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book reviews

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Foundations of Crystallography with Computer Applications. By Maureen M. Julian. Boca Raton: CRC Press, 2008. Pp. xxvi + 340. Price (hardback) GBP 55.00. ISBN 978-1-4200-6075-1.

The book *Foundations of Crystallography with Computer Applications* by Dr M. Julian is based on the crystallography course that the author has been teaching since 2000 in the Materials Science and Engineering Department at Virginia Tech, Blacksburg, Virginia. The book reviews the fundamentals of crystallography and is intended to provide a tutorial and a practical guide for university undergraduate and college students interested in crystallography and material sciences in general. The mathematical prerequisites for the book are reduced to an introductory knowledge of matrix algebra and familiarity with *MATLAB* or similar computer languages. This widens the potential readership of the book to students in biology, chemistry, physics, geological sciences and engineering.

The book consists of an introduction and seven chapters. The first five chapters develop the appropriate mathematical tools related to the basic geometrical and algebraic components of mathematical crystallography. Chapter 1 is devoted to the introduction of lattices and their mathematical description. In Chapter 2, the basis of unit-cell calculations is developed applying the metric-tensor formalism. After a detailed description of two-dimensional point groups, the three-dimensional point groups and their group–subgroup relations are discussed in Chapter 3. The first part of Chapter 4 deals with the 17 two-dimensional plane (also known as 'wallpaper') groups while the second part is devoted to the introduction of the 230 three-dimensional space-group symmetries. In Chapter 5 the reciprocal lattice is defined, its general properties are reviewed, and the relationships between direct and reciprocal lattices are derived. While the first five chapters provide an introduction to the principles of symmetry in crystallography, the last two chapters are devoted to more experimental aspects of crystallography: the discovery and the properties of X-rays and an introduction to X-ray diffraction phenomena are the subjects of Chapter 6. Finally, Chapter 7 focuses on atomic scattering factors and structure factors, and their application in calculations of electron-density maps. The book closes with a short reference and bibliography section, an appendix with definitions of important notions and terms used in the text, and a subject index.

In my opinion, the main strength of this book lies in the clear and pedagogical presentation of the material. The well set out didactic presentation of the individual chapters (*e.g.*, each chapter starts with a presentation of the learning objectives and closes with a list of the important terms defined in the chapter, the definitions and example problems are highlighted throughout the text *etc*.) is very beneficial for students and provides instructors with a good overview of the material to be covered. Care has been taken so that the essence of the topic is presented in an educational and concise fashion. For this, part of the more complex mathematics is very often truncated or greatly abbreviated, since the algebraic details (available elsewhere) can often obscure the salient facts. The large amount of space dedicated to explaining even the simplest concepts makes the book easy to read for undergraduates, including life-sciences students whose mathematical background, in general, is more limited. The author offers the reader a number of illustrative and worked-out examples within the text which reinforce understanding of the subject. Abstract and more complicated mathematical concepts are complemented by a visual approach, including a number of high-quality graphical presentations (more than 250 figures), numerous (more than 80) tables and panels with illustrative data that add a qualitative perspective to the problem being treated. For clarity and overall understanding the crystallographic ideas are first developed in two dimensions, which is then followed by a transition to three dimensions. Two model examples – hexamethylbenzene, a centrosymmetric crystal, and anhydrous alum, a noncentrosymmetric structure typical of ceramics and metals – are chosen as model crystals and are used throughout the book to explain symmetry, point groups, space groups, Bravais lattices, reciprocal lattices and diffraction maxima. At the end of each chapter there are exercises (in total more than 200), varying widely in level of difficulty, which provide practice and extend the student's knowledge. Among them one finds a number of computer-based exercises, accompanied by *MATLAB* starter programs for facilitating the necessary computing. The possible use of computer applications allows easy computation of important crystallographic quantities such as bond lengths, bond angles, unit-cell volumes, reciprocal-lattice constants, interplanar angles and *d*-spacings in all the crystal systems.

It is surprising that such a pedagogical presentation of the material is not accompanied by a more selective reference scheme to the corresponding literature. At the end of the book one can find a bibliography section but it would be much more useful for the students if each chapter closes with a list of references to the primary literature on the subject that has been treated, followed by a list of sources for further reading.

I find it very positive that the author makes frequent references to *International Tables for Crystallography*, Volume A, *Space-Group Symmetry* (referred to as ITA in the following). The conventions and notation used throughout the book are consistent with ITA. In addition, two sections of Chapter 4 are devoted to the interpretation of the space-group

symmetry data tabulated in ITA. It is a pity, however, that for these explanations the author has used sample pages from the fourth (1996) edition of ITA, and not from the most recent fifth edition (2002). See, for example, the pages for the space groups $P\bar{1}$ (Figs. 4.72 and 4.73) and $P321$ (Figs. 4.81 and 4.82).

The author should be congratulated for developing a website for the book (http://foundations-of-crystallography.com), which in principle offers unlimited possibilities for additional online material related to the book. On this website the reader can consult an updated list of corrections to the printed edition of the book. It is a bit disappointing that some of the pages of the website are still under construction. Apart from the solutions to the exercises, accessible under the 'Resources for the Instructor' link, the rest of the data provided online are limited to information already available in the printed book. [For example, there are four links under the 'Resources for Students' menu: two of the links are to pages which are under construction ('Crystal Examples' and 'Web Links'), while the other two – 'Starter Programs' and 'Homework Exercises' – repeat the data in the book.]

