

Recent advances in protein powder diffraction

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The central problem in using powder diffraction data for the solution and refinement of crystal structures is that the diffraction information is severely limited relative to that obtained from a single crystal covering the same region of reciprocal space. The scattering from a single crystal is represented in reciprocal space by an array of slightly broadened delta functions; their intensity measurement is a simple integration of the peak intensity above background. For a powder diffraction experiment, the reciprocal space picture is of a nested series of spherical shells broadened by sample and instrumental effects; the density of these shells increases quadratically with distance from the reciprocal space origin. Their intensity corresponds to that of the structure factor responsible for the shell and its multiplicity. Use of the individual structure factor intensities that form the powder pattern is then compromised by the increasing overlap of these shells. This is particularly acute for proteins as the diffraction patterns are made from a very large number of reflections. However, the unprecedented sharpness of protein powder pattern peaks and their position sensitivity to sample environment provides a means of overcoming this loss of information. This talk will present some recent results on the improvement possible from using combinations of protein powder patterns for Rietveld refinement.

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