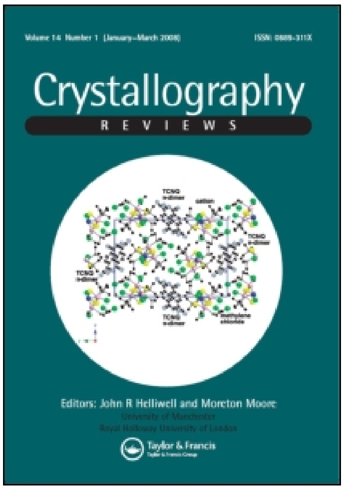

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Book Review

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BOOK REVIEW

Incommensurate Crystallography by Sander van Smaalen, Oxford University Press, IUCR Monographs on Crystallography No. 21, 2007, xviii + 270 pp., £68.00 (hardcover), ISBN 978-0-19-857082-0

Incommensurate crystallography is characterized by fascinating diffraction patterns with beautiful and sometimes confounding symmetry. Most crystallographers won't touch these crystals 'with a 10-foot pole'; as I was once advised. But then there is the brave and mathematically bent scientific community composed primarily of inorganic and organic chemists and physicists that truly love them and are pushing forward this cutting-edge of crystallography. Professor van Smaalen is an expert in this field and with this text he is sharing his wealth of experience with the community. This text book fills a need for the student and I mean students at all levels from graduate student, postdoc, senior scientist to professor. But be forewarned, as the preface indicates, it necessarily requires skills in advanced mathematics. This is not light reading. It gives an excellent presentation from start to finish of the structural analysis of aperiodic crystals. This is a difficult subject and the associated scientific literature is a difficult read, in particular the diagrams of concepts not found in other areas of crystallography, e.g. superspace and multi-dimensional diffractions. One thing I particularly like about this text is that complex diagrams are explained piece by piece. This careful explanation then allows one to read the scientific literature with much better understanding. This textbook is likely to push forward the field of incommensurate crystallography, making it attainable to the common crystallographer.

X-ray crystallographers normally solve 'periodic' crystal structures. In an ideal periodic crystal, the contents of the asymmetric unit are perfectly replicated by the unit translations and the symmetry operators of the space group. One particularly fascinating deviation from ideality results is the appearance of distinct 'satellite' reflections around the 'main' reflections. These satellite reflections are often as sharp as the main lattice spots and result from a structural modulation contained in 'aperiodic' or 'modulated' crystals. Modulated structures contain a variation that perturbs the short-range translational symmetry and can be thought of as a form of systematic or smoothly varying disorder. Clear diagrams of examples of modulated structures are provided in Chapter 1. The types of aperiodic crystals and how to distinguish them from periodic crystals are also well described in Chapter 1. This warms up the reader to the challenging concepts ahead. The mathematics used to describe the diffraction of periodic crystals is neatly reviewed here followed by the equations needed to describe the satellite reflections observed in aperiodic crystals. The concepts of the 'q vector' and multi-dimensional superspace are successfully introduced at the end of the first chapter. The reader can use Appendix B, which contains a glossary of the unique symbols and terms associated with incommensurate crystallography, to enhance their comprehension of the text.

The diffraction pattern of a normal, periodic crystal can be described with an orientation matrix and three integer indices that give the location of the observed main lattice reflections. A modulation can be 'incommensurate' or 'commensurate' with this main lattice. For the commensurate case, the modulation causes a special type of super-lattice; the distortion can be described with an integer-multiple relationship to the main lattice. Commensurate crystals can be indexed normally by three integer indices and then solved as a super-cell of the original unit cell. Then there is the incommensurate case, where the relationship with the main lattice is non-integral. Here the position of a reflection from a modulated crystal involves additional dimensions and the so-called q vector. In this way, a 'superspace' is defined for a (3+d)-dimensional reciprocal lattice. The locations of satellite reflections in superspace are defined using a 'q vector' to describe their direction and distance relative to the main reflections. The type of modulation within the crystal, commensurate *versus* incommensurate, can be distinguished by the spacing of the satellite reflection from the main reflection. This diagnostic information is held in the q vector. For commensurate crystals, all components of the q vector are rational and for incommensurate crystals at least one component is irrational. The direction of the structural modulation is given by the direction of the satellite reflections. Of course, the case of the commensurately modulated crystal is relatively easy to solve when compared to the incommensurate case. The term aperiodic includes both positionally and occupationally modulated crystals and composite crystals. Once you have a q vector, then you can integrate your satellite reflections and start worrying about what your 'superspace group' is. If you understand the symmetry involved in periodic space groups, then expanding your mind to the superspace groups is not so bad.

It is possible to determine the structure(s) housed in modulated crystals with modern software. Chapter by chapter the theoretical concepts are first introduced in this book (i.e. superspace, superspace groups and types of modulations possible) then the text becomes more applied and the concepts of structure refinement, electron density interpretation in superspace, superspace group determination and structure solution methods are described. The list of computer programs given in Appendix A is what is needed in practice for solving incommensurate crystals. A flow diagram of the crystal structure solution process is missing from this text and would be helpful to the 'application scientist'. Also, a section on how to diagnose modulations *versus* other common crystallographic ailments like twinning, etc. would have been appreciated. In addition, in depth step by step examples, with data processing examples, of each type of modulated structure would have made this a truly outstanding text.

In conclusion, this text is dedicated to describing the theory and methodology of incommensurate crystallography and Professor van Smaalen has produced an excellent text on a very difficult subject. Our relatively inexperienced group of incommensurate protein crystallographers will greatly appreciate this text. We particularly appreciate van Smaalen's success in building the concepts of incommensurate crystallography piece by piece into the whole picture. The references list is extensive and appears to be very complete and a useful tool for the student. Overall, Professor Sander van Smaalen has achieved the goal of filling the need of students, of all levels, who want to become practicing 'aperiodic crystallographers' or who are just plain fascinated by this area of crystallography. Furthermore, the book is an excellent presentation from start to finish of the structural analysis of aperiodic crystals. I just wish this text had been available 10 years ago!

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