Unfortunately, the book is not free from imperfections. One can find incorrect and inaccurate statements that, in my opinion, are unacceptable, especially in a book addressed to students. Some examples are given in the following. On p. 94, in the explanations of the Hermann–Mauguin symbol of the point group $2mm$ we read that the two m's in the symbol indicate that 'the two mirrors are perpendicular to each other'. On the next page we learn that 'There is only one m in the symbol of $3m$. This notation indicates that the mirror planes in $3m$ are not orthogonal.' Similar statements are given for $4mm$ (p. 98) and $6mm$ (p. 99). In fact, the Hermann–Mauguin symbols for the crystallographic point groups refer to the (sets of symmetrically equivalent) symmetry directions of the lattice point groups: the character in each position of the symbol designates the symmetry elements that occur for the corresponding symmetry direction. For example, the three different mirror planes in the group $3m$ are represented by one m in the Hermann–Mauguin symbol because they are equivalent due to the threefold axis.

The definitions of t- and k- subgroups of space groups given in the book are not correct (*e.g.* Chapter 4.8 and the definitions in the appendix). According to the author the t- (or k-) subgroups of space groups are maximal subgroups, which is definitely not true, as non-maximal subgroups can also be t- (or k-) subgroups. Similar errors are found in the discussions of t- and k- supergroups of space groups which, according to the definitions in the appendix, are limited to minimal supergroups only.

I agree that a pedagogical presentation of a problem often requires simplifications of explanations. However, such didactic simplifications should not lead to misunderstandings, especially when the text is addressed to inexperienced readers. Unfortunately this is the case when group–subgroup relations of crystallographic groups are treated. For example, consider the group–subgroup tree of point groups shown in Figs. 3.37 and 3.38, which is a simplified version of the point-group graph that can be found, for example, in ITA Fig. 10.1.3.1. I would accept that the terms conjugate and/or normal subgroups are probably not obligatory for the introductory level of presentation of the group–subgroup relations in this book. However, the author could at least have indicated that the graphs of Figs. 3.37 and 3.38 are of the contracted type, *i.e.* each node of the graph may correspond to different subgroups of the same type. For example, the node m of the graphs indicates three different (conjugate) subgroups for the group–subgroup pair $3m > m$, or two (normal) subgroups for $2mm > m$. Similar considerations apply to the graph given in Fig. 3.45.

Another example is related to the t-supergroups of space groups, which are discussed following the group–supergroup relations between the corresponding point groups (see *e.g.* Chapter 4.8). However, one should use this analogy with extreme care owing to the specific and more complicated structure of the space groups. For example, although there is just one supergroup of type 4 of the point group 2, there are two minimal t-supergroups $p4$ of $p2$: one with the origin coinciding with that of $p2$, and another one with an origin which is shifted by $\frac{1}{2}\mathbf{a}$ (or equivalently by $\frac{1}{2}\mathbf{b}$). Further, in considering group–supergroup relations between space groups that belong to different crystal systems, one should always check whether the lattice parameters of the group fulfil the corresponding lattice conditions of the supergroup. Otherwise, the supergroups do not represent space groups. For example, the plane group $p4$ is a minimal t-supergroup of $p2$ only if the lattice parameters of $p2$ satisfy the conditions $a = b$ and $\gamma = 90^\circ$. Bearing in mind the above comments on group–supergroup relations of space groups, I would definitely recommend that the author carefully reconsiders the text of Example 4.1 (Chapter 4.8) for the next edition of the book.

Some typographical errors, misprints and imperfections in the drawings are inevitable in a book like this. Some examples are given in the following: the stereographic projection for the point group 2 in Table 3.21 (p. 108) corresponds to the unique axis c setting, while the corresponding matrix–column pair description in Table 3.20 (p. 107) refers to the unique axis b setting; there is a similar problem with the data of group $2/m$ in Table 3.27; there seems to be a common typographical problem with the boundary lines of the asymmetric units: the bold lines that are used can be confused with symbols for mirror planes, *e.g.* Fig. 4.50 (p. 159); also in Fig. 4.50 the symbol and the asymmetric unit of $p4gm$ are not correct, and the choices of the asymmetric units of $p4mm$ and $p6mm$ do not coincide with the choices of ITA; a misprint in the formula for the area of the asymmetric unit (p. 160); an error in the general-position diagram of $P\bar{1}$, Fig. 4.72 (p. 183); several imperfections in the reproduction of the second page of ITA of $P\bar{1}$ in Fig. 4.73 (p. 184); an error in the symmetry-operation diagram of $P321$ in Fig. 4.81 (p. 191); and several misprints in the explanations of the subgroups of $P321$, Section 4.13.2 (p. 192).

Leaving these defects aside, my overall estimation of the book is positive. It is a highly illustrated, self-contained textbook covering the fundamentals of crystallography with a

clear didactic purpose for undergraduate and college courses within materials science and engineering. I believe that the drawbacks mentioned above can be remedied in a future edition without much effort and that the book can be useful for undergraduate and college students with an interest in crystallography.

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