any moment of data collection as a sum of diffraction intensities of crystal voxels taking into account the profile of the incident X-ray beam and the dose absorbed by each voxel. We will present development and applications of the methods which demonstrate feasibility of automated approaches and indicate a possibility of significant improvement in data quality in particular for membrane protein crystals grown in mesophase.

References:

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**Keywords:** BEST, MeshBest, Dozor**MS02-P03****VMXi – A new fully automated *in situ* and serial crystallography beamline at the Diamond Light Source**James Sandy<sup>1</sup>, Halina Mikolajek<sup>1</sup>, Juan Sanchez-Weatherby<sup>1</sup>, Thomas Sorensen<sup>1</sup>

1. Diamond Light Source Ltd., Chilton, Didcot, United Kingdom

**email:** [james.sandy@diamond.ac.uk](mailto:james.sandy@diamond.ac.uk)

The Diamond Light Source has a cohort of seven beamlines dedicated towards macromolecular crystallography (MX). The VMXi beamline is one of the most recent additions to this group of successful MX beamlines at Diamond. VMXi is a dedicated microfocus, high-flux, high-throughput beamline. VMXi has been designed to be a fully automated *in-situ* and serial crystallography beamline which breaks away from the standard MX user experience. Samples are delivered to the beamline and are imaged using a Formulatrix Rock Imager system. These images are viewed via the SynchWeb application which is already widely used for displaying experimental results.

Users can look at individual drops and mark either a region or a point where they would like to carry out an experiment. By applying simple parameters, the user can assign any number of experiments to a plate. Once all experiments are registered, the plate joins a queue and makes its way on to the beamline via a series of plate-handling robots. Plate transfer times have been optimised to minimise local heating effects on the samples. An internal plate storage hotel means that x-ray time is most optimally used by minimising shutter closed time. Samples are aligned using an image matching algorithm between images from the Formulatrix Rock Imager and visible light images collected on the beamline. Experiments are carried out and the experimental results are displayed in SynchWeb. Users are informed once data have been collected by an automated email service. At no point do users interact directly with the beamline. The beamline operates autonomously using the parameters that the user has specified.

We describe here some experiments carried out on the VMXi beamline, and validate the beamline as a place to quickly collect highly useful screening and experimental data, without having any manual interaction with the sample.

**Keywords:** VMXi, *in-situ*, beamline