



Crystallography of Modular Materials (International Union of Crystallography Monographs on Crystallography)

Giovanni Ferraris, Emil Makovicky, Stefano Merlino

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This is the first book to provide a comprehensive treatment of theories and applications in the rapidly expanding field of the crystallography of molecular materials. Molecules are the natural modules from which molecular crystalline structures are built. Most inorganic structures, however are infinite arrays of atoms and some kinds of surrogate modules, e.g. coordination polyhedra, are usually used to describe them. In recent years, the attention has been focused on complex modules as the basis for a systematic description of polytypes and homologous/polysomatic series (modular structures). This representation is applied to the modeling of unknown structures and understanding nanoscale defects and intergrowths in materials. The Order/Disorder (OD) theory is fundamental to developing a systematic theory of polytypism, dealing with those structures based on both ordered and disordered stacking of one or more layers. Twinning at both unit-cell and micro-scale, together with disorder, causes many problems, "demons", for computer-based methods of crystal structure determination. This book develops the theory of twinning with the inclusion of worked examples, converting the "demons" into useful indicators for unravelling crystal structure. In spite of the increasing use of the concepts of modular crystallography for characterizing, understanding and tailoring technological crystalline materials, this is the first book to offer a unified treatment of the results, which are spread across many different journals and original papers published over the last twenty years.

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