and a very helpful section on refinement strategy.

Following a brief but interesting historical account in Chapter 2, by H. M. Rietveld, of the development and acceptance of the method that now bears his name, some of the mathematical aspects of Rietveld refinement are summarized in Chapter 3 (E. Prince), including the method of least squares and its application to the Rietveld model, weights, constrained models, refinement procedures and estimates of uncertainty. In Chapter 4, T. M. Sabine considers processes that modify the flow of radiation in a polycrystalline material and derives simple expressions for absorption, multiple scattering and extinction that can be readily incorporated into the Rietveld model in the form of two refinable parameters: the effective specimen size and the size of the mosaic blocks. Chapter 5 (R. J. Hill) is the longest in the book and gives a comprehensive and pragmatic account of data-collection strategies for Rietveld refinement. Among the many important topics covered are the relative merits of laboratory X-ray, synchrotron X-ray and neutron diffractometers for different types of experiment, the choice of wavelength and resolution, the basic requirements of pattern analysis, how the choices of step increment and counting statistics affect the precision and accuracy of the refinement, and the application of Rietveld refinement to the quantitative analysis of multiphase materials. Background modelling in Rietveld analysis is addressed in Chapter 6, by J. W. Richardson Jr, who describes how a Fourier filtering technique can be used to correct time-of-flight neutron data with broad oscillations in the background caused by the presence of a noncrystalline component in the sample. Some procedures for analytical fitting of laboratory X-ray peak profiles in the application of Rietveld analysis are discussed in Chapter 7 by R. L. Snyder. The convolution of sample, spectral and instrumental contributions to the observed profile can be satisfactorily modelled by a split Pearson-VII function. Chapter 8 (R. Delhelz *et al.*) contains a detailed account of the effect of crystal imperfections on the shape and breadth of the peak profiles in a powder diffraction pattern and of the ways in which information about size and strain can be extracted by Rietveld refinement or pattern decomposition. In Chapter 9, P. Suortti shows how the instrumental profile function can be calculated from the known scattering geometry by ray-tracing or phase-space analysis techniques and also how the background contribution can be divided into an incoherent part that can be calculated explicitly and a coherent part that can be represented by a radial correlation function incorporating the salient features of the thermal and disorder diffuse scattering. In Chapter 10, C. Baerlocher points out how soft constraints, or restraints, can be used to improve the quality of the refinement of complex structures such as zeolites. These restraints, implemented in the form of approximate geometrical relationships in the least-squares minimization process, are now incorporated into several widely used programs. Chapter 11 (W. I. F. David and J. D. Jorgensen) reviews Rietveld refinement with time-of-flight neutron powder data. The power of this technique with a high-resolution diffractometer, such as the HRPD at the ISIS pulsed neutron source, is strikingly illustrated by examples of anisotropic line broadening in $LaNbO_4$ and a high-precision refinement of the structure of benzene. There are also advantages when special sample environments such as high-pressure cells and furnaces are required. In Chapter 12, R. B. Von Dreele (a co-author with A. C. Larson of the very versatile and widely used *GSAS* program) describes the extension of Rietveld refinement to a combination of X-ray and neutron powder diffraction data and illustrates how multiple data sets of this type may be the only way to determine the distribution of different atomic species among a number of crystallographic sites. F. Izumi, the author of another very versatile Rietveld refinement program (*RIETAN*), widely used in Japan, describes some of its features in Chapter 13, including the refinement of incommensurate structures from powder diffraction data and the use of multiple data sets of different types, as exemplified by a refinement of the modulated structure of the high-$T_c$ superconductor $Bi_2(Sr_{1-x}Ca_x)_3Cu_2O_{8+z}$. Chapter 14 (H. Toraya) gives an account of pattern-decomposition methods, which employ many of the features of Rietveld refinement but do not invoke a structural model. These methods are particularly useful in the initial stages of data analysis of materials about which little is known, and may allow the unit-cell parameters to be determined along with enough individual integrated intensities for *ab initio* structure solution. The fact that a structural model is not required may also be advantageous in microstructural analysis of size and strain parameters. In the concluding chapter, A. K. Cheetham covers the rapidly developing methodology for the *ab initio* solution of crystal structures from powder data, an exciting and challenging new area that owes much to the success of the Rietveld technique. He points out that the task of determining the unit-cell parameters and extracting enough integrated intensity data for structure solution by traditional methods is greatly facilitated by the high resolution available at a synchrotron source, whereas neutron data are likely to be most useful in the subsequent Rietveld-refinement stage for the precise determination of atom coordinates. However, the effect of the microstructural characteristics of the sample on the peak shapes will need very careful consideration if pattern decomposition and Rietveld techniques are to be utilized optimally for the determination of very complex structures.

