Book review

R.L Snyder, J.Fiala, H.J.Bunge: „Defect and Microstructure Analysis by Diffraction“

International Union of Crystallography, Oxford University Press, New York 1999, ISBN 0 19 850189 7.

This volume forms a part of a series of books sponsored by the International union of Crystallography (IUCr) and published by Oxford University Press. It has been conceived as an initiative of the Commission on Powder Diffraction of the IUCr dated as late as in 1991. Then, Commission on Powder Diffraction, chaired by Prof. R.A.Young, has made a specific proposal for a meeting in Czechoslovakia with the title „X-ray Diffraction Studies of *Real* Polycrystalline Materials“ (grain size, strain and texture). The conference was carefuly prepared and realized in Military Academy Liptovský Mikuláš, Slovakia in August 1995 with 120 attendants from 23 countries (SIZE-STRAIN'95). There were 25 invited lecturers there who agreed to work out texts that would be organised into an authoritative book on defect and microstructure analysis by diffraction to serve as a comprehensive, in-depth reference work on this topic for crystallographers and materials scientists. And, after another four years of great endeavour, the book finally appeared.

The book has 785 + XVII pages and consists of 31 chapters (written by 39 authors) which are grouped into seven parts: fundamentals of defect analysis by diffraction, experimental techniques, macrostress, texture, whole pattern fitting, restoring physical patterns from the observed variables, and applications. Some sixty per cent of the volume is devoted to the line-broadening effects observed in X-ray powder diffraction patterns since the early days of X-ray diffraction analysis when it was recognized that the diffraction line shape contains information about imperfections in crystalline phases. The second most important subject dealt with in the book is texture of polycrystalline materials as defined by the orientation distribution of its crystallities. The featuring chapter on texture, written by Prof. H.J.Bunge, the world's top specialist in texture analysis, represents, in fact, the best treatise on this subject matter ever published. The third issue, discussed in the volume and complementing the description of the materials real structure (microstructure), is macrostress, the measurement of which represents one of the most widespread and technologicaly important applications of X-ray difraction.

In fact, microstructural or „real-structure“ features, i.e. structural imperfections as well as the size, shape, spatial arrangement and orientational alignment of crystallities or domains, residual stress and strains are of utmost practical importance since the properties of many materials in daily life largely depend on these features. On the other hand, the diffraction pattern is relatively intensive to the microstructural features and that is why they are usualy studied in the real space by various microscopical methods. But X-ray diffraction provides much microstructural information in the reciprocal space which is unaccessible by microscopy, being at the same time very demanding from the technical point of view. In fact, defect and microstructure analysis is the most difficult branch of X-ray crystallography and the only work that attempted to cover comprehensively this field was the book of H.S.Peiser, H.P.Rooksby and A.J.C.Wilson „Diffraction by Polycrystalline Materials“ that was published by Chapman and Hall in London, 1960. The present volume, edited by Snyder, Fiala and Bunge, fills up the wide gap between 1960 and 1999 and brings an extensive and detailed review of what has been done. So, much is explained on various sources of diffraction line broadening like crystallite or domain size and size distribution, strain including anisotropic strain, structural mistakes, stacking faults and other planar defects, dislocations, dislocation manifolds and dislocation configurations, strain fields and paracrystallinity. The state-of-the art evaluation techniques for restoring (deconvolution of) physical patterns from the measured diffraction profiles, background subtraction, smoothing, sampling and interpolation, Fourier techniques, iterative solutions of integral equations, inverse filtering, regularisation and maximum entropy methods, maximum likelihood and Bayesian methods, are discussed in detail, too. The extensive theoretical passages are complemented with a number of chapters reporting numerous examples of practical applications related to inorganic chemistry, metallurgy, ceramics and organic polymers.

The volume points out the weak points of the conventional X-ray diffraction techniques for real structure analysis: the verification of structural models, indistinguishability of different structural models from the point of view of powder diffraction; the number of different real structure models that have been investigated in detail is very small and these models are rather simplified and far from reality. A new, very promissing technique for the study of microstructure is introduced in the chapter on X-ray diffraction imaging (XRDI). Unlike traditional powder diffractometry, where divergent and focusing X-ray optics are essential to collect information from an ensemble of all grains within the illuminated volume of the sample which is then analysed making use of a mathematical model of the assumed microstructure, a nearly parallel beam is employed in XRDI to observe and measure diffraction images from individual grains and component particles (grain-by-grain mapping, topography) providing thus ability to measure shape, size, orientation and strain without model-based analyses.

The book „Defect and Microstructure Analysis by Diffraction“ is a very useful, quite a unique work, invaluable both to practitioners of X-ray analysis and to all those involved in materials characterization.

Pavol Šutta