

Continuum mechanics in an atomistic frame: modelling strain effects in X-ray powder diffraction

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Abstract

X-ray powder diffraction (XRPD) is a flexible and powerful tool for the non-destructive analysis of polycrystalline materials. The position and intensity of the diffraction peaks bear information on the atomic arrangement and its periodicity, whereas the breadth and shape are intimately related to the microstructure. Microstructure can be quantitatively analysed via XRPD in terms of shape, size and size distribution of the crystalline domains and of distortions in the lattice, computed under continuum mechanics hypotheses.

The analysis of the XRPD of a realistic computer-generated microstructure simulated e.g. via molecular dynamics (virtual experiment), poses the problem of relating the discrete nature of the specimen (and of the atomic displacements) with the continuous description employed in the analysis.

With a suitable stretching of the definition of strain down to the atomic level, a consistent description of the diffraction effects is possible: the results offers a deeper understanding of the nature of defects, grain boundary and, in general, of local strains in nanocrystalline materials.