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Book Review

Mathematical Techniques in Crystallography and Materials Science

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Springer Verlag, Berlin, Heidelberg, New York 2004 (3rd Edition)
224 pages, 29 figures, bibliography and index, ISBN 3-540-21111-X

The third edition of this classical reference book provides an impressive confirmation of the proverb "The man who undertakes to solve a scientific question without the help of mathematics undertakes the impossible" (Gallileo, 1610).

Nowadays various mathematical techniques have to be applied in all fields of crystallographic research. This book is a reference book, where the fundamentals of mathematical crystallography are briefly summarized on the one hand, while modern mathematical procedures necessary for the daily work in crystallography are discussed on the other.

The book consists of 10 chapters. The first five familiarize the reader with the fundamentals in both mathematics and crystallography necessary for the understanding of crystals and crystal structures. Here the reader is introduced to the mathematics of matrices, vectors and tensors. The importance of these mathematical concepts is clearly illustrated by means of numerous practical examples. Furthermore, the fundamentals of group theory and representation of groups connected with the introduction to the symmetry of point groups are treated. A brief description of the symmetry of Bravais lattices and space groups completes the description of fundamentals of mathematical crystallography. In Chapters 6 to 8 the main problems connected with data handling and data analysis are described. The reader is introduced to techniques like data fitting and methods for estimating precision. In addition, questions related to the significance and accuracy of data sets are discussed in detail. In chapter 9 the mathematics of model fitting, discussed in a comprehensive way in the previous chapters, is vividly illustrated for crystal structure refinement. Since nowadays practically all computer programs use fast Fourier transform algorithms (FFT) for the calculation of the Fourier transform, an insight into the commonly used FFT algorithms is given in chapter 10.

Very useful are Appendixes A – F, where the following topics are briefly treated: the stereographic projection, Eigenvalues and Eigenvectors of (3 × 3) symmetric matrices, sublattices and superlattices, the probability integral, the Gamma function and related topics, and the harmonic oscillator in quantum mechanics, including Bloch theorem and symmetry restrictions on second, third and fourth rank tensors. Some useful computer programs written in Fortran concludes the book.

All in all this reference book represents a comprehensive introduction to the fundamentals of mathematical crystallography. The book is very carefully and clearly written. However, as a reader I was a bit sad about the list of references which is far from up-to-date. It is desirable to update the list of references in a forthcoming edition. Nevertheless the "Prince" will not only be a valuable aid for beginners in crystallography to become familiar with the fundamentals of mathematical crystallography. This paperback edition can also be strongly recommended as a practical guide and reference book to all scientists doing crystallographic research.

Wolfgang Neumann, Berlin