

Searching for a refinable model of a nanocrystal

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When elaborating a diffraction data of polycrystalline samples one has already in mind a model of the material's structure to which one refers to. In a routine procedure of diffraction data analysis of a crystalline material the model which one "has in mind" is a single crystal. An individual nanoparticle obviously shows a non-uniform structure with a unique atomic architecture, definitely more complex than that of a single crystal. There are several conditions for a successful investigation of nanocrystalline structures: (i) a (refineable) model of a nanocrystal, (ii), (the right) experiment and, (iii), (appropriate) data elaboration technique.

ad (i) A realistic "universal" model of a nanocrystal which could be described by a set of "refinable" parameters does not exist. A tentative core-shell model which is often used is a kind of a "substitute" which might help one to come up with some numbers which characterize an atomic architecture of the nanocrystal.

ad (ii) The appropriate experimental technique applicable to nanocrystals is powder diffraction. However, due to a complexity of nano-structures a reliable information on the atomic arrangements in nanograins requires collection of data at possibly large diffraction vector, much larger than available with standard laboratory diffractometers. Definitely "hot neutrons" or hard X-rays available at synchrotron sources are necessary to start structural analysis of such materials.

ad. (iii) Any software developed so far for elaborating the structure of crystalline materials and applied to nanocrystals might serve only for evaluation of "how poorly" single crystal lattice represents the actual structure of the current sample. Definitely, for nanocrystals we need a specific software dedicated to such materials.

At present, a practical and temporary solution for overcoming the limitations of not having an atomistic model of a nanocrystal might be achieved by building projections of nanocrystals in real and/or reciprocal spaces which would constitute a reproducible "footprints" of the examined nanomaterials. They might have a form of specific plots of experimentally derivable parameters from Bragg and/or PDF images. Tentative solutions will be discussed.