

STRUCTURE ANALYSIS FROM POWDER DIFFRACTION DATA SUPPORTED BY TOTAL ENERGY CALCULATIONS

Carlota Conesa-Moratilla¹, Max Petersen², Steffen Wilke¹

¹Accelrys Ltd, 334Cambridge Science Park, Cambridge, CB4 0WN, UK

²Accelrys, Inc., 10188 Telesis Ct., San Diego, CA 92121, USA

Successful structure determination from powder X-ray diffraction data (PXRD) is often limited by the amount of information that is contained in the experimental spectra. This holds in particular for large, flexible molecules, strong sample effects (crystalline size broadening, preferred orientation), or for atoms with low scattering cross sections (hydrogen atoms). In such cases, direct space and Rietveld methods might result in reasonable spectral fits but ambiguous or chemically non sensible solutions.

This paper reviews a hierarchical approach to include total energy considerations into the structure analysis of PXRD. For the sampling of large number of configurations during real space searches, a close contact penalty is included to favor chemical sensible structures. Once likely structures are found and standard Rietveld refinement is performed, total energies based on accurate force-fields can be included in an all atom refinement. These total energies are not only used to weigh the similarity measure, but can also be Pareto optimized to obtain the best combination of spectral fit and low energy configuration. Finally, quantum mechanical optimizations based on density functional theory are explored to obtain high quality structural information. Application examples will be discussed for each of these methodologies.