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book reviews

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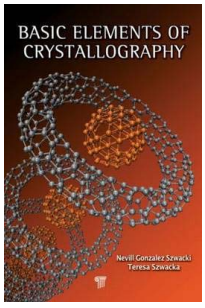

Basic Elements of Crystallography. By Nevill Gonzalez Szwacki and Teresa Szwacka. Pan Stanford Publishing, 2010. Pp. xi + 195. Price (paperback) GBP 49.99. ISBN 978-981-4241-59-5.

The well known difficulties in maintaining courses specifically devoted to crystallography in university curricula mean that researchers and technical staff often have to compensate for the lack of, or insufficient, crystallographic education in their academic career by *in-the-field* experience with a significant amount of self-training. The need for textbooks in crystallography is therefore self-evident, but, because of the multidisciplinary nature of our field and the huge number of subjects to cover, it is virtually impossible to find a single text covering everything. A large number of textbooks of crystallography have been published and continue to be published since Haüy's time, so we can expect that when a new book comes out, it either covers some aspects that have been insufficiently presented so far, or at least presents known facts in a different perspective, perhaps easier to approach by readers with a specific background. *Basic Elements of Crystallography* does not fit either criterion. Far from introducing something new, or even shedding new light on something well known, this text adds some more noise in a panorama where the signal (valuable texts of crystallography) is already endangered by a high level of noise (texts repeating common knowledge or even introducing macroscopic mistakes).

In the preface of the book, we learn that it 'is intended to be a complete and clear introduction to the field of crystallography for undergraduate and graduate students and lecturers'. Actually, it is neither complete nor clear; after carefully reading it, one even has reasonable doubts whether it may fit the term 'introduction'. The preface also states that 'The entire notation in this book is consistent with the *International Tables for Crystallography*': a commitment as unfaithful as the promises of a politician right before general elections. Indeed, *Basic Elements of Crystallography* is characterised by the absence (one could even say *systematic*) of almost everything one would expect in a book of crystallography. It is probably the only text where the notion of 'group' is absent – not even mentioned in the whole book (to be fully honest, the expression 'point-group symmetry' is mentioned in the preface, but immediately forgotten). It is also one of the few books on crystallography where matrices are completely absent (do not look for the metric tensor, you will not find any trace of it). The last, but not least, absence is diffraction: no trace of it whatsoever. So, what is this book about? In short, it is about Bravais lattices (Chapters 1 and 2, 65 pp.), and structure types of elements and of binary compounds (Chapters 3 and 4, 86 pp.), with a sort of appendix about the reciprocal lattice (Chapters 5 and 6, 30 pp.), whose presence, in a book that does not say a word about diffraction or morphology, is difficult to justify. A very narrow target even for a book aiming at giving only 'basic elements'.

Chapter 1 (pp. 1–15) is called *Crystal structure*, which is a far too ambitious title because it is essentially about one- and two-dimensional *lattices*, while the only direct reference to the *structure* is in the atomic 'basis' (read: number of atoms in the unit cell). The notions of translation vector, basis vector, and primitive and centred unit cell represent the bulk of this chapter. After a typographical error ('filed' for 'filled') which does not harm the reading, we learn about such a strange thing as the 'volume' of one-dimensional (p. 2) and two-dimensional cells (p. 4). On p. 5 the derailment begins, when we meet the terms *conventional primitive cell* and *conventional basis vectors*, which are used before being defined. We soon understand that these are *conventional* in the sense that they are those *conventionally used*, so that cells with the symmetry of the lattice and the primitive cell with a lower symmetry are both allowed to use the title of 'conventional': it is a pity that the *International Tables* give a precise definition of conventional unit cell that does not have much to do with the meaning given in this book. [A conventional unit cell is the smallest unit cell having its edges parallel to the symmetry directions of the lattice. This definition leaves some degree of freedom for low-symmetry lattices (oblique in two dimensions as well as triclinic and monoclinic for three dimensions: see Volume A, §2.1.3).] On p. 8 the hexagonal cell of the honeycomb structure has an interaxial angle of 60° ('The entire notation in this book is consistent with the *International Tables for Crystallography*', remember?), which, strangely enough, due to a different choice of axes, becomes 120° when the hexagonal lattice is shown on p. 10.

Chapter 2 introduces three-dimensional lattices, by graphic inspection of the unit cells chosen to represent these lattices. More than six pages are devoted to derive the symmetry axes (yes, only the axes) of the three types of cubic lattices. On p. 24 the concept of lattice system is introduced, but wrongly called 'crystal system'. Nowhere in the book are the crystal systems presented; it is always matter of lattice systems: wrong title. The confusion reaches its summit precisely where so many predecessors have fallen too: the *rhombohedral* lattice is called *trigonal* (that the primitive cell is a *rhombohedron* does not seem to raise any doubt in the mind of the authors).

