MS2. X-ray free electron lasers (XFEL) in macromolecular crystallography

Chairs: Janos Hajdu, Adrian Mancuso

MS2-O1 High-resolution native structure analyses of supramacromolecular complexes susceptible to radiation damage

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In protein crystallography, radiation damage free structure determination is not necessarily achieved, even when the data is collected at cryogenic temperatures. The active sites of metalloproteins are especially susceptible to radiation damage due to changes in the oxidation states of catalytically important ions. Therefore, native structural determination of the active site of such metalloproteins is an important challenge in protein crystallography.

Recently we successfully determined the radiation damage free high-resolution structure of bovine heart cytochrome c oxidase (CcO) [(1)] and cyanobacteria photosystem II (PSII) [(2)]. Both CcO and PSII are supramacromolecular complexes containing metal ions as catalysts of their redox reactions. Radiation damage free diffraction data was collected using femtosecond crystallography. To improve diffraction resolution, large crystals, as opposed to micro-crystals popular in serial femtosecond crystallography, were used. In this presentation I talk the goniometer based data collection system developed at SACLA (SPring-8 Angstrom Compact free-electron LAser) and the damage free crystal structures of CcO and PSII.

(1) Hirata, K. *et al.* (2014) *Nature Methods* **11**, 734-736, (2) Suga, M. *et al.* (2015) *Nature* **517**, 99-103.

Keywords: femtosecond crystallography, radiation damage, metalloprotein

MS2-O2 Data processing for serial crystallography: recent developments in CrystFEL

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The technique of serial femtosecond crystallography has emerged over the last few years as a particularly successful application of X-ray free-electron laser (XFEL) sources. Data processing for this technique, which starts with the diffraction patterns and from them derives estimates of the structure factor moduli, requires some modifications to the conventional methods and is an area of active and ongoing research. Very recently, exciting progress has been made towards increasing the quality of data which can be obtained from a given number of diffraction patterns in a serial crystallography experiment [1,2], which may eventually allow new types of experiment to be performed. The CrystFEL software suite [3] has been made available as free and open-source software to address the needs of this technique, including these recent improvements, in a user-oriented manner along with suitable documentation, tutorials and usage guidelines. This talk will discuss recent progress in this area, including a look at new features and improvements in recent versions of CrystFEL. [1] M. Uervirojnangkoorn, O. B Zeldin, A. Y. Lyubimov, J. Hattne, A. S. Brewster, N. K Sauter, A. T. Brunger, W. I. Weis. eLife 2015;10.7554/eLife.05421 [2] T. A. White. "Post-refinement method for snapshot serial crystallography". Phil. Trans. Roy. Soc. B 369 (2014) 20130330. [3] T. A. White, R. A. Kirian, A. V. Martin, A. Aquila, K. Nass, A. Barty and H. N. Chapman. "CrystFEL: a software suite for snapshot serial crystallography". J. Appl. Cryst. 45 (2012), p335–341.

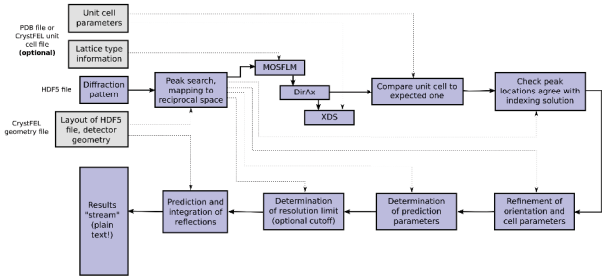

Figure 1. Fully automated indexing and integration pipeline implemented in CrystFEL for each frame of diffraction data, corresponding to one X-ray pulse.

Keywords: XFEL, serial femtosecond crystallography, data processing