Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (J. H. Robertson, School of Chemistry, University of Leeds, Leeds LS2 9JT, England). As far as practicable books will be reviewed in a country different from that of publication.

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International tables for crystallography. Vol. A. Edited by TH. HAHN. Pp. xvi+854. Dordrecht: Reidel, 1983. Price Dfl 385.00, US $165.00, £80.00; or, for individual crystallographers, Dfl 215.00, US $90.00, £45.00.

This book is a new version of the well known *International Tables for X-ray Crystallography*, Vol. I, *Symmetry Groups* (first edition 1952), familiar to every crystallographer. The difference in the titles of these two versions reflects the main aim of this new book - *IT*, Vol. A (1983), as we shall now refer to it - which, according to the editor's intention, is 'to provide data and text which are useful for all aspects of crystallography'.

The present volume deals with the symmetries of one-, two- and three-dimensional space groups and point groups in direct space without extension to 'generalized symmetry'. Its most striking feature is a considerable increase in size [854 pages, *i.e.* 53% more than in Vol. I (1952)], which is the result of an important extension of the contents. No wonder that such an impressive work had to be undertaken by an editorial team of experts three times larger than before.

A pleasant invitation to reading which we encounter immediately after opening the huge book is a short explanation of the space-group data given inside the front and back covers.

IT, Vol. A (1983) consists of two parts. Part I, 'Tables for Plane Groups and Space Groups', is designed mainly for practical use. Part II, 'Symmetry for Crystallography', contains the necessary theoretical background for all the topics which appear in Part I.

In Part I there are five short sections which should be read before making profitable use of the plane- and space-group tables given in Sections 6 and 7 respectively.

Section 1 (Th. Hahn) gives definitions of the symbols and terms which occur throughout the whole of Vol. A. It has important tables which contain printed and graphic symbols for symmetry elements in a clear form, much extended in comparison with *IT*, Vol. I (1952). They involve graphic symbols applied in the newly introduced diagrams of the cubic space groups as well as useful detailed definitions of all glide-plane symbols. As reviewers, we would, however, feel better if the definition of the rotation operations given in Table 1.3 were supplemented with a remark about the way of looking at the designated rotation axis. Such a remark is given in Part II, Section 11.2 (p. 788), but no reference to it is made in Section 1. It would also be good if the entry 'rotation sense definition, 788' were given in the Subject Index before 'rotation, sense of, 789, 790'. In the same table a footnote concerning the usage of the letter **g** for glide reflections should be added with a reference to Section 11 [11.2 (v)].

Section 2 (Th. Hahn & A. Vos, with contributions from other members of the Editorial Committee) is a guide to the use of the Tables.

A lot of work has been carried out to acquaint the reader with the considerably extended and completely revised symmetry tables. There are many novelties and some of them deserve special mention.

(i) In the classification of the space groups the term 'crystal families' has fortunately been introduced to good effect, especially in the case of the trigonal and hexagonal crystal systems and *hP* and *hR* Bravais lattices. It seems to be a nice solution of a long-lasting controversy between different schools of crystallographers.

(ii) The monoclinic space groups are treated with special care: synoptic descriptions of three cell choices are given with a complete demonstration of each of two settings. It seems to us that, for a practising crystallographer, of most importance are the three statements on the selection of the monoclinic cell on p. 38 which may be read as a summary of § 2.16.

(iii) Maximal subgroups and minimal supergroups are thoroughly described with many examples which help the reader to follow the rather difficult text.

(iv) No distinction has been made between 'independent' and 'included' reflection conditions which might be slightly disappointing for those who have become accustomed to these symbols.

Two slight changes we propose below could perhaps help in reading this section. In a paragraph about the symmetry elements not indicated in the full symbols of space groups (§ 2.4, p. 16), Tables 4.1.1, 4.1.2 and 4.1.3 containing additional symmetry elements should be mentioned, together with Tables 4.2.1 and 4.3.1 where extended full symbols are given. In § 2.7 (p. 21) instead of 'second description' ('second' in contrast to the 'first description' which corresponds to the centre of symmetry), we would prefer 'another description' because in the space-group tables the origin in the point of high site symmetry is always taken as origin choice 1.

