

1. Record Nr.	UNINA9910830141803321
Autore	Chateigner Daniel
Titolo	Combined analysis [[electronic resource] /] / Daniel Chateigner
Pubbl/distr/stampa	London, U.K., : ISTE Hoboken, N.J., : Wiley, 2010
ISBN	1-118-62264-2 1-118-62250-2 1-299-31555-0 1-118-62271-5
Edizione	[1st edition]
Descrizione fisica	1 online resource (517 p.)
Collana	ISTE
Disciplina	548.83 548/.83
Soggetti	Analytical chemistry Solid state chemistry Crystals
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Cover; Combined Analysis; Title Page; Copyright Page; Table of Contents; Introduction; Acknowledgements; Chapter 1. Some Basic Notions About Powder Diffraction; 1.1. Crystallite, grain, polycrystal and powder; 1.2. Bragg's law and harmonic reflections; 1.2.1. Bragg's law; 1.2.2. Monochromator; 1.2.3. Harmonic radiation components; 1.3. Geometric conditions of diffraction, Ewald sphere; 1.4. Imperfect powders; 1.5. Main diffraction line profile components; 1.5.1. Origin of g(x); 1.5.2. Origin of f(x); 1.5.3. Deconvolution-extraction of f(x) and g(x); 1.6. Peak profile parameters 1.7. Modeling of the diffraction peaks 1.7.1. Why do we need modeling?; 1.7.2. Modeling of a powder diffraction pattern; 1.8. Experimental geometry; 1.8.1. Curved Position Sensitive detector, asymmetric reflection geometry; 1.8.2. CCD or image plate detector, transmission geometry; 1.8.3. Curved-Area Position-Sensitive detector, transmission geometry; 1.9. Intensity calibration (flat-field); 1.9.1. Counts and intensity; 1.9.2. Flat-field; 1.9.3. PSD detector; 1.9.4. CAPS detector; 1.10. Standard samples; 1.10.1. Laboratory x-ray standards;

## 1.10.2. Neutron texture standards

1.11. Probed thickness (penetration depth)Chapter 2. Structure Refinement by Diffraction Profile Adjustment (Rietveld Method); 2.1. Principle of the Rietveld method; 2.2. Rietveld-based codes; 2.3. Parameter modeling; 2.3.1. Background modeling; 2.3.2. Structure factor; 2.3.3. Crystallites' preferred orientation (texture) corrections; 2.3.4. Peak asymmetry; 2.3.5. Peak displacements; 2.3.6. Lorentz-polarization correction; 2.3.7. Volume, absorption, thickness corrections; 2.3.8. Localization corrections; 2.3.9.

Microabsorption/roughness corrections; 2.3.10. Wavelength

2.4. Crystal structure databases2.5. Reliability factors in profile refinements; 2.6. Parameter exactness; 2.7. The Le Bail method; 2.8. Refinement procedures; 2.8.1. Least squares; 2.8.2. Genetic or evolutionary algorithms; 2.8.3. Derivative difference minimization (DDM); 2.8.4. Simulated annealing; 2.9. Refinement strategy; 2.10. Structural determination by diffraction; 2.10.1. The phase problem in diffraction; 2.10.2. Patterson function; 2.10.3. Direct methods; 2.10.4. Direct space methods; 2.10.5. Fourier difference map; 2.10.6.

Extension to aperiodic structures

Chapter 3. Automatic Indexing of Powder Diagrams3.1. Principle; 3.2. Dichotomy approach; 3.3. Criteria for quality; Chapter 4. Quantitative Texture Analysis; 4.1. Classic texture analysis; 4.1.1. Qualitative aspects of texture analysis; 4.1.2. Effects on diffraction diagrams; 4.1.3. Limitations of classic diagrams; 4.1.4. The Lotgering factor; 4.1.5. Representations of textures: pole figures; 4.1.6. Localization of crystallographic directions from pole figures; 4.1.7. Texture types; 4.2. Orientation distribution (OD) or orientation distribution function (ODF) 4.2.1. Pole figures and orientation spaces

## Sommario/riassunto

This book introduces and details the key facets of Combined Analysis - an x-ray and/or neutron scattering methodology which combines structural, textural, stress, microstructural, phase, layer, or other relevant variable or property analyses in a single approach. The text starts with basic theories related to diffraction by polycrystals and some of the most common combined analysis instrumental set-ups are detailed. Also discussed are microstructures of powder diffraction profiles; quantitative phase analysis from the Rietveld analysis; residual stress analysis for isotropic and anisotropic ma