MS1-P4 SONICC implementation at GM/CA-beamline 23IDB at the Advanced Photon Source

Michael Becker[1], Sergey Stepanov[1], Justin A. Newman[2], Shane Sullivan[2], Robert M. Everly[2], Christopher M. Dettmar[2], Scott J. Toth[2], Paul D. Schmitt[2], Stephen Corcoran[1], Dale Ferguson[1], Robert F. Fischetti[1], Garth J. Simpson[2]

1. GM/CA@APS, Argonne National Laboratory, Argonne, IL, USA
2. Dept. of Chemistry, Purdue University, West Lafayette, IN, USA

email: mbecker@anl.gov

Second order nonlinear optical imaging of chiral crystals (SONICC), based on femtosecond laser scanning microscopy, has been implemented at GM/CA@APS undulator beamline 23ID-B for rapid protein crystal localization and centering. The technique is based on infrared laser light impinging on non-centrosymmetric crystals of proteins, which may selectively yield a frequency-doubled, visible signal generated by the anharmonic response of the electron cloud of the protein in response to the laser field. One aim of this method is to locate small crystals grown in opaque crystallization media for centering in X-ray beams of only a few microns or less in cross-section, such as for membrane-protein crystals grown in mesophase [1]. The optical system implemented for generation and detection of Second Harmonic Generation (SHG) signals at beamline 23IDB has been described [2]. The system also provides the capability to scan visible laser light across the sample and detect two-photon excited UV fluorescence (TPE-UVF), which provides complementary contrast based on the native fluorescence of proteins. Recent efforts towards providing user-friendly capabilities include: increasing rates of data acquisition, providing bright-field laser imaging capabilities, and incorporation of laser-safety interlocks suitable for a user program. SHG imaging has also enabled direct experimental visualization of electric fields generated by photoelectrons that are produced as a result of X-ray absorption, which provides insight on X-ray damage in samples [3]. Recent advances will be presented.

[1] D. Kissick, C. Dettmar, M. Becker, A. Mulichak, V. Cherezov, S. Ginell, K. Battaile, L. Keefe, R. Fischetti, G. Simpson, Acta Cryst., 2013, D69, 843-851.

[2] J.T. Madden, S. Toth, C. Dettmar, J. Newman, R. Oglesbee, H. Hedderich, R. Everly, M. Becker, J. Ronau, S. Buchanan, V. Cherezov, M. Morrow, S. Xu, D. Ferguson, O. Makarov, C. Das, R. Fischetti, G. Simpson, J Synchrotron Rad., 2013, 20, 531-540.

[3] C.M. Dettmar, J.A. Newman, S.J. Toth, M. Becker, R.F. Fischetti, G.J. Simpson. Proc.Nat. Acad. Sci.USA, 2015,112, 696-701.

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MS1-P5 Multicrystal analysis with DIALS and BLEND

Pierre Aller[1], David Waterman[2], James Foadi[3], James Parkhurst[1], Luis Fuentes-Montero[1], Richard Gildea[1], Graeme Winter[1], Gwyndaf Evans[1]

1. Diamond Light Source, Harwell Science and Innovation Campus, OX11 0DE Didcot, UK
2. STFC Rutherford Appleton Laboratory, OX11 0DE Didcot, UK
3. Membrane Protein Laboratory, Diamond Light Source, Harwell Science and Innovation Campus, OX11 0DE Didcot, UK

email: pierre.aller@diamond.ac.uk

The recent developments of micro-focus beamlines[1] and *in situ* data collection[2,3] have led to a renewed interest in multiple crystal dataset analysis[4] . Although the availability of smaller beams is instrumental to the data collection of microcrystals, the impact of the radiation damage prevents the collection of a complete dataset from a single crystal. For a typical experiment on a micro-focus or sub micro-focus beamline we should expect to merge small wedges of data collected on multiple crystals in order to get a complete set. However, processing and merging small wedges of data from multiple crystals is not trivial and typically requires some analysis to establish isomorphous groups of data for merging.

Programs such as BLEND[5] have been developed to help and guide users to merge data from the isomorphous crystals together using cluster analysis. BLEND's cell dimension analysis can be improved by simultaneously analysing multiple crystals with DIALS (dials.diamond.ac.uk) to produce a more accurate set of unit cell dimensions. In this work we detail these recent developments and provide several examples of their application.

1 Evans, G., Axford, D., Waterman, D. G. & Owen, R. L. Macromolecular microcrystallography. *Crystallography Reviews* **17**, 105-142 (2011).

2 Aller, P. *et al.* Application of in situ diffraction in high-throughput structure determination platforms. *Methods in molecular biology* **1261**, 233-253, doi:10.1007/978-1-4939-2230-7_13 (2015).

3 Axford, D. *et al.* In situ macromolecular crystallography using microbeams. *Acta crystallographica. Section D, Biological crystallography* **68**, 592-600, doi:10.1107/S0907444912006749 (2012).

4 Smith, J. L., Fischetti, R. F. & Yamamoto, M. Micro-crystallography comes of age. *Current opinion in structural biology* **22**, 602-612, doi:10.1016/j.sbi.2012.09.001 (2012).

5 Foadi, J. *et al.* Clustering procedures for the optimal selection of data sets from multiple crystals in macromolecular crystallography. *Acta crystallographica. Section D, Biological crystallography* **69**, 1617-1632, doi:10.1107/S0907444913012274 (2013).

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