RECENT ADVANCES IN STRUCTURE SOLUTION FROM POWDER DIFFRACTION DATA

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Crystal structure determination frequently is a prerequisite for the rational understanding of the solid-state properties of new materials. While single crystal diffractometry is the preferred method for crystal structure determination, it is often impractical due to difficulties in growing appropriate size single crystals. High quality powder samples, on the other hand, are much easier to obtain. Subsequently, the ability to determine crystal structures from powder data is highly desirable. Using direct-space structure solution techniques, increasingly complex crystal structures can nowadays be solved directly from powder diffraction data. Combined with easy-to-use tools for model building and visualisation as well as molecular mechanics and first principles Density Functional Theory (DFT) calculations, crystal structure solution from powder diffraction data is becoming a routine task.

Recent advances include the determination of a preferred orientation correction during the structure solution search, parallel tempering as an optional global search algorithm along with the simulated annealing method, and treatment of special positions. A close contact penalty can be applied to ensure only chemically viable solutions are found without bad contacts between structural fragments. As a complementary technique, first principles DFT calculations have been used successfully to validate structure solutions and to aid the subsequent Rietveld refinement. A novel indexing program X-Cell has been validated to tackle various difficulties typically encountered in powder indexing, including contamination with impurity phases, strong peak overlap, peak position errors, zero-point shift and extreme cell geometries, when many existing programs fail.

In conclusion, structure solution from powder diffraction data is a viable alternative for crystal structure determination when single-crystal data is unavailable.