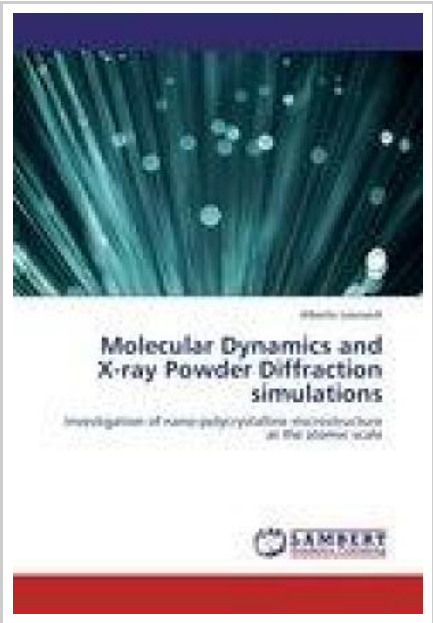

Molecular Dynamics and X-ray Powder Diffraction simulations

By Alberto Leonardi

LAP Lambert Academic Publishing Jul 2013, 2013. Taschenbuch. Book Condition: Neu. 220x150x10 mm. This item is printed on demand - Print on Demand Neuware - Atomistic simulations based on Molecular Dynamics were used to model the lattice distortions in metallic nano-polycrystalline microstructures. Complex microstructures were generated with a new modified Voronoi tessellation method which provides a direct relation between generation parameters and statistical properties of the resulting model. Line Profile Analysis (LPA) was employed to retrieve the microstructure information from the powder diffraction patterns. The study provided a new point of view on the role of the grain boundary regions in nano-polycrystalline aggregates, exploring the interference effects between different domains and between grain boundary and crystalline regions. Usual concepts of solid mechanics were brought in the atomistic models to describe the strain effects on the powder diffraction pattern. The new concept of Directional Pair Distribution Function (D-PDF) was developed. D-PDFs provide a representation of the strain field which is directly comparable with the results of LPA. The D-PDF opens a new chapter in powder diffraction as new insights and a more sound interpretation of the results are made possible with this new approach to diffraction LPA. 164 pp. Englisch.

Reviews

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