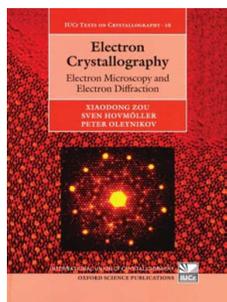


book reviews

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**Electron Crystallography. Electron Microscopy and Electron Diffraction.**

By Xiaodong Zou, Sven Hovmöller and Peter Oleynikov. Oxford University Press, 2011. Price (hardcover) GBP 52.50. ISBN-13: 978-0-19-958020-0.

Within the past ten years, the use of electron crystallography has had a revival. This renaissance is due to the commercial availability of the precession electron diffraction technique on one hand and the development of automated techniques for gathering electron diffraction patterns on the other hand. There are a multitude of books whose purpose is to teach either crystallography or transmission electron microscopy (TEM). In my experience, books teaching the topic of TEM are all more oriented toward general transmission electron microscopy, with little or no attention to the crystallography side of TEM. On the subject of electron crystallography, in recent years books have appeared that are a collection of short papers by different authors, but no up-to-date teaching text is available. The book reviewed here bridges the gap between these existing texts. With all the new arrivals in techniques in electron crystallography, such a text is certainly due. From my own experience in workshops with students of TEM, I have found that many do have the skills to take quality high-resolution images or spectroscopic data but do not have knowledge on how to use the crystallographic aspects of either their images or electron diffraction patterns (for example, basic indexing or determining cell parameters). Therefore, a good book on this topic is a timely and welcome publication.

The book under review covers essentially four main topics: basic crystallography, determining the unit cell from electron diffraction patterns, the effect of symmetry on both electron diffraction (ED) patterns and high-resolution TEM (HRTEM) images, and solving structures from ED and from HRTEM images using image processing. The text seems to have grown from the many lectures and workshops the authors have given over the years on these topics. As a consequence, it is mainly focused on the techniques related to the software developed by the authors themselves. However, even though it does not cover all of the main topics in electron crystallography, the content certainly fills a gap that exists in the available literature and brings useful knowledge to the reader. Moreover, the focus on the techniques used by the authors themselves allows them to give very clear step-by-step procedures accompanied by many explanatory figures.

The book is divided into 13 chapters, starting with a very short chapter on the history of electron crystallography. Thereafter, the text starts with basic crystallography in Chapter 2. A large part of the reasoning in this second chapter will not be understood if the reader does not already have a ready knowledge of point groups, space groups and all crystallographic notations. Nevertheless, this aspect fits the book since its focus is after all on electron crystallography and there is no need to repeat what is available in many other good textbooks. This chapter also differs from other basic crystallography texts in that every topic is illustrated using real electron diffraction patterns and HRTEM images. Even for readers who know basic crystallography, I would advise not to skip this chapter, as it is very instructive to see the connection between the images and ED patterns of a material and all these crystallographic definitions and considerations, such as the relation between reciprocal and real space and the effect of symmetry relations on reflections and HRTEM images.

Chapter 3 deals with the relation between crystal structure factors and symmetry. A clear explanation, and a detailed example, is given on what the phase of a reflection actually means for the possible atom positions, and how the knowledge of a small number of different reflections with their phases can often already give you a rough projected potential map. There is also a rigorous treatment of the amplitude and phase relations between symmetry-equivalent reflections. This is the clearest explanation on the consequences of symmetry for the reflections that I have ever read. This is a part that is rarely or never covered in other textbooks for microscopists. The addition of this part feels natural within the concept of this book, as it provides a clear understanding of how Fourier transforms of HRTEM images can help in determining the symmetry and ultimately in solving structures.

Chapter 4 is about the basics of transmission electron microscopy. It is not very detailed and indeed should not be too detailed, as there are enough books dealing in great length with these aspects. Basically, the use and purpose of different microscope components and techniques are mentioned, as well as how they differ from X-ray diffraction.

Chapter 5 is on electron diffraction. It contains a very good step-by-step treatment of how to index ED patterns and the different ways to determine the cell parameters of an unknown compound from the ED patterns. Again, excellent use is made of real ED patterns to explain some basic concepts, such as how a ring pattern is formed. A valuable addition here would have been an explanation on how to determine the extinction symbol from the electron diffraction patterns as a step towards the space group, either by deriving manually the reflection conditions or by giving the essence of the method using the higher-order Laue zones as described by

Morniroli & Steeds (1992). Without this, there is a gap between the knowledge presented in Chapter 3 on which symmetry element causes which reflection condition and how to determine this in practice from experimental ED patterns. Instead, the chapter switches to a very superficial treatment of convergent beam electron diffraction (CBED) (five pages, mostly images). It feels as if this section was added on just because the authors did not want to not mention CBED. For example, many new terms appear that are not explained or defined, and tables are presented although there is no clear explanation of how to use them. References are given for those needing a more detailed explanation, but the section feels incomplete.

