Introduction to crystallography

David A. Keen

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BOOK REVIEW

Introduction to Crystallography, by Frank Hoffmann. Springer International Publishing, Switzerland, 1st Ed. 2020, 319pp, ISBN-13:978-3030351090, Hardcover. Price GBP 56.18

David A. Keen[a]

[a]ISIS Facility, Rutherford Appleton Laboratory, Harwell Campus, Didcot, Oxfordshire OX11 0QX, UK

ARTICLE HISTORY
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I have a confession: although I have read biographies of crystallographers this is the first book on crystallography that I have read from cover to cover. I am one of those crystallographers who has 'learnt on the job' (or more accurately who is still learning on the job) and was never taught crystallography as a student in any depth. I expect that this is now the situation for most researchers who use crystallography as a means to understand their materials. We use the readily available crystallographic tools, whether they be programs for Rietveld refinement or single crystal structure determination or simple structure plotting, and we dip in and out of text books and online resources as needed to make sense of these tools, most of which do the crystallographic 'hard work' for us. The danger with this approach of course is that we can place our structural research on flaky foundations that, although usually sufficient, might at some point limit our ability to develop our crystallographic understanding fully. We might come unstuck when tackling a tricky sample or phase transition or fail to describe our results as effectively as we might with better understanding of the basics of crystallography.

As an example, the first structure I studied in my PhD was rocksalt-structured silver bromide, space group $Fm\bar{3}m$, a structure covered in some detail in Hoffmann's book. I could manipulate the structure, calculate correlation functions and structure factors and look for ways that atoms might move within the structure (one of the themes of my thesis), but it was only several years later that I properly understood the full meaning of "$Fm\bar{3}m$". At the time, for example, it was not necessary to know which viewing directions corresponded to the m, $\bar{3}$ and m of the space group symbol. Now, many more years later, I know that I would not have been alone in only having a fuzzy understanding of such key pieces of crystallographic knowledge.

In his preface to this English translation of his original German work '*Faszination Kristalle und Symmetrie*', Hoffmann says, "the most important thing is to try to make the *basic concepts* of a subject clear." He goes on to say that this is so "the quasi-natural curiosity of the learners is preserved as long as possible". In this he has succeeded; I stayed with him for almost all of the book, and it was only in the final chapter that my attention wandered a little (more on this later). The basic concepts are clearly and gently introduced and explained, each chapter building on previous

CONTACT D. A. Keen. Email: david.keen@stfc.ac.uk

ones, and the text is well-linked to excellent diagrams and relevant sections elsewhere in the book.

The book's chapters are well-organised and bring the reader on a journey from simple observations about crystals and symmetry to space groups and the IUCr International Tables for Crystallography. This is followed by descriptions of a small number of pertinent crystal structures (using the knowledge gained in the previous chapters) and discussions of some of the non-standard behaviour seen in crystals. In Chapter 1, Hoffmann introduces us to crystals in the general sense, what they are and how big they can be, how observing their sizes and shapes might help us understand their symmetry and how the concepts of a lattice and a unit cell give rise to the seven crystal systems. Chapter 2 goes into more detail about crystal shapes and how they arise from the lattice symmetry even if at first this is not obvious. Miller indices are introduced in the context of labelling the faces of a crystal, as are the fourteen Bravais lattices in the context of unit cell centring (and indeed why there are only fourteen). Face- and body- etc. centring naturally leads to the idea of atoms within the unit cell having fractional coordinates and hence how a crystal structure is described. Usefully this is done with reference to the crystallographic information file (CIF) and the freely available crystal structure drawing software VESTA. The final section of the chapter deals with the apparently awkward behaviour of the hexagonal crystal system.

Chapter 3 is the symmetry chapter, where symmetry elements are introduced and how they help us understand crystal shapes. The 32 crystal classes are described. It is also where a toy locomotive first appears in the book as a structure motif. Chapter 4, by returning to discussions of planar symmetry, may seem like a backward step. But this helps establish the symmetry of glide planes through its links to patterns in art and ancient culture – and wallpaper. The next two chapters, Chapters 5 and 6, deal with translational symmetry elements in crystals, glide planes and screw axes, and how these combine with the already established symmetry elements to build up the 230 space groups. Some of the nomenclature is introduced in Chapter 5 and then the way that this is codified within the IUCr International Tables for Crystallography is explained in some detail in Chapter 6, using a small number of examples. The helpful toy locomotive is also still much in evidence. Chapter 7 gives some helpful examples. Chapter 8 looks at ways that the 'forbidden' symmetry within quasicrystals may be understood by going to higher dimensions and Chapter 9 discusses how some crystals might be understood using ideas about topology and networks.

Two things that mark this book out against older introductions to crystallography are the links to resources on the author's web-pages and the suggestions for using specific pieces of software to demonstrate the crystallographic concepts throughout the book. Both of these are really helpful enhancements that complement the excellent diagrams throughout the text; there is no real substitute for creating physical crystal models and/or being able to rotate and otherwise manipulate structures on the computer screen. It is also very well written. Initially I was unsure of the writing style as it started a little clunkily to my way of reading but it quickly improved—or I happily became used to it—and I enjoyed the clear descriptions, the care to cover the oddities and to explain the apparent exceptions, and the interesting and useful asides along the way.

There were other things that I was less sure about. I didn't entirely understand the rationale for including the final chapter in the book. It seemed somewhat out of place in the context of the rest of the work and this was the only part of the book that I skimmed through. Instead I would have preferred a discussion of how we understand crystals which are imperfect. There was a passing discussion of incommensurate

structures in Chapter 8, but no discussion of the effect of temperature or other disordering effects. Indeed the author discusses the phase transitions of $BaTiO_3$ in Chapter 7 in terms of symmetry changes to the TiO_6 octahedra, whereas it is becoming more accepted that these octahedra remain in their low-symmetry form, with the central titanium ion always offset towards an octahedral face at all temperatures. On heating each titanium ion can displace towards an increasing number of such faces, thus progressively raising the average symmetry (which in turn leads to a misunderstanding of the local structure). This would have been an ideal place to introduce concepts of disorder. I also think that a stronger link to diffraction, and the reciprocal lattice, would be expected in a book with this title. Instead it is mostly only discussed in the context of quasicrystals. I realise that this would probably have necessitated a greater amount of mathematics but crystallography is so dependent on the way that crystal structures are measured that the book would have been improved with a chapter on this. But maybe the very general title of the English version of the book gave me false expectations; had a literal translation of the German title been used I might not have anticipated such a chapter.

So who might gain most benefit from this book? It would be an excellent companion to undergraduate-level crystallography courses as it is very accessible to the different disciplines which have crystallographic content. Although many of the examples have a mineralogical bias—largely because of the easy access to good specimens displaying clear crystal morphologies—researchers in other fields should not be put off by this. The links to other areas of science and culture would also make it suitable to those with a general, or even only passing, interest in crystallography; it is certainly very readable and easily followed and, as the author intended, contains hardly any mathematics. I also feel that—maybe because this was the approach I was thinking about when reading it—it can help firm up the basic understanding of those researchers who use crystallography as tool; those who have become expert in crystallographic *methods* will find their work further enriched by this book. In this context did I learn anything new and fill in some more crystallographic gaps? A few, yes, particularly about crystal morphology which I have never needed to consider before. And did my foundational understanding become more firmly embedded? Definitely.