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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. Wavelength2.4. 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 structuresChapter 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 materials