We have some personal feelings about the newly introduced terminology for reflection conditions: we are not enthusiastic about 'integral' and 'serial' reflection conditions, though we fully accept 'zonal' ones.

Section 3 (A. Vos & M. J. Buerger) provides a discussion on the determination of space groups from diffraction patterns. Here the most important item is Table 3.2 which lists reflection conditions, diffraction symbols and possible space groups, and is much extended in comparison with that in *IT* (1952). The terms used in this table are briefly considered including possible sources of errors in the space-group determination, and some additional methods which give appropriate information about the space group of the crystal structure under consideration.

Section 4 (E. F. Bertaut) contains the synoptic tables of space-group symbols, extended with respect to older versions of *IT*. They are completed with the tables of additional symmetry elements [suppressed in *IT* (1952)] and many examples which show how to use them. These examples are easier to follow when Section 12 from Part II is taken into account and this should be pointed out in a footnote.

This section also gives instructive examples of group-subgroup relations in the cases when maximal subgroups can be recognized from extended and full space-group symbols.

We noticed on p. 60 two printing errors which might be confusing for some readers, namely symbols: '$\begin{matrix} P2_1\,2\,2(51) \\ m\,m\,a \end{matrix}$' instead of '$P\,2_1/m\;2/m\;2/a$ (51)' and '$P2_1/n11$ ($P2/c$)' instead of '$P2_1/n11$ ($P2_1/c$)'.

Section 5 (H. Arnold) deals with transformations in crystallography emphasizing transformations of coordinate systems, while the detailed description of the symmetry operations themselves is given in Section 11. Some important invariants are also considered. As an illustration of rules for the coordinate system transformations the very good example of the relation between low-cristobalite and high-cristobalite structures is presented. A useful list of selected transformation matrices and their inverse matrices makes up Table 5.1, complete with diagrams.

Sections 6 and 7 were prepared with the use of a computer. All the programs for crystallographic calculations and the computer typesetting of the tables were carried out by D. S. Fokkema while the other authors supplied such data for each of the 17 types of plane group and 230 types of space group as headline, Patterson symmetry, origin description, asymmetric unit indication, list of symmetry operations, generators, oriented site-symmetry symbols, maximal non-isomorphic subgroups, maximal isomorphic subgroups of lowest index, and minimal non-isomorphic supergroups. Many of these are new features of the space-group description. Extremely valuable are new types of diagrams for triclinic, specially treated monoclinic, and orthorhombic space groups. Also, cubic space groups are provided with elaborate diagrams including stereodiagrams for the general positions. No wonder that a standard layout requires two pages per space-group type. As reviewers we are delighted by the results of the efforts made to modify the plane- and space-group tables: they are much more informative than the previous versions of *IT*.

Part II consists of sections 8 to 14 and it seems to be important for a more profound understanding of what is going on in the space-group tables.

Section 8 (H. Wondratschek) gives basic concepts and terms used in the modern approach to crystallographic symmetry as well as to classifications of space groups, point groups, lattices, and group–subgroup relations.

Of this useful section the most elegant, clear and instructive chapter is that which treats the coset decomposition of a space group and shows how it can be used in establishing the relations between space and point groups. In connection with this chapter we would like to remind crystallographers of the work of Opechowski and coworkers (Opechowski & Guccione, 1965; Opechowski & Dreyfus, 1971) whose contribution on the application of the coset decomposition formalism in classifications of magnetic structures seems to us quite remarkable.

It is worth mentioning that the definition of such terms as space-group types, arithmetic and geometric crystal classes, Bravais classes of matrices and Bravais types of lattices, Bravais flocks of space groups as well as crystal families, which were not given in *IT* (1952), are presented in a very thorough manner. It is good to have them collected in one section in case one needs a reliable source for this part of crystallographic theory.

The relationships between crystal systems and Bravais systems are well described, which is especially important in the case of the hexagonal family of space groups.

Among other topics, the discussion of sub- and supergroups, with many examples, deserves the special attention of those who study structural relationships and phase transitions.

