Oral Contributions

[MS2-03] Data Collection Options at the Macromolecular Crystallography Beamline I04 at Diamond Light Source Ralf Flaig[a], Pierpaolo Romano[a], Dave Hall[a],

Macromolecular Crystallography Group[a]
[a]Diamond Light Source, Harwell Science and Innovation Campus, Chilton, Didcot, Oxfordshire, OX11 0DE, UK.
E-mail: ralf.flaig@diamond.ac.uk

Diamond Light Source [1] is the UK third generation synchrotron facility located south of Oxford and started with the user programme in early 2007. I04 is one of a suite of seven MX beamlines at Diamond providing state of the art facilities to the user community [2].
Beamline I04 has undergone various upgrade programmes and is always developing in order to improve the experimental capabilities. In standard mode the beamline offers a focused beam of 90 x 45 microns over the whole energy range provided by newly repolished KB mirrors. The bimorph control allows for defocusing to adjust the beam size to the sample size or to select a different focal plane, e.g. on the detector. The beamline is also equipped with compound refractive lenses (CRLs) which provide a beam size between 8 x 2 and 200 x 200 microns depending on energy. Currently, we are exploring the combination of mirrors and CRLs which should provide beam sizes in between the microfocus and standard mirror beam. The user also has the option to select different apertures, currently 10, 20 and 200 microns.
The flexible beamline design allows for an easy change between standard cryo or room temperature experiments as well as experiments under humidity control.
Recently, the beamline has been upgraded with a Pilatus 6M-F detector allowing acquisition rates of up to 25 Hz. This also benefits fast line and grid scans for sample characterization.
The beamline can be accessed and controlled by remote users with the fast sample changer having a capacity of 160 samples and we provide automatic loop finding and alignment after sample mounting to streamline the user experience.
A mini kappa goniometer is now in optimization mode on the beamline. The crystal reorientation capability helps to achieve a better spot separation for samples with long cell axes. MAD experiments could benefit from collecting Bijvoet pairs on the same frame. This increases the chance to get a more accurately determined anomalous signal especially for radiation sensitive samples. For the SAD method it is easier to achieve data sets with higher multiplicity with different crystal orientations which provides multiple independent measurements. Software is available to calculate alignment angles for different crystal orientations and multi-axis data collection strategies for various types of experiments are being developed further.
Data collection strategies and crystal and diffraction image characterization are provided automatically. Very shortly after the data collection has finished the results from our automatic data processing routines are available and we also provide difference electron density map, molecular replacement and experimental phasing pipelines.

[1] http://www.diamond.ac.uk
[2] http://www.diamond.ac.uk/mx-home/

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