X-ray Powder Diffraction Characterization of Nanoparticles

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Nanometer size particles show chemi-physical properties which largely differ from those of the parent bulk material. Because of the complexity and novelty of these materials, a fundamental simple task, such as determining and controlling the NP size distribution needs a complex experimental work, which often requires the combination of different characterization techniques. Among the most widely used, X-ray powder diffraction has shown a great potential to meet the increasing demands of microstructural material characterization. Indeed, powder diffraction data analysis methods – exported from micrometer-sized polycrystalline materials characterization research field – have to be specifically tuned for particle size falling much below 100 nm. In fact, even for crystalline NPs, due to the small size, Bragg peaks may be so much broadened to be hardly separated and many approximations, commonly accepted for micrometer size domains, fail. In addition, surface-related strain fields and size effects cannot easily be separated and affect both peak position and width. In the most complex cases, also non-crystallographic structures may occur. In these extreme cases, the classical crystallographic formalism becomes quite useless, being the Debye scattering function (that is, the direct evaluation of the NP structure factor from the interatomic distances) the only possible choice.

We will present examples on several nanoparticles, namely Au, II-VI compounds and CeO_2. Based on the specific material and data analysis demand, we will make use of a shape-convolution method to calculate the diffraction pattern of the NPs powder or alternatively of a computing approach based on the Debye scattering function.

Keywords: nanoparticles, x-ray powder diffraction techniques, quantitative x-ray analysis