DIFFRACTION ANALYSIS AND ATOMISTIC MODELLING OF THE REAL STRUCTURE OF NANOCRYSTALLINE MATERIALS

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Despite the considerable importance of nanostructured materials in science and technology, the common approach to their characterization by diffraction techniques is still far from being satisfactory. Most current analytical methods are based upon a perturbative approach, according to which small crystallites are thought as pieces of matter carved from an ideal, infinite crystal lattice: each further deviation from ideality can be added as a perturbation, and a completely consistent theory can be built on this basis.

However, this approach is not appropriate to real nanocrystals. Particles clearly demonstrating this inadequacy are the so-called non-crystallographic nanoparticles, like decahedra, icosahedra or tetrapods, frequently observed at the nano scale. In those cases the tridimensional periodicity typical of a perfect crystal is lost, and traditional crystallography (and diffraction) methods can hardly be used. Besides those striking examples, this issue concerns any small object: in order to minimize the free energy, nanostructured materials commonly relax their lattice in a rather complex way and often introduce defects like arrays of twins. Nanoparticles, whether crystalline or not, should thus be considered as large single molecules more than the usual stacking of unit cells: for an accurate and fruitful modelling of diffraction patterns the atomistic nature of those objects should be considered. This is the paradigm of the Debye Scattering Function (DSF), which is the most direct and accurate way to describe the diffraction pattern from a powder of objects, just knowing the positions of atoms and their scattering power. In the past years much has been made to relieve the major problem of the DSF being computationally heavy. While this problem is still a subject for active research, much less is made to improve the description of the nanocrystal models.

In our view, an atomistic model (like those used in Molecular Dynamics or similar techniques) should be the guide for a correct modelling of the diffraction data. This to the benefit of a more realistic description of the nanoparticles, also supported by energetic considerations. The present contribution addresses the complex problem of refounding diffraction Line Profile Analysis on the basis of atomistic models of nanocrystals.