

INTRODUCTION TO STRUCTURE ANALYSIS OF MODULATED AND COMPOSITE CRYSTALS. V. Petříček and M. Dušek, Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, 18221 Praha 8, Czech Republic.

Modulated and composite crystals represent an example of general aperiodic crystals. The superspace theory, as developed by deWolff, Janssen and Janner [1], gave crystallographers a natural tool for their description as a periodic matter in 3+d dimensional space and enabled generalization of standard crystallographic procedures for structure solution and refinement. Structure solution techniques are strongly dependent on amplitudes of the modulated atoms. With increasing modulation, more advanced methods are to be used. A recently developed powerful solution technique called “charge flipping” [2], which can be applied also to aperiodic crystals, has provided a revolution in the field.

Modulations in the crystal, affecting various structural parameters (site occupancies, atomic positions and also atomic displacement parameters), can usually be described as a combination of continuous harmonic functions. There are cases, however, when the continuous harmonic model is not sufficient as the modulation has a discontinuous character. Such cases can be recognized already in the diffraction pattern by the presence of strong higher-order satellites, and for proper description needs special modulation functions of crenel or saw-tooth shape [3], [4]. These functions have been introduced in the Jana program, and recently a new algorithm has been developed that facilitates their application.

The superspace description can be also used for commensurately modulated crystals. Here, it plays also an important role in the systematic description of structural families. Different members of such a family of various composition and symmetry can be generated from a common parent structure defined in the superspace using different q-vectors and origin positions of the internal space. Thus, new structural crystal types can be defined in (3+d) dimensional space.

The program system Jana2006 can refine regular, twinned, modulated and composite structures. It can perform full structure analysis from single or powder crystal data from either neutron or X-ray diffraction. The latest version also allows joint refinement against diffraction data from different sources, typically combining neutron and X-ray data.

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