

CLOSE CONTACT PENALTY FUNCTIONS IN DIRECT SPACE METHODS AND ENERGETIC CONSIDERATIONS IN STRUCTURE REFINEMENT

Carlota Conesa-Moratilla, Colin Ross, Steffen Wilke

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

When solving crystal structures from powder diffraction data using direct space methods, all available information (i.e., molecular structure and space group symmetry) is used to limit the number of degrees of freedom. When the quantity of information available from a powder diffraction diagram is limited (due to, e.g., broad peaks, preferred orientation, positions of weak scatters like H atoms...) and/or the number of degrees of freedom is large, it may be necessary to add extra chemical information to the process in order to obtain a solution. This extra chemical information can be introduced by requiring the generated structures to be energetically stable. In this scenario, the potential energy contributes to a combined figure of merit alongside the powder pattern similarity, Rwp. Higher energy structures then have a higher value for the combined figure of merit and are therefore penalised during the optimisation process.

One of the most basic pieces of chemical information that can be incorporated into a structure determination is to utilise the fact that viable solutions should not contain overlapping atoms. Adding a simple close contact penalty that prevents solutions with non-viable intermolecular interactions from being generated is adequate for the global optimisation process, which aims at locating a rough, refinable solution. The close contact penalty model implemented in MS Reflex Plus will be discussed including a number of case studies where the use of this feature has made the derivation of crystal structure solution possible.

During refinement an accurate description of the potential energy (e.g. a good force field) should be used in combination with the Rwp in a weighted optimisation process. The *a priori* determination of the weighting factor might not be intuitive; in such cases a Pareto optimisation (a *posteriori* preference articulation) can be used to obtain an appropriate value. It will be demonstrated, how the use of the Rwp factor in conjunction with energies derived from a force field expression can be used in an all-atom Rietveld refinement process to determine structures that are both chemically viable and in close agreement with the experimental powder pattern.