Poster Presentation

MS36.P01

A reshaped approach for protein nanocrystal structure analysis from XFELs

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The size and quality of protein crystals are critical limiting factors in conventional X-ray crystallography structural studies. Serial femtosecond X-ray crystallography (SFX) presents new opportunities through the use of submicron and nano-scale crystal samples. SFX experiments with X-ray free-electron lasers have demonstrated success (Chapman, 2011). While new instances are arising for the study of poorly crystallizing proteins, fresh examination must also be made of their analysis. Significantly, the smallness of the crystal samples creates broad integrated intensity distributions that require careful consideration for the accurate reconstruction of high-resolution protein crystal structures. Structural imperfections are also expected to play significant roles in the formation of SFX diffraction patterns (Dilanian, 2013). We present preliminary results from a new approach for SFX data analysis. As motivation, it is observed that significant similarities lie between merged SFX data-sets and powder diffraction patterns. The merged Bragg peak-shape distributions in SFX diffraction patterns are characterised by the shape, size and disorder distributions of the large crystal sample set. Powder diffraction peak-shape distributions are formed similarly by a collection of independent scatterers of such varying characteristics. The presented method utilizes an established powder diffraction analysis tool, the Le Bail method (Le Bail, 1988), for extension and application to SFX data. It is shown here that the continuous whole-pattern fitting technique, combined with variable peak-shape functions, can be used to closely model simulated SFX patterns and to extract integrated intensities. The presented approach is posed as a new analysis method for SFX experiments in which both crystal size and structural disorder variations can be incorporated.

[1] *A. Le Bail, H. Duroy, J.L. Fourquet, Mat. Res. Bull., 1988, 23, 447-452,* ***[2]*** *H. N. Chapman, P. Fromme, A. Barty, et al., Nature, 2011, 470, 73-77,* ***[3]*** *R. A. Dilanian, V. A. Streltsov, H. M. Quiney, K. A. Nugent, Acta Cryst., 2013, A69, 108-118*

Keywords: Nanocrystallography, Xfel