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Trigonal is an adjective that characterizes a crystal system, not a lattice. It is to be noted that the unit-cell parameters for all the lattice systems are called a_1, a_2, a_3, $\sphericalangle(a_1, a_2)$, $\sphericalangle(a_1, a_3)$, $\sphericalangle(a_2, a_3)$ ('The entire notation in this book is consistent with the *International Tables for Crystallography*', remember?). The next ten pages are devoted to a graphical presentation of the Bravais lattices: *nihil sub sole novi*, Bravais did a better job in 1850. Suddenly, the reader is introduced to the coordination number (for a lattice? Yes, for a lattice!), which is applied for the rest of the chapter, where some demonstrations (only for cubic lattices) that would have pleased *Monsieur de La Palisse* are presented: that the volume ratio of a centred cell and a primitive cell coincides with the number of nodes in the former; that different lattice nodes within a unit cell have equivalent positions in the lattice described by that cell. The narration proceeds with the most stunning performance in the whole book. An unconventional rhombohedral *I*-centred cell is introduced on p. 47 as an alternative, double cell for the description of the cubic primitive (called 'simple cubic' or *sc*) lattice. This cell is in fact used as an intermediate in the description of 'monoatomic' simple cubic structures (that 'monoatomic' means 'made by a single atom' is a venial sin with respect to what follows). Here we have a cubic primitive lattice containing only one atom in the unit cell (called '1-atom basis': the atom must of course occupy a special position of the highest site-symmetry group, but we already know that the concept of 'group' is foreign to this book) giving rise to a 'simple cubic crystal structure'. Because the aforementioned *I*-centred rhombohedral unit cell (double cell of the same lattice) has interaxial angles of 60°, the conclusion is drawn that it corresponds to a *cF* lattice. In other words, by a wave of a magic wand half of the lattice nodes disappear! Obviously, the node at $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ of the double cell has been forgotten in this statement, and this oversight leads to the astonishing conclusion that a *cF* lattice with two atoms in the unit cell gives the same 'simple cubic structure' introduced above. That this is not just a wrong expression but a real misunderstanding is confirmed by the explicit statement that the *cP* lattice 'is not the only Bravais lattice that we can propose to describe the *sc* structure'. *Monsieur de La Palisse* would object that to a given structure only one lattice can be assigned, whatever cell is used to describe it. But the nightmare is not over, because the above expression is immediately applied to the structures of elemental As, Sb, Bi and Hg, which all crystallize in the rhombohedral holohedry. The first three elements have interaxial angles close to 60°, so it is concluded that their structure is close to *simple cubic*: of course, the rhombohedral cell being primitive, the structure is close to *face-centred cubic*. The circle of evil is complete. Chapter 2 ends with a short discussion about the hexagonal axes for a 'trigonal' (read *rhombohedral*) lattice and with the construction of Wigner–Seitz cells for the three cubic types of lattices.

Chapters 3 and 4 introduce some elementary crystal chemistry applied to the structure of elements and binary compounds. A significant amount of space is devoted to tables of cell parameters taken from the literature, given without standard uncertainty. The classical sphere packing is introduced together with the filling factor, computed geometrically by using the radius of the spheres. The awkward expression 'two-dimensional layer of spheres' (with several variations) occurs throughout these chapters. A sphere being a three-dimensional object, a layer made of spheres cannot of course be two-dimensional: either the layer is made of circles, or it is three-dimensional, although diperiodic. The interstices formed by the stacking of layers are briefly introduced before proceeding to the analysis of simple structures in the classical ABC notation (Zoltai and Stout, in their 1984 book *Mineralogy: Concepts and Principles*, introduced a much better systematization of the topology of sphere packings and the resulting coordination polyhedra).

Chapter 4 starts with the upper and lower limit on the ratio of the ionic radii for a given coordination number: Pauling derived this as his first rule in 1929. Then, the structures of ZnS, CaF_2, NaCl, NiAs, TiAs and CsCl are presented. The percentage of ionic bond is given precisely, but with no indication of how these values have been computed. It would have been interesting to know how a 62% ionic bond has been calculated for ZnS (p. 108), which is an intrinsic semiconductor, although with a wide gap. A calculation shows that sphalerite and wurtzite have the same number of nearest neighbours and next-nearest neighbours: *Monsieur de La Palisse* would not expect that much, given that the two structures are polytypic.

Chapter 5 introduces the reciprocal lattice, which 'plays an important role in the description of the physical properties of crystalline materials'. Pity that none of these properties is ever mentioned. The scalar product of direct and reciprocal basis vectors gives 2π as a result, and the cell parameters are measured in 'meters' and 'inverse meters' ('The entire notation in this book is consistent with the *International Tables for Crystallography*', remember?). The calculation of the reciprocal of a triclinic type of lattice and of the cubic types of lattices ends this chapter.

The last chapter presents Miller indices and the interplanar distance. Curly brackets are introduced to indicate lattice planes that are equivalent 'by symmetry of the *lattice*': the notions of merohedry and of symmetry group being unknown in this book, the reader is led to think that lattice planes cannot be equivalent under a symmetry lower than that of the lattice. It is easy to imagine their surprise when they approach a more serious book and learn the concept of crystal form and of symmetry-related diffraction intensities.

The book contains several nice drawings and is completed by a series of exercises at the end of each chapter. This effort does not compensate for the flaws, mistakes and limits of the whole content. It remains an alert for academic authorities who should wake up and understand the desperate need for solid crystallographic education, without which books like this will continue to be produced. It is far from being the first accident in the crystallographic literature, and unfortunately it will not be the last.

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To conclude, if you happen to see this book in a store, follow Virgil's recommendation to Dante when they met the Uncommitted in the vestibule of Hell: 'Let us not speak of them – look and pass by'.

Massimo Nespolo

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