

The basics of crystallography and diffraction

By Christopher Hammond.

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This book is the third in the series of IUCr Texts on Crystallography. As the title implies, the book covers 'ideas of symmetry, structures, lattices and the architecture of crystals', and 'the interpretation of diffraction patterns'. It excludes any discussion of the solution of crystal structures, a topic covered in the second book in the series, C. Giacovazzo's *Fundamentals of Crystallography*, which also includes much of the material covered in this volume. Hammond's book therefore joins a long succession of introductory works. It consists of ten chapters and six appendices. Chapter 1 describes some of the early history and development of crystallography and introduces crystal structures through closest packing of spheres. There is a good description of the tetrahedral and octahedral interstitial sites in close-packed arrays and of how crystal structures are built up by occupation of these sites. Chapter 2 introduces the concept of lattices and unit cells in two dimensions and allowed two-dimensional symmetry elements. Combination of all the allowed symmetry elements is then used to derive the 17 plane groups. An excellent flow diagram is included to help the student identify the plane group to which a particular pattern corresponds. A number of intriguing one-dimensional plane patterns are included that challenge the reader's skill in properly assigning the correct symmetry. However, I believe that the introduction of color symmetry at this stage is inappropriate. Chapter 3 is a short description of the 14 Bravais lattices and seven crystal systems. Crystal shapes, point groups, three-dimensional symmetry and space groups are covered in Chapter 4, which, to my way of thinking, is much too perfunctory. Thus, the author mentions stereographic projections but never tells the reader what they are nor does he represent a point group by one. He treats only one space group, *Pba2*, and neither derives nor gives the equivalent points. He might also, when explaining how screw axes and glide planes arise, have described the effect of perpendicular translations on rotation axes and mirror planes; such information helps in comprehending space-group diagrams.

Chapter 5 treats Miller indices, zones and zone axes, and transformation matrices. This is followed in Chapter 6 by a short treatment of the reciprocal lattice. The use of vectors and vector notation is introduced with a general introduction to vectors and complex numbers provided in Appendix 5. A relatively lengthy Chapter 7 treats the diffraction of light, lenses and microscopy. The treatment is clear and helpful in understanding X-ray diffraction and much of this material is often omitted from X-ray texts or treated in less detail. Chapter 8 presents both the Laue and Bragg equations, contrasts their use in the treatment of X-ray diffraction, and includes the use of the Ewald sphere and reciprocal lattice to identify diffracted-beam directions and patterns. The difference between the Bragg and Laue methods is nicely, if briefly, illustrated. Chapter 9 continues the treatment of diffraction by providing an introduction to film methods. The structure-factor equation, with examples of its use and an introduction to electron diffraction, is also treated in this chapter. However, systematic absences and how they arise are left to Appendix 6. A brief treatment of peak broadening and diffraction from thin films is also presented. The book concludes with an adequate chapter on powder diffraction methods and their applications to accurate measurement of lattice parameters, phase identification, crystal-grain-size determination and elastic strain. Included in the appendices are a guide to suppliers of crystal models and model building kits, mostly in the UK, information on computer programs, biographical notes on many of the major contributors to our knowledge of crystallography and a compilation of some useful crystallographic relationships.

The book is not without its defects. As a text directed at students, it could use more examples to help illustrate the important points in the various chapters, and would benefit from additional problems. This is particularly true for Chapters 3, 4 and 6. The student may find some notations confusing. Thus, in Chapter 4, Hammond uses the symbols x, y, z to specify axial directions and x', y', z' for positional coordinates and later, in Chapter 9, he uses u, v, w to specify positions in real space, practices at variance with the usage adopted in *International Tables for Crystallography* and in most standard X-ray texts, where x, y, z denote real-space positions and u, v, w denote positions in Patterson space. In Figure 1.5, intended to illustrate the unit cells of simple hexagonal structures, there are more atoms in the diagrams than are present in the unit cells. It would be appropriate to outline the unit cells to accord with the figure caption. I also am not fond of 'pm' as a unit for interatomic distances; the Å remains the norm in crystallography. There are also a number of typographical errors in the text, but none that are serious. However, emission of light from a laser is 'stimulated' not 'simulated' (p. 109) and there is no Laue photograph on p. xii (p. 125).

Notable for its omission is any treatment of crystal structure solutions. In this regard, the title means what it says: the author has treated the basics in a style that should be readily comprehended by the beginner with a little help from a more experienced practitioner. In teaching any course in crystallography for chemists (my own interest in this book), however, Hammond's text would need to be supplemented by other works. Chemistry students, in general, are exposed to very little solid-state chemistry and physics and perhaps only a superficial treatment of X-ray diffraction. As a result, they are not adept at spatial visualization and three-dimensional thinking. Yet chemists are beset by thousands of crystal structures that are published each year, some of which are related to their own research. It is important that they be able to read such papers with comprehension and we must find ways to make that happen. I intend to use Hammond's book in my own course, supplemented with computer modules, material on structure determinations and my own notes. We shall see if this accomplishes the desired end. For those seeking a comprehensive single-volume treatment of fundamentals combined with structure determination, at an introductory level, *Crystal Structure Analysis*, by Glusker & Trueblood (Oxford University Press, 1996), places its main emphasis on the latter but contains much of Hammond's material in appendices. Neither that text nor Hammond's

treats X-ray generation or spectra, topics treated in the third edition of *Structure Determination by X-ray Crystallography*, by Ladd & Palmer (Plenum Press, 1997), a text that provides a comprehensive coverage of all the essential topics for an introductory course.

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