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book reviews

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Crystallography of modular materials. By Giovanni Ferraris, Emil Makovicky and Stefano Merlino. Pp. x + 370. Oxford: Oxford University Press, 2004. Price Hardback GBP 75.00. ISBN 0-19-852664-4.

This book appears as the fifteenth volume in the series *IUCr Monographs on Crystallography* with the aim to provide a unified treatment of results concerning the crystallographic nature of modular structures scattered across different journals and original papers, mainly within the last 20 years. This endeavor resulted in the *first comprehensive* book of this sort. It contains five chapters whose authorship is not given explicitly (also the list of references is common), but the style of Chapters 1 and 3, Chapter 2, and Chapters 4 and 5 is typical for E. Makovicky, S. Merlino and G. Ferraris, respectively. The individual chapters are *de facto* revised and extended chapters of these authors in the European Mineralogical Union Notes in Mineralogy 1: *Modular Aspects of Minerals*, edited by S. Merlino and published for the EMU School of Mineralogy in Budapest in December 1997. The authors should be congratulated for their work.

A crystallographic approach to modular structures depends largely on the personality and individual taste of the respective scientist. Therefore, the following characteristics of the five chapters reflect my personal opinion.

Chapter 1: *Modular series – principles and types* (126 pages, 71 figures, 28 tables, ~390 references). The most important part of this chapter is the homologous series – those of sulfosalts cover the dominant part of the author's research which started in the sixties, together with Vladimir Kupčík in Bratislava, using material from the Slovak polymetallic ore deposits, and which later gained him an international reputation. Accretional homologous series are considered to be more general than polysomatic series, and their quantitative characteristics are defined. The reader will appreciate that the results scattered hitherto in the literature are concentrated here. The relatively strict rules governing homologous series are then relaxed (*mero-* and *plesiotypes*) so that this enables classification of a wide variety of modular configurations to understand mutual relations as well as to predict new modular structures. It is commendable that also some consequences of a modular build-up in the reciprocal space are indicated. This line of research should deserve more attention in the future.

The author displays here in an impressive way his knowledge and overview over a huge amount of material and the chapter has great encyclopedic value. It is not easy to read. Figures of some structures without additional editing are illustrative rather than informative and the hierarchy of sub-headings is not always consistent. The terminology concerning symmetry properties is a bit 'liberal' (*e.g.* Structures ... contain 2-fold axes and −1 as operators ..., Table 1.12), and the use of the suffix *-typy* instead of the commonly used *-typism* seems to have a 'Russian accent'. The content of Section 1.4.1 dealing with various *cell twinnings* shows – I feel – a development of Ito's (1950) original ideas into a non-transparent territory. By the way: Ito introduces *twinning groups* but he does not mention OD groupoids (p. 2).

Chapter 2. *OD structures* (80 pages, 52 figures, 5 tables, ~120 references). The author starts with some motivations leading to the concept of OD structures which became a theory of symmetry of polytypic structures. To introduce the reader to the terminology and procedures, the author uses wollastonite which played a prominent role in Ito's *Studies on polymorphism* (1950) and which, in turn, was also among the inspirations leading Dornberger-Schiff to the foundation of her OD theory. Basic terms and definitions are given for OD structures of equivalent layers and also for those of M kinds of layers, accompanied with numerous, both artificial and real, examples and figures, either conventional with coordination polyhedra or symbolic ones, showing just the relevant symmetry. A treatment of the tobermorite family – the author's favorite – illustrates the heuristic power of the OD approach, not only within this family but later also between OD families of different substances but with the same OD groupoid family. The chapter contains also a table of monoclinic and orthorhombic OD groupoid families and an example of how to calculate the Fourier transform of the wollastonite family, explaining its diffraction patterns.

This chapter is well written and suitable for acquiring basic knowledge for reading OD papers. Shortcomings are rare: the OD groupoid family of clinotobermorite should be that of category II (not I, as given), not all generating τ operations are MDO-generating operations and the usage of hyphens (-) instead of dots (.) to indicate missing symmetry in the symbols for coincidence operations, is a bit unusual.

