Computing VI
Materials Research

MS03.06.01 STRUCTURE PREDICTION, Clive M. Freeman, Alan M. Gorman and Steve M. Levine, MSI 9685 Scranton Road, San Diego CA 92121, USA.

Techniques for predicting and solving crystal structures based on powder diffraction data and simple descriptions of interatomic interaction have advanced dramatically in recent years. Such procedures exploit the standard techniques of computer simulation in combination with hybrid potential energy functions to yield structures which are sterically and experimentally plausible. These methods have been especially useful in the investigation of microcrystalline framework structured solids for which powder diffraction may be the primary experimental route to structural information. In contrast to traditional refinement procedures, which use rapidly convergent but locally biased least squares methods, analogy with physical simulations has prompted the use of simulated annealing as an optimization method in the majority of studies. Metropolis Monte Carlo or Molecular Dynamics based annealing procedures provide significant 'searching' capabilities which yield global minimization properties. Applications to framework structured solids, condensed metal oxides and molecular crystal structures will be described.

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MS03.06.02 CONVENTIONAL DESCRIPTIONS OF NEW PHASES FROM RESULTS OF HIGH PRESSURE INORGANIC STRUCTURE MODELLING, Y. Le Page, D.D. Klug and J.S. Tse, National Research Council of Canada, Ottawa, Canada K1A 0R6. E-mail: yvon.le_page@nrc.ca.

Results of ab-initio inorganic structure modelling are often in the form of Cartesian coordinates of atoms in a large, periodical and in general oblique simulation box containing hundreds to thousands of atoms. The contents of that box may correspond to a single crystal, a twin, a mixture of phases or a disordered block of matter. It may also include point, line or plane defects.

The problem of extracting the corresponding crystallographic description, a necessary step in view of full quantum calculations and possible publication, is different from the familiar problem of extracting crystal symmetry and structure from experimental diffracted intensity data. The computer-aided method developed at NRC over the years is based on eye identification on a stereo plot of three pairs of atoms related by conjugate translations in a same single-crystalline region, followed by derivation of fractional coordinates for the atomic content of the corresponding primitive cell. Running this data through the MISSYM program discloses potential symmetry elements of the structure, with their corresponding crystallographic directions.

These potential elements are then critically examined and accepted either as symmetry or pseudo symmetry based on comparison of coordinate deviations between related atoms with the expected magnitude of thermal motion. The conventional cell and space group are then derived from the accepted symmetry elements. All calculations described here can be performed with the NRCVAX system of programs. Examples of simulation boxes and Cartesian models for new members of structural families will be detailed.