There are, however, some misleading fragments concerning the definitions of vector space, point space, vector lattices and point lattices (in Section 8.1.3) which might cause confusion rather than build a bridge between mathematicians and theoretical physicists on one side and crystallographers on the other. One of the troublesome notions seems to be the concept of 'finite number of interpenetrating infinite point lattices' which, according to the author, may be used for a description of a crystal structure. It is difficult to infer from the text whether this concept has an old, often-criticized meaning (*e.g.* Fischer, Burzlaff, Hellner & Donnay, 1973) or whether it concerns the lattice complexes introduced in *IT* (1983) in Section 14. We also wonder if the term 'linear part', used for the rotation part of a motion or transformation, here and throughout the whole volume (*e.g.* Section 5), should not be replaced by 'homogeneous part' for the sake of mathematical precision. For the same reason we would suggest adding in a footnote a remark that the 'augmented matrix' can be described as a semiproduct of rotation and translation.

Section 9 (H. Burzlaff, H. Zimmermann & P. M. de Wolff) is a description of crystal lattices and their properties. It also gives the rules for selection of the conventional crystallographic bases on one side and of reduced bases on the other, as well as the relationships between their metric tensor coefficients. Two tables, very helpful in everyday practice, deal with the 44 lattice characters and are a guide for immediate recognition of the lattice symmetry and Bravais type from the reduced basis, and also for the transformation to a conventional basis.

Section 10 (Th. Hahn & H. Klapper) on point groups and crystal classes is remarkably rich both in size and in content. A new feature of the presentation of the point groups is a treatment similar to that for the space groups, *i.e.* each of the 10 two- and 32 three-dimensional point groups is characterized by its Hermann–Mauguin and Schoenflies symbols, a pair of stereographic projections (one displaying a general form and point form and the other with the framework of the symmetry elements), matrix representation of the group-symmetry operations, as well as general, special and limiting forms classified into Wyckoff positions; even the symmetries of special projections are added. There is also a useful table which reviews the 47 face forms and point forms, taking into account their eigensymmetries and occurrence in the crystallographic point groups. Subgroups and supergroups of the crystallographic point groups are also discussed and depicted in the form of family trees for two and three dimensions. As an extension of the concept of geometric crystal classes the 'general classes', *i.e.* the classes of non-crystallographic point groups, are considered and classified into systems for two and three dimensions. For one of these systems, icosahedral, two of its point groups are tabulated in the same manner as the crystallographic point groups. This section is concluded with a brief but informative survey of the relation between point-group symmetry and physical properties of crystals with two very clear and elegant tables: one on the occurrence of specific physical effects and the other on polar and non-polar directions in the 21 non-centrosymmetric crystal classes.

The whole of Section 10 seems to us very important in view of the recent revival of crystal morphology in connection with the development of crystal physics.

The only confusing fragment is that on p. 766 (in the right-hand column below the diagram of the 23 point group). It concerns the block arrangements of the Miller indices for the cubic point groups. The text suggests that for each of these groups four blocks can be found, but in fact all four of them are present only in the groups $\bar{4}3m$ and $m\bar{3}m$. Only two blocks are in 432 (left and right block) and $m\bar{3}$ (upper and lower block) while in 23 only one block exists. It seems to us that the description of this arrangement should start with the group type of the highest symmetry and then the blocks in each of the groups should be enumerated.

We also noticed a kind of inconsistency in regard to the names of the prismatic point forms given in Table 10.2.2. The statement on p. 767 that prisms are among the open forms seems to contradict the next sentences ('A point form is always closed') because some point forms are listed in the table as 'prisms'. Accordingly, we think that the name of a prismatic point form, such as the *tetragonal prism* of $8c1$ in $4/m$ (p. 754), should be completed with 'cut off by pinacoid', as given for other point forms; or a statement should be added that in the case of point forms the term 'prism' means a closed form.

As to the references in this section, we would prefer, instead of the mention of 'the well-known books by H. S. M. Coxeter', a few chosen references to the newest editions of these books.

