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Foundations of Crystallography

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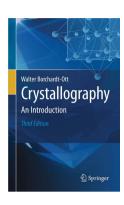
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#### book reviews

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**Crystallography – An Introduction**, 3rd ed. By Walter Borchardt-Ott. Springer, 2012. Pp. xvi + 357. Price (paperback) EUR 42.75. ISBN 978-3-642-16451-4.

The third edition of *Crystallography – An Introduction* is the English version of the seventh edition of the German book *Kristallographie*, which was first published in 1976. It is the result of the author's several decades of experience of teaching in Münster. The strength

of this book is clearly in the solved exercises (more than a hundred) and in the presence of 22 patterns for polyhedra that the reader can copy, cut and paste to obtain a three-dimensional paper model, which is certainly useful for self-study when wooden models are not available. The text itself has quite modest ambitions, being a rather intuitive and less formal introduction to classical geometric crystallography with the addition, in the last edition, of a limited discussion of X-ray diffraction (mainly powder) and elementary crystal chemistry.

The presentation is clearly for beginners and the target readership is students with a weak background in mathematics. In fact, the formalism is reduced to a minimum, as shown by the absence of a fundamental tool like the metric tensor. The concept of a group is introduced only at page 237, but it is mentioned and used well before, although in an intuitive way. This choice is clearly anti-pedagogical: one may guess that it comes from the intention to avoid scaring readers less prone to abstract thinking, but with the risk, nevertheless, that they may be puzzled by the use of an undefined notion. A serious sin of this book is the use of the term 'crystal system' to indicate three different concepts: the crystal family, the lattice system and the (true) crystal system. It is far from being a defect exclusive to this text, but it is highly regrettable that this widespread confusion still affects a textbook published so recently.

The bulk of the book consists of geometric crystallography. Chapter 1 is just a one-page introduction. Chapter 2 (*The Crystalline State*, 6 pp.) is a nice presentation of the states of matter with obvious emphasis on the crystalline state. Chapter 3 (*The Lattice and Its Properties*, 13 pp.) presents one-, two-and three-dimensional lattices, introduces standard notations for lattice directions and Miller indices of planes, and ends with the zonal equation. Only primitive cells are introduced and thus only co-prime Miller indices are allowed. Unfortunately, when centred cells are introduced later (Chapter 7), the consequences on the relative values of Miller indices are not shown.

Chapter 4 (Crystal Structure, 6 pp.) starts with a problematic statement: 'In order to progress from a lattice to a crystal, the points of the lattice must be occupied by atoms, ions or molecules.' This affirmation is a trap for a beginner, who is led to think that atoms can sit only on lattice nodes, a mistake that is unfortunately much more widespread than one may think. The atomic content of a unit cell is called a *basis*, which again easily raises confusion with the basis used to define the lattice vectors: an unfortunate choice of terms. A generic example composed of three types of atoms is used to illustrate the concept of crystal structure: one sitting at the origin and two others in general positions, but all with multiplicity 1. Only two concrete examples are given, which are again far from being of general type:  $\alpha$ -polonium and caesium iodide. The beginner certainly does not get an idea of how complex crystal structures can be.

Chapter 5 (*Morphology*, 31 pp.) presents in detail the classical topics of crystal morphology, in particular the stereographic projection, the Wulff net and the procedure for indexing the faces of a crystal, with some consideration of the reflecting goniometer and the gnomonic and orthographic projections. The relative length of this chapter with respect to the briefness of the previous one on crystal structure clearly contrasts with the relative importance of these two topics in contemporary crystallography.

Chapter 6 (*Principles of Symmetry*, 14 pp.) introduces symmetry elements. In the presentation of rotation axes confusion is made between two- and three-dimensional spaces. The term 'axis' clearly indicates the latter (in two dimensions they would be rotation *points*), but then we read that 'the lattices resulting from sixfold and threefold axes are, in fact, equal', which is true only in two dimensions.

Chapter 7 (*The 14 Bravais Lattices*, 44 pp.) owes its length to the presence of many figures. The chapter is affected by a frustrating confusion between 'lattice' and 'crystal system', which produces a monster like 'trigonal *R*-lattice' to indicate the conventional triple cell (hexagonal setting) of a rhombohedral lattice. Space-group diagrams are given to show the symmetry of lattices *before* the notion of a group (let alone a space group) is introduced much later. Furthermore, the diagrams are incomplete, showing only symmetry elements without screw or glide components, because these are 'irrelevant' to the discussion of the symmetry of lattices. The simplification effort clearly goes too far.

Chapter 8 (*The Seven Crystal Systems*, 4 pp.) defines (wrongly) the crystal systems, already used in the previous chapters. The definition given corresponds to the crystal family, which obviously leads to problems when considering the split of the hexagonal *system* (actually *family*) into the

hexagonal-trigonal pair (of *crystal systems*) and into the hexagonal-rhombohedral pair (of *lattice systems*).