Chapter 6 is the only chapter that contains more formulae than figures. It leads up to a statement 14 pages further that it is thus 'possible to obtain accurate structure projections from HRTEM images combined with crystallographic image processing, contrary to common belief among many scientists in the field' (p. 145). Having witnessed several discussions between the first author of the book and microscopists opposing this idea in workshops, I understand the need for the authors to add the extensive background in this case and not to present a black box tool. The authors do suggest to the reader the possibility to just skip to the conclusions. The chapter also contains equations explaining the possibility of retrieving the contrast transfer function from the Fourier transforms and how to ultimately obtain the crystal structure factors and the structure image. The end of the chapter clarifies the different uses of the term 'phase' within the TEM community in an attempt to avoid future miscommunication between microscopists.

Chapters 7 and 8 explain how to solve crystal structures from HRTEM images through crystallographic image processing. The former chapter treats the theoretical background, while the latter focuses on how structure solution is done in practice. This is one of the aspects for which the authors themselves are well known and for which they have created extensive software packages. All these software packages are also referred to in the text. Together with the worked example in Appendix 6, the reader is clearly told why and how each step should be performed. For all the microscopists that use the software, this chapter is definitely a must. This is one coherent text, eliminating the need to make a literature study of all the separate papers published by the authors over the years on this subject.

Chapter 9 gives a brief overview of how structures can also be solved from electron diffraction. Of course, a large part of this information is the same for electrons as for X-rays, like the parts about normalized structure factors, the Wilson plot, direct methods, the Patterson method and charge flipping, so the authors have kept this short and to the point, with references to the original papers about these techniques and to more general textbooks on this subject. It is good that these sections are present to point out the existence of these aspects. The chapter ends with the strong-reflections approach, which is again more electron diffraction specific.

Structure refinement from electron diffraction is treated in Chapter 10. The chapter is rather short (ten pages), maybe because this is an area still in development. With the coming of precession electron diffraction and the three-dimensional electron diffraction techniques that scan reciprocal space avoiding main zones, dynamical diffraction can now be reduced sufficiently to allow refinements straight from electron diffraction data using the kinematic diffraction theory (dynamical diffraction refinement is also possible but is computationally heavy). However, the available publications do not yet agree on which method is best and how data should be treated first to get the best results, so an elaborate text on a unique procedure could not be expected at this moment. In the book, several pieces of advice are given for those wanting to try. A few words are also said about the advantages of combining electron diffraction data with a refinement from X-ray diffraction data.

This is followed by Chapter 11, which is an extension of earlier chapters and adds how to solve structures in three dimensions by combining series of ED patterns and HRTEM images along many different zones.

The final two chapters are rather short: Chapter 12 is on the subject of simulating images and electron diffraction patterns. It briefly demonstrates the two most commonly used methods, *i.e.* multislice and Bloch wave, and compares them. Chapter 13 shows examples of specific compounds that were solved using electron crystallography.

There are several appendices, of a wide diversity. The most noteworthy is the first one, which contains a suggestion for the formulation of learning outcomes for electron crystallography courses. I have put the book itself to the test to see if the suggested learning outcomes are reached and found that basically the book indeed covers all self-suggested topics, although some goals are defined vaguely, like 'have an idea about...', 'know some...', 'have some basic knowledge about...', where it is of course then subjective whether the level 'some' is reached. A second appendix called *Tables for Space Group Determination* corresponds to those tables from *International Tables for Crystallography*, Vol. A (Hahn, 2002), where the reflection conditions are systematically listed, together with the extinction symbols and possible space groups. As an introduction to this appendix, there is a very short text on determining the space group. This introduction would be more useful to the reader if it were in Chapter 5 and expanded with some examples. Appendices 5, 6 and 7 contain exercises. For the first and last the correct answers are included; for Appendix 6 I could not locate the answers in the book. It would be useful to correct this slight oversight in a next edition. The other appendices mainly give some extra practical information on specific content covered in the chapters.

In conclusion, the book has a very different focus from other books for transmission electron microscopists; for many of the topics it is the first time that I have found them in a clear student-oriented text. The authors also do not spend too much time re-explaining aspects that are already well covered in

other basic texts. It is certainly a worthy addition to the library of any transmission electron microscopist who deals with structure solution and refinement and a book to suggest to TEM students. A basic knowledge of crystallography before starting the book is recommended.

References

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