m29.o05

Analysing Stacking Disorder with a Genetic Algorithm

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Keywords: diffuse scattering, disordered molecular structures, genetic algorithms

A disordered stacking of layers is described in terms of probabilities governing the addition of new layers to a stack. The diffuse scattering exhibited by such stacks takes the form of diffuse lines perpendicular to the layers and can be represented as a function of the stacking probabilities in closed form [1]. The corresponding expression becomes increasingly unwieldy, as the number of layers affecting the probabilities increases. In this work we have determined the probabilities with a numerical procedure based on a genetic algorithm.
The crystal structure of tris(bicyclo[2.1.1ηexeno)-benzene, **1**, shows layers of coplanar molecules with layer symmetry *p6bar2m*. Consecutive layers may assume one of three positions with probabilities depending on the position of the three preceding layers. Initially the probabilities have been estimated by visually comparing measured diffuse intensities with those calculated from a complicated analytical function of the probabilities [2].
We have redetermined these probabilities using an adaptation of a genetic algorithm described earlier [3]. The mean values and their standard deviations from 20 sets of three probabilities obtained after 113 generations of optimization are 0.08(1), 0.60(4) and 0.46(4) in good agreement with the values derived from the analytical approach, 0.08(2), 0.56(6) and 0.46(10). Although the general structure of maxima and minima is reproduced well (Fig.1), their relative heights indicate room for further improvement of the structural model, e.g. by tilting the molecules out of the plane and adjusting the displacement parameters. These quantities are presently optimized with the genetic algorithm.

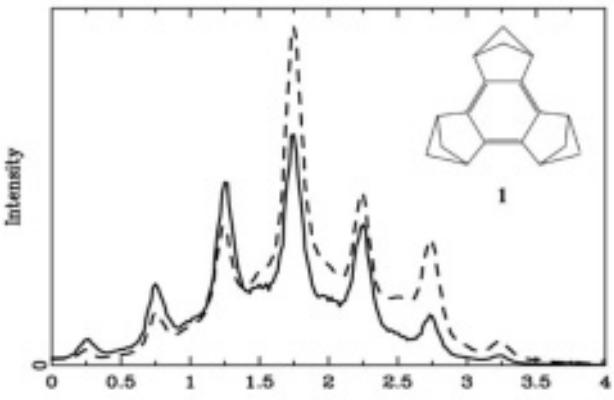

Fig. 1 Observed (dashed) and calculated (solid) 02L profile; molecular graph (inset).

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m30.o01

'Pushing the Boundaries' of Evolutionary Algorithms in SDPD - A Cultural Differential Evolution approach

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Keywords: powder structure determination, structure solution methods, computer algorithms

The development of direct space structure solution techniques is an important factor in the increasing number of crystal structures determined by PXRD [1]. These methods involve the assessment of trial structures based on comparison of the calculated powder profile to the experimental pattern, and the use of a global optimisation algorithm to locate the optimum structure solution ie. that lying in the global minimum.
Many optimisation techniques such as Monte Carlo, simulated annealing and genetic algorithms have been applied to this problem. Our work has focussed on the development of the Differential Evolution (DE) method, which is an evolutionary algorithm that is simple to implement and offers a robust searching of minima [2,3]. In DE, a population of trial structures is mated and mutated over a number of generations until the global minimum is located. This mutation and recombination process is carried out in a single step with only three parameters needed to control the optimisation process. The inherent use of maximum and minimum boundaries in the DE process also allows the search to be restricted to specific areas of parameter space without disrupting natural search pathways. However, in the original implementation of DE, the boundary values remain constant throughout the calculation. In our implementation of the Cultural Differential Evolution hybrid approach (CDE), we invoke the experience of previous generations to influence subsequent generations using dynamic boundaries to shadow the evolution and clustering of a population as it progresses through the generations. Our use of an underpopulation threshold at each generation ensures that our boundaries can also expand as the calculation proceeds, helping to avoid convergence in a local minimum. Early tests show an average 40% improvement in efficiency through shorter convergence using the CDE method, illustrating the advantages of a technique that combines the concepts of biological and sociological evolution [4].
This presentation describes our development and application of the DE algorithm to the structure solution of molecular materials from powder diffraction data, and modification of the basic DE algorithm to combine the concepts of genetic and cultural evolution, CDE. We will examine the effects of this modification on the behaviour and efficiency of the DE algorithm, and present examples of structures studied using this technique.

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