Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (R. F. Bryan, Department of Chemistry, University of Virginia, McCormick Road, Charlottesville, Virginia 22901, USA). As far as practicable, books will be reviewed in a country different from that of publication.

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Mathematical techniques in crystallography and materials science.

Second edition. By EDWARD PRINCE. Pp. xi + 223. New York and Berlin: Springer-Verlag, 1994. Price US $79.00. ISBN 3-540-58115-4.

The second edition of this book will certainly engage the lively interest of crystallographers in various specialities – both those who know the first edition and those who are only now looking for a mathematical guide to help them in their work. To bring his book up to date, the author has added a new chapter about the fast Fourier transform, so the present edition contains the following chapters: 1. Matrices: definitions and fundamental operations; 2. Symmetry of finite objects; 3. Symmetry of infinitely repeated patterns; 4. Vectors; 5. Tensors; 6. Data fitting; 7. Estimation of uncertainty; 8. Significance and accuracy; 9. Constrained crystal structure refinement; 10. The fast Fourier transform. Moreover, improvements have been made to the original chapters, and two new figures have been added. As the first edition of the book has already been reviewed in *Acta Crystallographica Section A* [*Acta Cryst.* (1984), A**40**, 86–87], I shall concentrate mainly on the new Chapter 10.

Although the fast Fourier transform (FFT) is an important component of popular crystallographic program systems, probably only a few of their users know what causes it to be fast. To explain the mechanism of FFT calculations, the author starts with the definition of the Fourier transform, one of the basic concepts in crystallography, proceeds to the discrete Fourier transform (DFT) in matrix notation, and so gets immediately at the substance of the computational problem, avoiding the customary considerations of conditions for existence and other inessential (in this context) properties of the transform. Next, the reader's attention is directed to the somewhat complex transformations of the DFT matrix. These are performed to express the DFT matrix as a product of matrices that are both sparse (having many zero elements) and have many elements equal to either ± 1 or $\pm i$, which makes the calculations easier and faster. Progress in the subject is demonstrated by successive solutions, such as the Good–Thomas, the Cooley–Tukey and the Rader field algorithms.

Next, the discussion about economy of calculation in the Fourier transform is transferred to the native field of crystallography and to three-dimensional space. The author conveys to his readers, or reminds some of them of, the reduction in computation that results when one deals with real – in most cases – values of the density of scattering matter, and the presence of symmetry elements in the given crystal structure.

The proper selection of material, illustrated above, and the didactic aspect of the book are worth emphasizing. The author himself seems to be present during one's reading. He knows how the reader is thinking – makes useful comments, places numerical examples, takes care on the correct usage of certain terms, gives some historical details and, sometimes, tells relevant anecdotes. Owing to its clear organization, well aimed wording, pictorial comments and handy index, this book may be used for various purposes. The whole book can be highly recommended for beginners in crystallography, as complementary reading while they are going through the fundamentals. More advanced crystallographers may concentrate on selected problems that interest them – to widen, brush up or systematize their knowledge. For 'outsiders', the book may serve as a dictionary of basic mathematical and crystallographical terms. A short but well chosen bibliography points the reader to the relevant literature. The detailed Fortran programs, enclosed as Appendix *G*, will certainly be useful; but it seems to me that the mathematical formulae alone, well arranged within the main text, are very likely to inspire crystallographers to write their own programs. I found few errors or misprints. The lack of the minus sign in one exponent of the sequence of formulae on page 141 should be quickly spotted, but the equation accompanying Definition 15 on page 4 may cause a little more trouble.

To sum up, the author's aim 'to write . . . a *vade mecum* for active research workers' has been fully achieved. His approach invites active crystallographers on a comfortable journey through mathematical problems specially selected for them – with a reasonably light luggage of necessary formulae and definitions, and with a competent guide.

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Resonant anomalous X-ray scattering – theory and applications.

Edited by G. MATERLIK, C. J. SPARKS and K. FISCHER. Pp. xii + 688. Amsterdam: North-Holland, Elsevier, 1994. Price Dfl 350, US $200. ISBN 0-444-82025-6.

The intention of this book is to review, in a single volume, the present status of theory and experiments in X-ray resonant scattering from gases to solids. The book is a reference work, with 39 articles, on many different fields of research, chosen from contributions presented at the International Conference on Anomalous Scattering held in Malente, Germany, in 1992.

An earlier book on anomalous scattering, edited by S. Ramaseshan and S. C. Abrahams (Munksgaard, 1975) presented what then appeared to be a well understood field of X-ray science. The last twenty years, however, have seen a rapid development of synchrotron X-ray sources, and completely new experimental details can now be observed using