Poster Presentation

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Serial snapshot crystallography with a non-monochromatic microbeam

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X-ray free-electron laser (XFEL) sources create X-ray pulses of unprecedented brilliance and open up new possibilities for the structural characterization of crystalline materials. By exposing a small crystallite (100nm-10µm) to a single ultrafast pulse, a diffraction pattern can be obtained before the crystal is damaged. If such single-pulse diffraction patterns, collected sequentially on many randomly oriented crystallites, are combined, it is possible to determine the structure of the material accurately [1]. One of the drawbacks of this approach is that only a single position of the Ewald sphere is accessed in each pattern, so, because reflections have a finite width, the diffraction condition is not satisfied completely for any of the reflections recorded. The new XFEL source that is being developed in Switzerland (SwissFEL) will provide a broad-bandpass mode with an energy bandwidth of about 4% [2]. By using the full energy range of the SwissFEL beam, a new option for structural studies of crystalline materials becomes possible. In a recent study based on simulated data, we showed that a diffraction experiment with stationary crystallites in such an 'extra pink' beam not only increases the number of reflection intensities that can be collected in a single shot, but also overcome the problem of 'partial reflection' measurement [3]. To test the viability of the data processing with experimental data, attempts to simulate this 4% bandpass have been carried out on SNBL at ESRF and on the microXAS beamline at SLS. On SNBL, a single crystal was rotated over 360˚ and a continuous scan of the monochromator over the 4% energy range was performed every 1˚. At SLS, a mirror was used to cut off the higher energies of the undulator beam and the energy threshold of a Pilatus detector to eliminate the lower ones. With this setup, a series of randomly oriented crystallites were measured. A comparison of the analysis of these datasets will be presented.

[1] *H. N. Chapman, et al., Nature, 2011, 470, 73–77.,* ***[2]*** *B. D. Patterson, R. Abela, H. H. Braun, et al., New J. Phys., 2010, 12, 035012.,* ***[3]*** *C. Dejoie, L. B. McCusker, C. Baerlocher, et al., J. Appl. Cryst., 2013, 46, 791-794.*

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