# Book Reviews

*Works intended for notice in this column should be sent direct to the Book-Review Editor (R. F. Bryan, Department of Chemistry, University of Virginia, McCormick Road, Charlottesville, Virginia 22901, USA). As far as practicable, books will be reviewed in a country different from that of publication.*

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**Modern crystallography.** Vol. 1. **Fundamentals of crystals. Symmetry, and methods of structural crystallography.** (Second enlarged edition.) By BORIS K. VAINSHTEIN. Pp. xxii + 480. Berlin: Springer-Verlag, 1994. Price DM 119. ISBN 3-540-56558-2.

This book, written by one of the most respected crystallographers in Russia, is the second edition of a work that first appeared in English translation in 1981 (originally published in 1971 as *Sovremenaia kristallografia*; *Simmetriia kristallov. Metody strukturnoi kristallografii* by Nauka Publishing House, Moscow). As the first of a four-volume set, it is a comprehensive overview of crystallographic symmetry, as well as of methods for data collection and structure analysis. Chapter 1 is a general discussion of the crystalline state, showing how crystalline habit follows from the packing of a repetitive motif. (There is a small update on the concept of quasicrystals, a research topic that has emerged since publication of the first edition, with more information given in the final chapter of the book.) Chapter 2 is a comprehensive treatment of symmetry, including cylindrical groups, which are rarely considered by other authors. Chapter 3 is an overview of crystal geometry, viewed in real and reciprocal space. Chapter 4 then treats the theory of scattering from crystals and discusses how the diffracted radiation is used for structure analysis. This second edition contains enlarged or new sections to this part; in the areas of electron diffraction, electron microscopy and surface probe microscopy. A new Chapter 5 discusses topics that have advanced to the forefront of crystallographic research since publication of the original volume.

Little need be said here about the first three chapters, since they are essentially the same as those in the first edition. The material is covered very thoroughly by Professor Vainshtein and, indeed, much could be said for purchasing this book even if the symmetry and geometry components were its only contents. Obviously, there is much in these chapters that originates from Professor Vainshtein's personal experience, particularly in discussions of periodic objects that do not correspond to the usual concept of a three-dimensional crystal mounted on an X-ray diffractometer.

Similarly, the discussions of structure analysis in Chapter 4 have a breadth not seen in many other crystallographic textbooks. There is a nice overview of scattering theories for X-rays, neutrons and electrons by crystals, showing how they are related to one another, and how each radiation can be used to find different kinds of structural information. The deviation from the single-scattering approximations is also described in terms of dynamical theories. Apparatus for obtaining diffraction information from crystals is described for all radiation sources. It is significant that a discussion of electron microscopy and image analysis is presented along with the conventional diffraction analyses to emphasize that crystal structure analysis is really a branch of optics, conveniently visualized in terms of Fourier-transform pairs (a concept also not touched on in many books on X-ray crystallography). The use of electron micrographs as a source of crystallographic phase information independent of conventional phasing techniques has become increasingly important in recent years. Optical principles are also important for understanding other aspects of diffraction, including the effect of finite crystallite size, *via* the shape transform, as well as the overall effect of disorder, first as a Gaussian distribution of mass centers around space lattice sites, which Fourier transforms to another Gaussian function that limits diffraction resolution by the sifting operation. A discussion of scattering from noncrystalline objects is also presented. The need for a conservation of scattering from disordered crystalline specimens, expressed as a diffuse component added to the Bragg diffraction, is also stated.

It is appropriate that electron diffraction techniques are discussed more thoroughly in this volume as a technique for structure analysis, given the significant pioneering effort in this area by the author. (Sadly, his 1964 book, *Structure Analysis by Electron Diffraction*, remains out of print.) Also, it is timely to mention the scanning-probe microscopies such as scanning tunnelling microscopy (STM) and atomic force microscopy (AFM) in a crystallographic text, given the recent success in characterizing both inorganic and organic surfaces by these techniques.

Although Chapter 5 does not have the coherent organization of the preceding ones, it can be regarded as a current-topics section, treating new developments that eventually could be incorporated into the preceding chapters in later editions. The discussion of quasicrystalline symmetry is particularly interesting and is well presented. Newer concepts in the treatment of powder diffraction data by profile analysis are given in the presentation of the Rietveld method. Applied research areas that have been made available by the use of high-intensity synchrotron sources and improved detectors are also described, including the study of crystalline surfaces and the use of extended X-ray absorption fine-structure spectroscopy to study the local environment of a chemical element in a crystal.