Section 11 (W. Fischer, E. Koch & H. Arnold) sums up the matrix approach to symmetry operations with many examples and a very convenient table which collects all matrices for point-group symmetry operations taking into account the orientation of corresponding symmetry elements referred to in the seven Bravais coordinate systems.

Section 12 (H. Burzlaff & H. Zimmermann) reveals the information hidden behind the space-group symbols, among them the properties of international symbols in comparison with other notations such as those invented by Schoenflies, Shubnikov, Hermann and Mauguin. The most impressive is the huge table which consists of standard space-group symbols in different notations and of the symbols given in 1935 and present editions of *IT*, with useful comments. An interesting novelty is the remarks on the formal matrix approach to the systematic absences.

However, in one case the authors do not follow the notation adopted throughout the whole volume and given in Section 5 (p. 70) for the matrix $\mathbf{w} = (w_1/w_2/w_3)$. Instead they use $(w^1/w^2/w^3)$, which seems rather infelicitous. We would also replace the sentence (p. 796): 'For centred cells the vectors to the centring points are given first' by 'For centred cells the centring vectors are given first'.

Section 13 (Y. Billiet & E. F. Bertaut) gives a detailed discussion on isomorphic subgroups of space groups. For each plane- and space-group type the explicit forms of the transformation matrices from the conventional unit cell to the basis vectors corresponding to an isomorphic subgroup are given. This is arranged in two steps: the first reveals the restrictions imposed on the matrix coefficients by the space-group symmetry and the other lists the derived matrices according to the order of the space-group numbers in *IT*.

There are several slips which should be corrected:

(i) instead of the determinant symbol |Det S| (p. 810, left column) we would suggest 'det (S)' as *e.g.* in Section 11 (p. 789) or '$|S_{ij}|$';

(ii) the missing number '(3)' for the general expression of the matrix S (p. 810, the top of the right column) should be added, because there is a reference to it on p. 811 (right column, line 9 from the bottom);

(iii) the space-group symbol, $P4/mmc$ (p. 812, left column, line 2 from the bottom) should be changed to $P4/mcc$.

Section 14 (W. Fischer & E. Koch) introduces for the first time the idea of lattice complexes into *IT*. This is very important for many applications such as the study of the geometrical properties of point configurations and relationships between different crystal structures. Characteristic features of lattice complexes are discussed and their descriptive symbols are given in each plane- and space-group type. The descriptive symbols of lattice complexes look rather complicated, but the authors point out several useful properties of these symbols.

In the text describing Tables 14.1 and 14.2 (p. 844, left column) we read '...the Wyckoff letter (column 1), the multiplicity (column 2)...', which contradicts the layout of this table where the Wyckoff letter is in column 2 and the multiplicity in column 1.

Taken as a whole *International Tables for Crystallography*, Vol. A, *Space-Group Symmetry* (1983) is an excellent well of information organized in a clear and coherent manner, with a great deal of internal consistency. It seems to us that the misprints are remarkably few considering the size and complexity of this volume of *IT*. The references to the literature contain the titles of papers which is very helpful for users. The thoroughness with which they have been prepared is quite impressive. In the Subject Index one can find, without much difficulty, most of the terms used in the book. Last but not least, the creamy background of the print and its good quality makes reading easy except for the 'heights' above the projection plane indicated on the cubic space-group diagrams, which are very faint. Unfortunately, the cover of the book, of beautiful blue colour with golden letters, does not seem to be joined well enough to the heavy bulk of almost 900 pages, so it is not too suitable for frequent use.

Thinking about future editions of *IT*, (i) we feel a necessity to consider a symmetry treatment suitable for describing the phases intermediate between nematic and crystalline, *i.e.* the cholesteric, blue and smectic phases [a complete classification through the combination of the continuous and discrete groups has been published by Kléman & Michel (1978)], (ii) we suggest the introduction of a uniform mathematical approach to ordered media with the use of rigorous definitions of vector space, point space, and their transformational properties [it seems to us that the concept of condensed matter could be further developed on the basis of papers by Michel (1980) and Thom (1981)], and (iii) it might also be fruitful to take into account the possibility of derivation of the space groups from Lie groups as their discrete subgroups, as was done by Raghunathan (1972).