Chapter 3: *Polytypes and polytype categories* (20 pages, 16 figures, 1 table, ~60 references). This is the most problematic chapter. In an effort to adapt the terminology to 'everyday usage', the definition of polytypes is widened to such an extent that polytypism becomes no more than a special case of polymorphism and its notion deviates significantly from the original ideas of Baumhauer who introduced in 1912–1915 the terms *polytype* and *polytypism* (by the way, the confusion of a *lattice* for a *crystal structure* was also 'everyday usage' in the past and it persists even today).

When referring to OD structures, the author is quite generous in his terminology, which often deviates from convention (*e.g.* OD layers become also *unit layers*, a pair of adjacent OD layers appears also as *two distinct configurations on interlayer contact*). Assertions that some structures are OD structures, given without proofs or references, are hardly reliable. An attempt to range isochemical OD polytypes belonging to different OD families (gibbsite/bayerite, polytypes within the serpentine–kaolin group) into a category of *non-OD polytypes* is controversial. In contrast to crystal chemical modules, OD layers are *disjunct* units defined from the point of view of symmetry, and thus also the statement that – *mutatis mutandis* – the choice of OD layers may destroy coordination polyhedra, is not appropriate because *e.g.* the choice of a unit cell may do the same. OD theory is a theory of symmetry, an OD interpretation does not compete with crystal chemical analysis of a structure; actually it follows from it and thus it cannot substitute a 'penetrating structure analysis' (p. 213).

Chapter 4: *Application of modularity to structure description and modelling* (53 pages, 36 figures, 2 tables, ~230 references). The author treats modular structures as polysomatic series and stresses the advantages of this approach, *e.g.* the fact that, in principle, each module may exist as an end member. This indicates the structural stability of some modules and explains why they occur in numerous compounds. The most important factor ruling the mutual fitting of modules together is the *dimensional* one. In the special part, the author groups polysomatic series according to the dominant modules, especially those of perovskite (including high-temperature superconductors), spinel and mica. Very useful also is the section dealing with relatively new modules which can serve not only for structure descriptions but also as inspirations for tailoring new materials.

The chapter has a logical build-up and the didactic and encyclopedic aspects are balanced. Figures are instructive and those illustrating concrete structures and drawn by computer are edited so that they are better understandable, even if the labeling of crystal axes is missing. The use of references in the figure captions is not consistent.

Chapter 5: *Modularity at crystal scale – twinning* (29 pages, 5 figures, ~70 references). This chapter has two dominant parts: classification of twins and consequences of twinning. The classification follows the French school based on the geometrical properties of the lattice and repeats the main terms and definitions. The second part is the author's favorite: how twinning influences the diffraction pattern and how this can be 'detwinned'. Numerous examples of successful structure solutions of twinned crystals are presented and the author's message is clear: don't use a computer as a 'black box', and first analyze thoroughly the diffraction pattern of your crystal!

The positive aspects of the second part hide somewhat a flaw in the first part: the ideas of Buerger (1945) on the role of a concrete atomic structure in the twinnig process are just mentioned but not developed. The ideas of Holser (1958) concerning the structure and symmetry properties of the 'slice' common to both twin individuals and, closely related to them, the OD twinning would also deserve some attention (the latter is treated only in Chapter 2).

For its very high informational value, this book is recommended to a wide community of mineralogist, chemists, physicists and materials scientists, and its second edition appears to be only a matter of time. Therefore, the authors might start working on some improvements to facilitate orientation in this extensive material:

- include a complete list of contents with sub-headings at all hierarchical levels;
- include an author index;
- revise thoroughly the subject index: in its present form it is superficial and does not unify the individual chapters;
- improve cross references between chapters;
- some entries in the list of references are not indicated in the main text and in tables and *vice versa*, there are also some discrepancies in the dates of publication;
- remove errors in the running titles in Chapters 2 and 3;
- the terms (symmetry) *operation* and (symmetry) *operator* are used as synonyms at random throughout the book. Since this phenomenon appears also elsewhere and *this is an IUCr publication*, the authors should define the difference between these two terms and state explicitly in what context they should be used.

As a whole, this is, also due to the effort of the publishers at Oxford, a handsome book and the authors are thanked for their pioneering work.

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