As an overview of modern crystallographic research, this is an excellent resource to have at one's disposal. Generally speaking, it seems hard to find any area of crystallography that does not interest Professor Vainshtein, and his approach is encyclopedic. Inevitably, some will feel that certain areas are less thoroughly covered than others, but to do complete justice to all would require a book at least twice as large. Inevitably, one looks for more in one's own areas of interest. For myself, I found the discussion of direct phasing techniques to be somewhat perfunctory, given that this is now the major method for the solution of small-molecule structures, and, given the new discussion of high-resolution electron microscopy in this book, I would have expected some mention in that section of its relevance to the phase problem. It is valuable to have electron-diffraction structure analysis and high-resolution electron microscopy discussed

in a crystallography book from a positive standpoint, and I heartily applaud Professor Vainshtein for doing this. However, I think that a realistic perspective of the difficulties could also have been presented. The Russian school of electron diffraction has often relied on the use of texture diffraction patterns for data collection from a large specimen area, sampling a relatively wide distribution of crystal orientations. Cowley has pointed out that this approach minimizes nonsystematic dynamical interactions, so that the two-beam dynamical theory is often adequate for such data sets. This is not necessarily the case for selected-area electron diffraction, where the sampled crystal area is generally much smaller and corrections must account for multiple-beam interactions. It is even less true for convergent-beam methods where a virtually flat specimen area is being used for the electron-diffraction experiment. More than a cursory mention of zone-axis convergent-beam diffraction patterns could have been made, particularly since they are quite useful for the determination of crystal point-group symmetries. While examples depicting a near correspondence to the weak phase object approximation in high-resolution electron micrographs of inorganics is valuable, this is a topic of considerable controversy nowadays. More than a passing mention of multislice calculations might have been given, with a frank discussion of where experimental images will cease to be useful for direct structure interpretation. At a different level of criticism, better copyediting would have corrected some minor deviations from standard spelling. In the newer sections, some references are out of sequence and some of the index citations are unreliable.

In general, I find this book to be a refreshing and comprehensive approach to crystallography in a style that could be imitated more often by other authors. While it will not, by itself, replace all other crystallography books on the shelf, each having its own strengths, it well deserves to be placed among them, especially in its newer version.

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**Crystallographic computing 6. A window on modern crystallography. (IUCr Crystallographic Symposia** No. 6.) Edited by H. D. FLACK, L. PÁRKÁNYI and K. SIMON. Pp. x + 310. Oxford: IUCr/Oxford University Press, 1994. Price £40.00. ISBN 0-19-855788-4.

This volume is the proceedings of an International School of Crystallographic Computing held at Balatonfüred, Hungary, in June 1992. It contains 19 chapters by 19 authors (two chapters have two authors, and two authors contributed two chapters each) and extended abstracts of nine submitted contributions. The topics of these chapters cover a wide range, from practical nuts-and-bolts details, such as a description of the crystallographic information file (CIF) by B. McMahon and descriptions of particular programs (*SHELXL*-92, by G. M. Sheldrick, and *CRYSTALS*, by D. J. Watkin) to advanced concepts, including a discussion of likelihood as a phasing tool, by C. Gilmore, and of the particular problems posed by incommensurate structures and quasicrystals, by W. A. Paciorek. In between, there are discussions of various topics of interest to working crystallographers, including direct methods, restrained refinement, powder diffraction, order–disorder, isomorphous replacement, charge-density determination, program structure and databases. With such a broad range of material, it is unlikely that any one reader will find every chapter useful, but there is something for almost everyone, and the book has the advantage over a collection of journal articles that it is not a mixture of articles on completely different subjects; it is also less restricted by space constraints than a journal.

With all of the contributors to this volume being innovative users of computers, it is somewhat surprising that the authors submitted their copy in camera-ready rather than machine-readable form. Before the computerization of the publishing industry, manuscripts were traditionally double-spaced to allow insertion of instructions to the typesetters by copyeditors. Most of these chapters appear to have been produced by similar wordprocessing systems and similar printers, and they have generally similar styles. The fact that this style contains extra space between the lines may improve readability slightly, and does not detract from the value of the volume, but it surely increases the cost. The most unfortunate effect of camera-ready copy, however, is that it reduces the role of the editors to putting the pages in order and writing a preface. The authors of several of the chapters are not native speakers of English, and in some of these chapters there are errors of punctuation and grammar that could have been removed by editing. This would presumably have delayed publication had it been necessary to return manuscripts to their authors for correction.

In spite of these reservations, this book contains useful information, and it is a worthy addition to the library of any group that is actively involved in crystallographic computing.

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**Point group theory tables.** By S. L. ALTMANN and P. HERTZIG. Pp. xii + 704. Oxford: Oxford University Press, 1994. Price £90.00. ISBN 0-19-855226-2.

This is, as the title states, a book consisting primarily of tables; not only for the crystallographic point groups, but also for the icosahedral group, the infinite dihedral and cyclic groups, and the finite dihedral and cyclic groups for axes up to order 10. For these groups, the authors give diagrams, character tables, representation matrices, product and branching rules