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Editorial note: A list of some twenty errata is supplied by the publishers with the book; a table listing other typographic errors is obtainable from the authors of this review.

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Diffusion in crystalline solids. Edited by G. E. MURCH and A. S. NOWICK. Pp. xv+482. New York: Academic Press, 1984. Price US $73.00.

This book focuses upon progress in diffusion research since about 1975, when the book *Diffusion in Solids: Recent Developments*, edited by A. S. Nowick and J. J. Burton, was published in the same series. It provides an update in an area where good textbooks and monographs have been missing for over a decade. As the editors state, a number of subjects have been selected that have reached a certain state of maturity - judged from a broad 'agreement on their scope and interpretation'.

The book contains eight chapters, each with a list of contents and references, one even with a list of symbols. The subject index is useful if information on specific materials is sought; some of the other entries do not serve the purpose of enlightening the reader on the subject.

In chapter 1, S. J. Rothman describes the experimental techniques for the measurement of tracer diffusion coefficients in solids, mainly inorganic materials. The reproducibility of a few percent reached by the sectioning technique is the result of a long, careful development.

Chapter 2 (by W. Frank, U. Gösele, H. Mehrer and A. Seeger) gives a detailed account of the mechanisms of diffusion in Si and Ge, including doping and oxidation effects on self- and foreign-atom diffusion.

In chapter 3, A. S. Nowick reports on the principles of atom transport in oxides of the fluorite structure, a relatively open structure which tolerates high levels of disorder (dopants and/or deviation from stoichiometry), with correspondingly complex diffusion properties.

Chapter 4, by H. Baker, deals with tracer diffusion in concentrated alloys, including intermetallic phases with the $B2$, $D0_3$ and $L1_2$ structures.

While chapters 2-4 are devoted to selected technologically important groups of materials, chapters 5 and 6 concentrate on special diffusion paths along dislocations and grain boundaries. A. D. Le Claire and A. Rabinovitch (chapter 5) describe the mathematics of the (continuum) analysis of diffusion in crystals containing dislocations, illustrated by some experimental results, while R. W. Balluffi (chapter 6, based on the 1982 Institute of Metals lecture) reviews the current knowledge of the structure of grain boundaries and experiments relevant to boundary diffusion, including the interplay of diffusional (atomic) and boundary motion.

Finally, chapters 7 and 8 report on Monte Carlo simulation of diffusion kinetics (G. E. Murch) and the statistical-mechanical treatment of point defect diffusion based on lattice dynamics calculations (G. Jacucci). These chapters illustrate the new developments which are possible with the use of large computers.

The book should be useful to all those who are interested in the current state of diffusion science.

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Creep of crystals. By J.-P. POIRIER. Pp. xiv+260. Cambridge Univ. Press, 1985. Price hardback £27.50, US$ 49.50; paperback £10.95, US$ 22.95.

Creep is the appearance of a plastic deformation (strain rate $\dot{\varepsilon}$) under the influence of an external stress σ at a given temperature T and a hydrostatic pressure P (which may all vary with time t). A general constitutive equation may read $\dot{\varepsilon} \equiv \dot{\varepsilon}(\sigma, y, T, P)$, where y is an internal state variable which may depend on ε, $\dot{\varepsilon}$, $\ddot{\varepsilon}$, ... and represents the microstructure of the sample produced along the total more or less complex deformation path. If y can be uniquely related to σ, $\dot{\varepsilon}$, T, P, then $\varepsilon(t)$ can be calculated, *i.e.* a mechanical equation of state exists. Geologists in particular, but also materials scientists, are interested in predicting $\varepsilon(t)$ for times t inaccessible in the laboratory and therefore much work is devoted to establishing the laws of plasticity where they can be observed in order to extrapolate with some reliability. The earth scientist is obviously in the most severe situation as characteristic time scales are in the range of millions of years.

Poirier's book appears in the Cambridge Earth Science Series but is equally useful for materials scientists as it