

MS39-O3 The EIGER detector for macromolecular crystallography

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Single photon-counting devices developed in recent years have represented a major breakthrough in detector technology enabling noise-free detection and novel acquisition modes. The Dectris EIGER detector offers a pixel size of $75 \times 75 \mu\text{m}^2$, frame rates up to 3 kHz and a dead-time of 3.8 μs . An EIGER 1M prototype was tested at the Swiss Light Source beamline X10SA for its application in macromolecular crystallography. The combination of the fast frame-rate and the very short dead-time enables finer data collection plus the numerous advantages associated to higher rotation speeds. A careful analysis of the image summation of extremely fine phi-sliced images yields the best overall statistics/data and can also be used to optimize the dose by finding the best the balance between diffraction and radiation damage. Data collected on both test and challenging crystals will be presented. In addition, the latest results obtained with an EIGER 16M will also be reported.

Keywords: Hybrid pixel detectors

MS39-O4 Neutron macromolecular crystallography at the Institut Laue-Langevin

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Neutron crystallography allows direct determination of the hydrogen and/or deuterium atom positions of a macromolecule, providing complementary information to that gained via X-ray crystallography. Knowledge of the protonation states of amino-acid residues, along with the positions and orientations of individual water molecules, can often be crucial towards understanding the macromolecule's specific function and behaviour. At the Institut Laue-Langevin, recent improvements to instrumentation for neutron macromolecular crystallography (*i.e.* the quasi-Laue cold neutron diffractometer LADI-III and the monochromatic thermal neutron diffractometer D19) are extending the limits of the field. Sub-mm³ crystals are now regularly being used for data collection, structures have been determined to atomic resolution, and much larger unit-cell systems (cell edges >100 Å) are being studied. Data collection at cryogenic temperatures is also possible, allowing a wider array of experiments, including studies of cryo-trapped enzymatic intermediates. To illustrate the improved performance and capabilities, examples of recent studies [1-6] from the two complementary neutron diffractometers will be presented.

[1] Weber *et al.*, (2013) *J. Med. Chem.*, **345**, 193-197.
[2] Cuypers *et al.*, (2013) *Angew. Chem. Int. Ed. Engl.* **52**, 1022-1025. [3] Casadei *et al.*, (2014) *Science*, **345**, 193-197. [4] Langan *et al.*, (2014) *Structure* **22**, 1287-1300. [5] Haupt *et al.*, (2014) *IUCrJ*, **1**, 429-438. [6] Howard *et al.*, (2015) *Proc. Natl. Acad. Sci. U.S.A.*, submitted.

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