Chapter 6
Evaluation Methods of Line Profiles

ABSTRACT

The evaluation procedures of X-ray line profiles are overviewed in this chapter. These methods can be classified into four groups, namely (1) the most simple methods that evaluate only the breadths of diffraction peaks, (2) procedures using the Fourier-transforms of line profiles for the determination of the parameters of microstructures, (3) variance methods evaluating the restricted moments of peaks, and (4) procedures fitting the whole diffraction pattern. The crystallite size distribution and the densities of lattice defects cannot be determined from the peak width alone as the rule of summation of breadths of size, strain, and instrumental profiles depends on their shape. However, the breadth methods can be used for a qualitative assessment of the main origins of line broadening (size, dislocations, planar faults) (e.g. for checking the model of microstructure used in whole powder pattern fitting procedures). The application of Fourier and variance methods is limited if the diffraction peaks are overlapping. In the case of pattern fitting procedures, usually a microstructure model is needed for the calculation of the theoretical fitting functions. The reliability of these methods increases with increasing the number of fitted peaks.

DOI: 10.4018/978-1-4666-5852-3.ch006

INTRODUCTION

The main goal of line profile analysis is to determine the parameters of the microstructure (e.g. crystallite size distribution, dislocation density, planar fault probability etc.) from the diffraction peak profiles. The nature of line broadening caused by crystallite size, dislocations and planar faults are essentially different which enables to separate these effects and determine their characteristic parameters. In chapters 2-4 the theory of the line broadening caused by the finite crystallite size, the lattice strains and the planar faults are reviewed and the theoretical profile functions related to these effects are given. On the basis of these functions several methods were elaborated for the extraction of the parameters of the microstructure from peak profiles. In the early years of the history of line profile analysis, mainly the peak breadths are used to determine the average crystallite size and the average lattice strains in the investigated material. The most frequently applied classical method for the evaluation of peak widths is the Williamson-Hall method (Williamson & Hall, 1953). Later, this procedure has been improved to handle the anisotropic strain broadening of line profiles caused by dislocations (Ungár & Borbély, 1996). The strain anisotropy means that the strain broadening component of the peak width is strongly and characteristically dependent on the indices of reflection *hkl*. Similar improvement has been made on the other very important evaluation procedure referred to as Warren-Averbach analysis (Warren, 1990). The modified version of this method was capable to give the characteristic parameters of the dislocation structure and the planar fault probability besides the crystallite size (Ungár, Ott, Sanders, Borbély, & Weertman, 1998). The procedures mentioned above need more than one diffraction peak for the successful evaluation. However, a single peak method has also been developed which is referred to as variance method (Wilson, 1955; Groma, 1998). This procedure uses the restricted moments of an intensity profile for the determination of the crystallite size and the characteristic parameters of the dislocation structure (Borbély & Groma, 2001; Groma, Tüzes, & Ispánovity, 2013). The latest improvement of the methodology of line profile analysis is the development of pattern fitting methods which was enabled by the increase of the power of computers. There are several line profile fitting procedures for the evaluation of the diffraction pattern of polycrystalline materials such as MAUD (Lutterotti, Matthies, & Wenk, 1999), FULLPROF (Rodríguez-Carvajal, 2001), FOX or MStruct (Matej, Nichtová, & Kuzel, 2008), MWP (Ungár, Gubicza, Ribárik, & Borbély, 2001; Ribárik, Ungár, & Gubicza, 2001), WPPF (Scardi & Leoni, 1999), WPPM (Scardi & Leoni, 2002) and CMWP (Ribárik, Gubicza, & Ungár, 2004; Balogh, Ribárik, & Ungár, 2006; Balogh, Tichy, & Ungár, 2009). It is noted that MAUD and MStruct can also be applied for thin films as they account for thin film absorption correction and asymmetrical diffraction geometry. In the following the most

Related Content

Investigations on Materials Used for Manufacturing the Rolling Rolls in Few Durability Experiments

Imre Kiss (2013). *International Journal of Surface Engineering and Interdisciplinary Materials Science (pp. 46-56).*

www.irma-international.org/article/investigations-materials-used-manufacturing-rolling/75565

Modeling Simulation-Based Agents for Reducing Operative Deferral in Oncology in a Virtual Scenario using Ergonomics

Adriana García, Alberto Ochoa-Zezzatti, Juan Luis Hernández Arellanoand Aide Aracely Maldonado Macías (2018). *Handbook of Research on Ergonomics and Product Design (pp. 48-54).*

www.irma-international.org/chapter/modeling-simulation-based-agents-for-reducing-operative-deferral-in-oncology-in-a-virtual-scenario-using-ergonomics/202646

Durability of Manufactured Sand (m-Sand) Concrete: A Review

Ankit Singh Beniwal, Nirbhay Mathurand Ram Vilas Meena (2025). *Tools, Techniques, and Advancements in Engineering Materials Science (pp. 157-166).*

www.irma-international.org/chapter/durability-of-manufactured-sand-m-sand-concrete/366819

Parametric Analysis of Different Grades of Steel Materials Used in Plastic Industries through Die Sinking EDM Process

Goutam Kumar Boseand Pritam Pain (2016). *International Journal of Materials Forming and Machining Processes (pp. 45-74).*

www.irma-international.org/article/parametric-analysis-of-different-grades-of-steel-materials-used-in-plastic-industries-through-die-sinking-edm-process/143657

An Overview of 3D Printing (Additive Manufacturing in Powder-Based Methods) Materials, Methods, Mechanical Properties, and Applications

R. Raffik, Raghavan Santhanam, Chamandeep Kaur, S. Seenivasanand K. Somasundaram (2023). *Handbook of Research on Advanced Functional Materials for Orthopedic Applications (pp. 14-28).*

www.irma-international.org/chapter/an-overview-of-3d-printing-additive-manufacturing-in-powder-based-methods-materials-methods-mechanical-properties-and-applications/329743