book reviews

Two-dimensional X-ray diffraction. By Bob Baoping He. Pp. 426. Hoboken: Wiley, 2009. Price (hardcover) GBP 76.95. ISBN 978-0-470-22722-0.

In many sections of science, buzzwords are mushrooming. One of the less felicitous, though widespread, examples is surely 'two-dimensional X-ray diffraction', used as the title of the present book. Of course, the book deals exclusively with three-dimensional diffraction phenomena, but concentrates on the recording of powder diffractograms with 'two-dimensional' area detectors. The title 'X-ray powder diffraction with area detectors' might have been more appropriate. One gets a very positive first impression from looking at the table of contents. It implies a comprehensive overview of modern powder diffraction methods from a pioneer of technical applications, Bob B. He, Director of Research and Development of the Bruker AXS company, which continues the powder diffractometry heritage of Siemens and Enraf–Nonius, amongst others.

The book begins in Chapter 1 with the terminology of the different aspects of X-ray diffraction, an introduction to the geometry of crystals, the principles of X-ray diffraction in real and reciprocal space, and, finally, a short résumé of 'two-dimensional X-ray diffraction'. Reading this introductory chapter, one experiences a first surprise when learning on p. 3 that 'a lattice point represents the location of the center of an atom', a wrong understanding of the term lattice. In the fast run through crystallography basics which follows, symmetry is only considered as lattice symmetry: there is no mention of crystal classes, Laue symmetry or space groups. However, we learn: 'The reflection plane divides the crystal into two sides.' Later on we read: 'these seven types of unit cells are called primitive cells and labeled by P or R'. In Table 1.1, however, the P lattice is named 'simple' instead of 'primitive'. Fig. 1.3, showing the unit cells of the 14 Bravais lattices, gives a monoclinic cell with the unconventional setting $\beta < 90°$, and the C-centered cell is labeled A. Fig. 1.4 creates confusion, as some directions are not drawn from the origin of the cell. In Fig. 1.6, the zone axis [001] is correctly drawn, but in the caption we read [100]. §1.2.3, *Atomic arrangement in crystal structure*, is restricted to the three simple sphere packings body-centered cubic, face-centered cubic and hexagonal close packing. The inattentive composition of drawings continues in Fig. 1.12, where the $b*$ axis is obviously wrong. The series of errors culminates in §1.3.1, *Bragg law*, with the explanation of the higher orders n of reflection as being caused by 'harmonic energies two or three times the fundamental energy (of X-rays)'! In conclusion, it would have been better to omit this chapter. It is one of the reasons why this book cannot be recommended to students.

Chapter 2 gives the mathematical scaffold for the description of X-ray diffraction on different goniometers with cylindrical and flat area detectors. Chapter 3 deals with the generation, collimation and monochromatization of X-rays, and with X-ray mirror systems. In Chapter 4, radiation detectors are discussed, with the focus on different types of area detectors. Here, much attention is given to the renaissance of the multiwire proportional counter in the form of the 'microgap detector' preferred by Bruker AXS for some applications. Chapter 5 shows the necessary goniometer and sample-stage configurations for measurements with area detectors, and Chapter 6 gives a detailed overview of the different calibration and correction techniques necessary to obtain correct diffraction data from an area-detector system. For researchers applying powder diffraction methods, these chapters provide a lot of technical and mathematical details on the setup of goniometers, sample stages and detectors that cannot easily be found elsewhere. For people that are responsible for the technical maintenance of diffractometers, it may be of great value to know about the necessary adjustments, calibrations and corrections to obtain optimum experimental data. In these chapters, many helpful drawings and photographs support the reader. It is, of course, not surprising that the discussion of the various detector systems concentrates mainly on the types used in Bruker AXS diffractometers, and that image-plate systems are mentioned on one page only.

Under the heading of Chapter 7, *Phase identification*, an introduction is first given to structure factors. For unknown reasons, the symbols u, v, w instead of the usual x, y, z are used for the atom parameters and it is stated that these values 'are between zero and less than unity' – another reason to hope that this text may never come into the hands of students! Thereafter, various influences of diffraction, sample geometry and texture on the intensities are discussed, and it is shown how measurements with area detectors have to be processed to obtain data sets with 2θ angles, peak profiles and intensities, suitable for handling with conventional phase-analysis programs. The methods of phase analysis itself are not treated.

Much space is devoted to the handling of texture effects (Chapter 8, 30 pages with 17 figures) and especially of stress measurements (Chapter 9, 80 pages with 33 figures). Here, it becomes obvious that the author moves into his own area of research. Many details of mathematical treatment going back in part to the author's thesis are listed. So, we find a two-page table with coefficients for a polynomial fit to calculate the pole density function for a fiber texture of a cubic structure. For both applications, texture analysis and stress measurements, helpful advice for measurement strategies is given, assisted by many figures and photographs. However, even in these

chapters, one has the impression that this book was prepared in a hurry, with insufficient proofreading. Otherwise, it would have been detected that the discussion of the pole density distribution function is given twice, in §7.5 and in §8.3.2. Equations 7.31–7.34 are identical to equations 8.9–8.11 and 8.3. Furthermore, in Fig. 4.3, curves B and C are interchanged, and in Fig. 4.16, the inset shows α_1/α_2-splitting of corundum lines, while the frame itself is obviously from some other sample. It is unfortunate that several alternative methods of texture and stress analysis in the literature are not considered here.

Chapter 10 gives a short overview of small-angle X-ray scattering (SAXS) with area detectors, including some interesting variations, 'scanning SAXS' and a vertical SAXS system. Chapter 11, *Combinatorial screening*, shows some examples of fast powder diffractometry on sample libraries in reflection and transmission modes. Chapter 12, *Quantitative analysis*, is confined to the measurement of 'percent crystallinity' and the determination of particle size; the austenite/martensite phase mixture is given as an example of quantitative phase analysis in industry. The application of the Rietveld method for structure refinement and semi-quantitative phase analysis, implemented in all powder diffraction software suites and widely used in research laboratories and industry, is surprisingly not in the scope of this book.

In Chapter 13 a survey of future developments is given, such as a scanning line detector, or a three-dimensional detector where the third dimension means additional energy resolution at a two-dimensional area detector. An interesting and promising concept of 'pixel direct diffraction analysis' is presented at the end. The way outlined (proposed also by other people in the past) is to use directly the information of each pixel or volume increment in reciprocal space instead of transforming it to integrated reflections or one-dimensional diffraction profiles, and this is surely the future way of crystallographic analyses.

The book competes with other recent monographs like *X-ray Diffraction by Polycrystalline Materials* by R. Guinebretière (ISTE 2007, see review in *J. Appl. Cryst.* **41**, 826) and *Powder Diffraction, Theory and Practice* edited by Dinnebier & Billinge (RSC Publishing 2008, see review in *Acta Cryst.* A**65**, 51), where the use of area detectors in modern diffractometers is also treated, though less extensively. Given the errors in teaching the crystallographic basics, this is not a book for students. The book will probably find its main readership among Bruker AXS users who want to experience what happens inside their devices.

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