In a book like this, it is inevitable that there is some unevenness in the length and degree of detail in the chapters and that some important topics receive inadequate attention. I would like to see, for example, a more exhaustive discussion of specimen preparation and diffraction geometry, accuracy and significance of the results, the tendency towards empiricism in modelling the peak shapes and the use of symmetry-adapted spherical harmonics to correct for preferred orientation and anisotropic line broadening. However, these are not serious criticisms and I recommend this book as a necessity for any diffraction library or for the personal collection of anyone with a serious interest in the application of the Rietveld technique.

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*J. Appl. Cryst.* (1994). **27**, 441–442

**X-ray diffraction at elevated temperatures: a method for *in situ* process analysis.** By *D. D. L. Chung*, *P. W. DeHaven*, *H. Arnold* and *D. Ghosh*. Pp. viii + 268. Weinheim: VCH Verlagsgesellschaft mbH, 1993. Price DM 158. ISBN 0-89573-745-0.

Books of this type, which bring together materials relating to a specialized technique, can be very helpful to new users of a method. The primary literature may be widely dispersed,with pertinent information appearing only as a minor section of a research paper. In many cases, a diligent search is required to find these references and a cursory electronic perusal may

miss much information that is not mentioned in either the title or abstract of the primary reference. Matters are even more difficult when, as in the present case, the technique is used by several disciplines, such as solid-state physics, materials science and mineralogy, further dispersing the literature references. We should therefore expect to welcome this text, but I find it flawed in two important respects – content and editing.

In terms of content, much of the material presented is unnecessary in a work of this kind. Thus, the first chapter, nearly 28% of the book, is devoted to a *Review of X-ray diffraction*, which consists of sections entitled *Introduction to X-ray diffraction*, *Symmetry*, *Theory of diffraction*, *Production of X-rays and their characteristics* and *Diffractometers and Cameras*. Although many solid-state scientists lack a sound level of training in the formalism of crystallography, one may assume that this would not be the case for potential users of this specialized crystallographic method. Even if it were the case, it is not clear that books such as this should try to remedy that deficiency. Better that the authors should state the level of background knowledge that has been assumed and suggest a standard text to be used when that knowledge is absent. Much of the space taken up by their elementary presentation of basic principles could have been used to pursue the main objectives – the performance and interpretation of high-temperature experiments or, by its omission, have served to reduce the price of the book. A similar criticism may be offered of the discussion of instrumentation; more than half of the chapter is devoted to the description of standard single-crystal devices, such as diffractometers and oscillation and precession cameras, even though the main thrust of the later chapters describing experimental procedures treats mainly the powder method.

Lack of clear editorial oversight is evident in the unnecessary repetition of material as well as in poor cross-referencing between chapters. For example, the design of position-sensitive detectors is discussed, by different authors, in both Chapter 3 (pp. 111–128) and Chapter 4 (pp. 162–164), with considerable repetition. However, in Chapter 7, where the use of these detectors is discussed, the cross-references are exclusively to the same author's shorter Chapter 4 rather than to the more definitive Chapter 3.

Despite these faults, the last four chapters, or about half of the book, are enough to make it useful as a text for new practitioners of the art of high-temperature diffraction. These chapters describe the equipment and the analysis of the data in enough detail for a newcomer to be able to make a start. But even here a criticism must be offered. The chapter on thermal expansion omits the methods needed to analyze the behavior of non-cubic materials. The derivation of the strain ellipsoid of thermal expansion from the lattice constants at two different temperatures has been known since the early 1970's. This technique is presented in at least one reference that the present authors cite in another context, and should have been included here. One final word of warning: the preface is dated May 1992, so the book presumably went to the printers in mid-1992. It is quite disturbing, therefore, that literature coverage appears to stop in early 1990.

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## Books Received

*J. Appl. Cryst.* (1994). **27**, 442

*The following books have been received by the Editor. Brief and generally uncritical notices are given of works of marginal crystallographic interest; occasionally, a book of fundamental interest is included under this heading because of difficulty in finding a suitable reviewer without great delay.*

**Electron diffraction techniques.** Vol. 2. (**IUCr Monographs on Crystallography** No. 4.) Edited by *John M. Cowley*. Pp. vi + 423. Oxford: Oxford University Press, 1993. Price £45.00. ISBN 0-19-855733-7. A review of this book, by Douglas L. Dorset, has been published in the March 1994 issue of *Acta Crystallographica Section A*, pages 258–259.

**Modern powder diffraction. Reviews in mineralogy**, Vol. 20. Edited by *D. L. Bish* and *J. E. Post*. Pp. xi + 369. Washington, DC: The Mineralogical Society of America, 1990. Price (paper) US $25.00. ISBN 0-939950-24-3.A review of this book, by James A. Kaduk, has been published in the March 1994 issue of *Acta Crystallographica Section A*, page 259.