

## RECENT ADVANCES IN STRUCTURE SOLUTION FROM POWDER DIFFRACTION DATA

**C. Liang<sup>a</sup>, M. A. Neumann<sup>b</sup>, F. J. J. Leusen<sup>b</sup>, G. E. Engel<sup>b</sup>, S. Wilke<sup>b</sup>,  
C. Conesa-Moratilla<sup>b</sup>**

<sup>a</sup>Molecular Simulation Inc. 9685 Scranton Road, San Diego, CA 92121, USA

<sup>b</sup>Molecular Simulation Ltd. 230/250 The Quorum, Cambridge CB5 8RE, UK

Crystal structure determination is in general a prerequisite for the rational understanding of the solid state properties of new materials. Even though single crystal diffractometry is the method of choice when it comes to crystal structure determination, this approach is often impractical because of the difficulties involved in growing single crystals of appropriate size. High quality powder samples, on the other hand, are much easier to obtain. Using direct-space structure solution techniques, increasingly complex crystal structures can nowadays be solved directly from powder diffraction data. Guided towards the best solution by global optimization algorithms, huge amounts of trial structures are generated and compared to the experimental data until a solution is found. Apart from a small number of internal degrees of freedom, the geometry of molecules and molecular ions is kept fixed during the structure search to reduce the number of degrees of freedom. Combined with easy-to-use tools for model building and visualization 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. To illustrate the applicability of direct-space Monte Carlo techniques to the crystal structure solution of organic and inorganic compounds, a variety of structure solutions with the program Powder Solve<sup>1,2</sup> will be presented.

Recent advances include the determination of a preferred orientation correction during the structure solution search and the use of parallel tempering, a newly implemented global search algorithm. As a complementary technique, first principles DFT calculations have been used successfully to validate structure solutions and to aid the subsequent Rietveld refinement.

<sup>1</sup>G. E. Engel, S. Wilke, O. König, K.D.M. Harris and F.J.J. Leusen, *J. Appl. Cryst.*, **32**: 1169 - 1179 (1999).

<sup>2</sup>G. Stephenson, *J. Pharm. Sci.*, **89**: 958-966 (2000)