Chapter 9 (*Point Groups*, 66 pp.) should have been preceded by the definition of a group. Crystal forms are analysed in detail and classified into *general*, *special* and *limiting* forms (the counterpart *basic* is not used); the eigensymmetry of forms is given for tetragonal forms but is not used to classify them into characteristic (a term used twice but not defined) and non-characteristic forms. A brief glimpse of molecular symmetry is followed by a set of criteria for determining the point group, the results of which are collected in Table 9.10. Possible physical properties associated with each point group (enantiomorphism, optical activity, piezoelectricity, pyroelectricity) are briefly analysed. Table 9.11 gives, for each type of point group, one molecular and one crystalline example. A short note on non-crystallographic point groups and on Platonic solids closes this chapter.

Chapter 10 (*Space Groups*, 33 pp.) presents a short introduction to glide planes and screw axes, followed by a very quick discussion of space groups (actually, *types* of space groups), which culminates in a compact table. The rest of the chapter discusses general and special positions and site symmetry, and shows the intuitive generation of a few space groups as a combination of symmetry operations, with a non-standard tail added to atoms in the projection, and explains how to obtain the number of formula units.

Chapter 11 (Symmetry Groups, 22 pp.) gives the matrix representations of symmetry operations and finally the definition of a group, where a serious slip occurs when the combination of symmetry elements (instead of operations) is mentioned. The term Abelian is used without being defined; on the previous page the term commutative is used instead.

Chapter 12 (Fundamentals of Crystal Chemistry, 31 pp.) presents the types of chemical bonds, common coordination polyhedra, sphere packings and ionic radii. The term lattice energy is used without being defined. Pauling's third rule is mentioned, the others are applied without making reference to Pauling. A reasonable account of isomorphism, polymorphism and types of phase transitions – without reference to thermodynamics, however – completes the chapter.

Chapter 13 (Studies of Crystals by X-ray Diffraction, 16 pp.) gives a very brief introduction to a subject which is so widely treated elsewhere that its presence here, in such a reduced form, is hard to justify. Nothing is said about the physics of the interaction of radiation with matter; Bragg's law is introduced in an axiomatic way; and the only method presented is the Debye–Scherrer method (the precession method is mentioned en passant and in the caption of the only diffraction pattern shown). After a geometric introduction to the reciprocal lattice and Laue groups, the possible placements of atoms of binary compounds (SnO<sub>2</sub> and CsI) in the unit cell are derived on the basis of simple crystal–chemical considerations

(avoiding overlap and respecting the stoichiometry): this heuristic procedure, presented under the section title *The determination of a crystal structure*, may give the beginner the wrong impression that solving a crystal structure is an easy task which can be performed using a pencil and ruler. Nothing is said about structure factors, systematic absences, data treatment, structure solution or refinement: the usefulness of this chapter is limited.

Chapter 14 (*Crystal Defects*, 8 pp.) is a short qualitative presentation of point, line and planar defects. Chapter 15 (*Appendix*, 20 pp.) contains a summary of symbols; a table of formulas for interatomic distances in the six crystal families which the reader will not be able to understand without the metric tensor; drawings of crystal forms; and the already mentioned paper models. The final chapter contains the solutions to the exercises and is followed by 49 references (17 in German) and a detailed index.

Several non-standard notations are used throughout the book. Direction indices [uvw] and Miller indices (hkl) are almost always given in roman typeface instead of italics. The end of a polar rotation axis is indicated by white symbols. The circle of projection in the stereographic projection is drawn dashed, following the American convention instead of the international standards. Similarly for the cross used instead of filled dots in some but not all of the figures in Chapter 9. Angular brackets to indicate symmetry-related directions are also used for axis labels (example: (a)). Crystal classes are considered synonyms for crystallographic point groups, whereas (1) a class is not a group, and (2) there exists an isomorphism between crystal classes and types of point group, not point groups. Fig. 9.3 is a distorted copy of Fig. 10.1.3.2 in Volume A of International Tables for Crystallography, giving the group-subgroup relations for point groups. To reproduce a figure about symmetry groups with an affine deformation invites a smile.

The author's background in mineralogy is clearly evident from the way the topics are organised and presented, with the balance of morphology *versus* structure too much in favour of the former. The presence of many solved exercises is definitely a positive aspect of this book. The paper models for studying morphology are nice but probably of limited interest for the majority of the readership that would be attracted by the general title of the book. The intuitive way in which the topics are introduced may meet the favour of a reader uncomfortable with a more rigorous formalism: the *rendezvous* is, however, only postponed and unavoidable if they want or need to go beyond the surface.

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