Acta Crystallographica Section A
Foundations of Crystallography
ISSN 0108-7673

book reviews

Works intended for this column should be sent direct to the Book-Review Editor, whose address appears in this issue. All reviews are also available from **Crystallography Journals Online**, supplemented where possible with direct links to the publisher's information.

Powder Diffraction. Theory and Practice. Edited by R. E. Dinnebier and S. J. L. Billinge. Cambridge: RSC Publishing, 2008. Pp. xxi + 582. Price (hardcover): GBP 59.00. ISBN (online): 978-1-84755-823-7; ISBN (print): 978-0-85404-231-9.

In this book, the editors cover the broad field of powder diffraction by wide-angle X-ray scattering. This book condenses the knowledge of renowned experts in the field into an authoritative overview of the applications of powder diffraction in modern materials research. After a basic introductory chapter entitled *Principles of Powder Diffraction* by the two editors, the book covers data-collection strategies using modern-day apparatus including synchrotron sources with chapters on *Experimental Setups* by J. K. Cockcroft and A. N. Fitch and also *Two-dimensional Diffraction Using Area Detectors* by B. Hinrichsen, R. E. Dinnebier and M. Jansen. I would have enjoyed a discussion here of details of how to improve the performance of the apparatus and when to use a particular arrangement of components to solve a particular problem.

The Intensity of a Bragg Reflection by R. B. Von Dreele and J. Rodriguez-Carvajal and *The Profile of a Bragg Reflection for Extracting Intensities* by A. Le Bail are described in two separate chapters. In the first, the main concern is the scattering from a modulated crystal lattice and neutron magnetic moment scattering, while the second is completed by a discussion of the limitations of extracting microstructural details from the profile of a Bragg reflection. *General Data Reduction* by R. Allmann is a classical chapter on data reduction and peak-search algorithms with a survey of the standard reference materials.

Ab initio structure determination from powder diffraction data and quantitative phase analysis by the Rietveld method are covered in four chapters, namely: *Indexing and Space Group Determination* by A. Altomare, C. Giacovazzo and A. Moliterni; *Crystal Structure Determination* by R. Caliandro, C. Giacovazzo and R. Rizzi; *Rietveld Refinement* by R. B. Von Dreele; and *Quantitative Phase Analysis* by I. C. Madsen and N. V. Y. Scarlett. The classical Patterson and direct methods are contrasted with more recent direct-space methods before concluding with the prediction of a crystal structure without the use of experimental information. One also finds much more specialized themes that are not treated in as much detail elsewhere: *Instrumental Contributions to the Line Profile in X-Ray Powder Diffraction. Example of the Diffractometer with Bragg–Brentano Geometry* by A. Zuev, which is an approach to the calculation of the total instrumental function with an exact analytical solution for the contribution of each incident ray to the intensity registered by a detector of finite size, and *The Derivative Difference Minimization Method* by L. A. Solovyov, which allows full-profile refinement independently of the background.

Two chapters are dedicated to microstructural properties, these being *Texture and Macrostress Effects* by N. C. Popa and *Lattice Defects and Domain Size Effects* by P. Scardi. After a clear distinction concerning the main applications of texture analysis, namely quantitative texture analysis and the problem of preferred orientation of crystallites in Rietveld refinement, the recent developments of the spherical-harmonics approach for the analysis of the macroscopic strain and stress by diffraction are developed with a thorough description of the mathematical background. In the second of these chapters, the traditional methods (integral breadth methods and Fourier methods) of line-profile analysis are contrasted with whole-powder-pattern modelling involving the use of physical models for the size and the strain modelling as well as other broadening sources. A further chapter is devoted to *Powder Diffraction under Non-ambient Conditions* by P. Norby and U. Schwarz, a subject which is usually absent in many textbooks and which concerns powder diffraction with a special emphasis on applications at high pressure. An introduction to *Local Structure from Total Scattering and Atomic Pair Distribution Function (PDF) Analysis* by S. J. L. Billinge completes the survey of the different approaches to scattering. The book ends with a chapter dedicated to *Computer Software for Powder Diffraction* by L. M. D. Cranswick, which presents a very useful list complete with internet addresses for software and resources.

This book is not intended to cover a basic introduction to crystallography and diffraction from crystals: fundamentals of the crystalline state, for example, are ignored. It is more an advanced introductory text about current methods and applications of powder diffraction in this active area of research. In this respect, this book contains essential theory and introductory material for students and researchers wishing to learn how to apply the basic and frontier methods of powder diffraction, although one would have enjoyed a chapter on small-angle X-ray scattering to complete this presentation. The good bibliography readily provides for further exploration of the fundamental research in powder diffraction.

Emmanuel Garnier

Laboratoire de Catalyse en Chimie Organique
UMR CNRS 6503 – Université de Poitiers
40 Avenue du Recteur Pineau
86022 POITIERS Cedex
France

 doi:10.1107/S010876730802850X