

SYNCHROTRON X-RAY POWDER DIFFRACTION AS IT BEGINS TO MAKE AN IMPACT IN STRUCTURAL BIOLOGY

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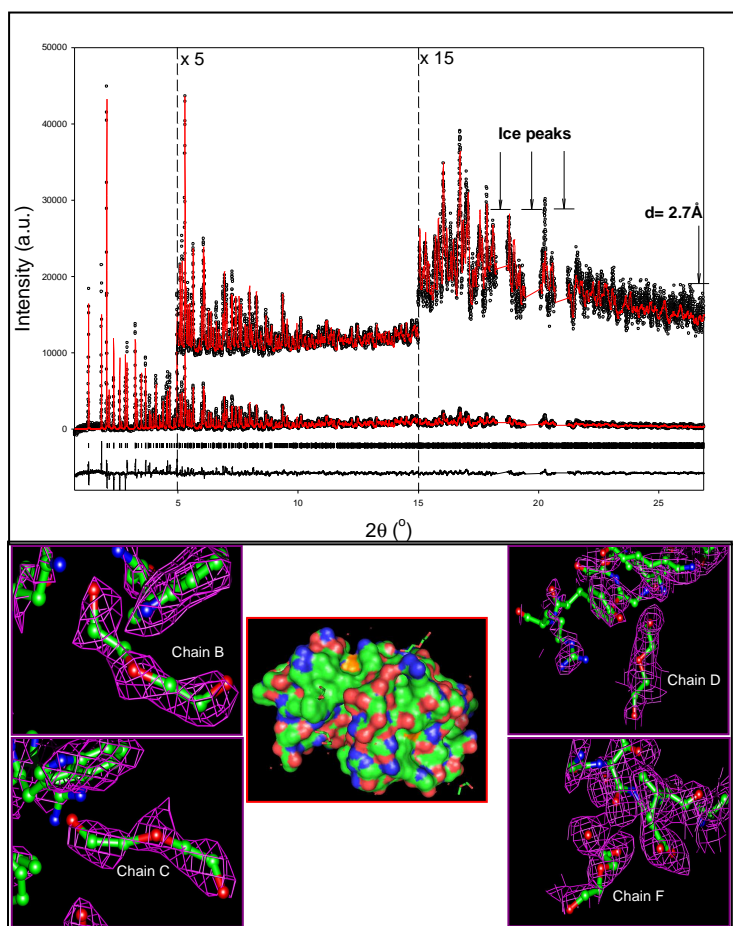


Figure 1. *Upper panel:* The Rietveld fit for tetragonal HEWL at 100K with a mixture of PEG 400 and methanol added for cryoprotection ($\lambda = 1.250845(23)\text{\AA}$, ID31- ESRF, GSAS: $R_{wp} = 6.80\%$, $R_F^2 = 10.12\%$). *Inset:* The refined molecular conformation of HEWL illustrated as surface. Three additional PEG molecules were identified in total omit maps to be bound on HEWL at 100K. *Lower panel:* Perspective views of selected regions around the 3 PEG chains of the total omit map at 2.7\AA resolution with the contour level at 1σ .

Many materials (often those of major industrial or pharmaceutical importance including zeolites, polymers, pharmaceuticals *etc.*) cannot be easily crystallized and exist only as powders. The solution and refinement of structures with diffraction data from polycrystalline samples has undergone a revolution in the last two decades: once a phase identification tool used primarily in the industrial setting, this technique currently is also used for fundamental investigations of new and complex materials. The requirement to solve increasingly complex structures from powder diffraction data alone demands access to the best available diffraction data. The aim of this talk is to describe the frontier of powder diffraction as it begins to make a significant impact on structural biology. Issues which will be discussed include: (a) application of the molecular replacement technique and structure refinements of selected proteins [1, 2] (b) methods for successful cryocooling (**Fig. 1**) [3] (c) radiation damage (d) experimental phasing and modelling of solvent envelopes (e) high throughput automated data collection (robotic sample changer) allowing systematic investigations such as screening and phase diagram mapping [4] and (f) ligand binding [1, 5].

References:

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