[MS26] Crystallography of nanoparticles, including strain broadening

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[MS26 - 01] Strain broadening effects in nanostructured materials

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X-ray Diffraction (XRD) patterns from nanostructured materials are directly affected by the size, shape of the crystalline domains and lattice distortion therein. Characteristic line broadening effects result from the interference between different crystalline domains and the strain field at the atomic level within each of them.
Atomistic modelling of nano-polycrystalline microstructures provides useful insights in the interpretation of the XRD line broadening. The atomistic point of view accounts for a large variety of contributing effects, usually considered as independent by traditional Line Profile Analysis methods. In this way, a direct explanation of the LPA models and their approximations can be provided, validating the corresponding results.
In the present contribution, the meanings of LPA results are discussed in terms of the strain field in an atomistic model of a nano-polycrystalline microstructure. The particular structure of grain boundaries and the interference between independent crystalline domains are singled out as diffuse scattering and broadening of Bragg peaks. The concept of Directional Pair Distribution Function (D¬PDF) is introduced, as an effective tool to study the strain broadening caused by the local atomic displacements in atomistic microstructures. The latter is thus discussed in terms of local deformation in continuum mechanics and different strain types, also accounting for the anisotropy of defects and elastic medium.