Maximising the Information Obtainable from Diffraction Experiments

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In this presentation I will describe some of the methods we have been developing in recent years for the analysis of both single crystal and powder diffraction data. In particular I will address how using modern and flexible software, such as the Topas-Academic package written by Alan Coelho, one can perform innovative analysis without needing access to source code. Complex analytical approaches can then be rapidly developed to address specific problems by those without high levels of computational expertise.

To illustrate the importance of software flexibility I will describe how simulated annealing techniques widely use for structure solution from powder diffraction data can be used to solve complex oxide superstructures from single crystal data. I will also describe methods we've developed for "surface fitting" diffraction data. By treating a set of variable temperature/time/pressure powder or single crystal data as an ensemble rather than as unconnected individual measurements, one can dramatically increase the useful information extractable from experimental data. Whilst specific examples will be used to highlight possibilities, the methods to be described have wide ranging applicability.

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