Keynote Lectures

[KN16] PDF of Nanocrystals,
Reinhard B. Neder

Crystallography and Structural Physics, University Erlangen, Staudtstr. 3., 91058 Erlangen,Germany
E-mail: reinhard.neder@fau.de

Due to the small size of nanocrystals, their powder diffraction pattern are characterized by very broad reflections that overlap considerably even at small diffraction angles. Common defects like surface relaxations, stacking faults, which destroy the long range order of the crystal will furthermore lead to an increased reflection width even more at larger diffraction angles. Thus he information content that appears to be present is reduced and standard structure determination and refinement procedures do not work any longer. The shape and continuous intensity distribution of these peaks do hold, however, a lot of information on the particle size and defects, which can quantitatively be interpreted by appropriate whole pattern matching. If the diffraction pattern is measured to very high values of Q, above some 20 $Å^{-1}$, a lot of further information about the sample is collected, despite the fact hat the diffraction pattern at high Q does not contain any sharp features but broad oscillations at best. With this high Q range, he powder pattern can be transformed via a sine Fourier transformation into the pair distribution function (PDF). The PDF, in analogy to the Patterson function, shows peaks at interatomic distances. Their heights correspond to the number of neighboring atoms, their positions and their widths are a direct measure of the interatomic distance and distance distribution. Thus the PDF can be interpreted likewise for crystalline, nanocrystalline and highly disordered materials.
Despite the few features in a diffraction pattern, the PDF of a nanocrystal usually shows sharp peaks that reflect the local crystal structure, which can easily be refined. Due to the finite size, the longest observed peaks in the PDF of a nanocrystal correspond to the nanocrystal diameter. With appropriate full modeling techniques an anisotropic shape can
be determined as well. The analysis of the peak width as function of distance gives an insight into a defect model of the nanocrystal. Their determination and the distinction of different models is much easier compared to reciprocal space methods. An exception is chemical short range order that is actually difficult to determine, as contrasting models give a very similar PDF. A particular strength of a joint X-ray and neutron diffraction data derived PDFs is the observation of peaks at distances that correspond to the distances between the inorganic core and the organic shell of a nanocrystal.
Current specialized beam lines allow true in-situ measurements. As an example the nucleation and growth of ZnO nanocrystals from a precursor phase via initial clusters of few atoms to the final nanocrystal will be presented.