FA1-MS01-T01

Locating, characterizing and measuring from microcrystals. A versatile beam for variable samples. G. Evans

FA1-MS01-T02

Femtosecond X-Ray Protein Nanocrystallography.
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The ultrafast pulses from X-ray free-electron lasers have opened up a new form of protein nanocrystallography. In this "diffract and destroy" method [1,2] the specimen is completely vaporized by the intense focused pulse but that destruction only happens after the duration of the pulse without affecting the recorded diffraction pattern. This allows crystallography to be carried out at a dose much higher than the Henderson limit [3], allowing the study of radiation sensitive proteins and those that do not crystallize to large sizes. Ultrafast pump-probe studies of photoinduced dynamics can also be studied. We have carried out experiments in coherent diffraction from protein nanocrystals, including Photosystem I membrane protein, at the Linac Coherent Light Source (LCLS) at SLAC. The crystals are filtered to sizes less than 2 micron, and are delivered to the pulsed X-ray beam in a continuously flowing liquid jet. Millions of diffraction patterns were recorded at the LCLS repetition rate of 30 Hz with pnCCD detectors [4]. Tens of thousands of these have been indexed [5] and we have analysed the effects of pulse duration and fluence. Details of these first LCLS experiments and analysis will be discussed.
This work was carried out as part of a collaboration, including CFEL DESY, Arizona State University, SLAC, Uppsala University, the Max Planck Institute for Medical Research, and the Max Planck Advanced Study Group (ASG) at the CFEL. The names and addresses of all do not fit on one page. The experiments were carried out using the CAMP apparatus, which was designed and built by the Max Planck ASG at CFEL. The LCLS is operated by Stanford University on behalf of the U.S. Department of Energy, Office of Basic Energy Sciences.

[1] Neutze, R et al. Nature, 2000, 406, 753. [2] Chapman, H.N. *Nature Mat.* 2009, 8 299. [3] Henderson, R. Proc. R. Soc. London Ser. B, 1990, 241, 6. [4] Strüder, L. et al. Nucl. Meth. A. 2010, 614, 483. [5] Kirian R. et al. Opt. Express, 2010, 18, 5713.

Keywords: protein crystallography, nanocrystals, radiation damage studies

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MX automation: Towards a new sample holder standard for frozen crystals.
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The definition of the SPINE sample holder standard has been essential to make the automation of MX beamlines a reality in Europe. Appropriate for the smooth transition from manual to automatic operation, the SPINE design now appears to be a limiting factor. To cope with the demand of future crystal screening facilities, a new sample holder standard with smaller footprint and better intrinsic precision needs to be defined. Storage density could be then increased, transport costs reduced and the crystal centring step accelerated or even made unnecessary for screening.
Solutions are being investigated to develop a new sample holder with 100/10 µm crystal pre- and re-positioning precision and with a size that allows transporting up to 800 frozen crystals in a CX100 Dewar. Technical challenges as well the impact on the handling process will be shown. Interest of better sample holder for the future automated crystal harvesting systems will be illustrated.

Keywords: Biological-Crystallography, Sample Holder, Automation

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Application of an *in situ* crystal screening system at BESSY-MX BL14.1.
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One of the major bottle-necks in the structure solution of a biological macromolecule is the determination of optimal conditions for crystal growth. Although the process is largely automated using HT-methods like crystallization robots, manual human effort is required to pick these crystals from 96 well crystallization plates to characterize them. A novel approach is to expose freshly grown crystals in crystallization plates directly in an X-ray beam. It is possible to obtain data with high level of completeness and hence even the macromolecular structure can be determined [1]. We present the implementation of an *in situ* crystal screening using the CATS robot at BL14.1. Data from various protein crystals belonging to different crystal systems and the optimization of data collection parameters will be presented.

[1] Jacquamet, L., Ohana, J., Joly, J., Borel, F., Pirocchi, M., Charrault, P., Bertoni, A., Israel-Gouy, P., Carpentier, P., Kozielski, F., Blot, D., Ferrer, J., *Structure*, 2004, 12, 1219.

Keywords: in situ crystal screening, synchrotron, crystallization of macromolecules

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Diffraction Cartography: multi-crystal and multi-position data collection.
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Crystals of biological macromolecules often exhibit considerable *inter* and *intra* crystal variation in diffraction