Characterisation of Nanoparticles

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Powder diffraction pattern of ZnO as well as CdSe/ZnS core shell nanoparticles were obtained and analysed with respect to particle size, defect density and local structure. The pair distribution function was successfully used to analzse the local structure.

The ZnO pattern were refined by the Rietveld method using a wurtzite structure. The moderate agreement shows that the particles are of anisotropic shape and have a stacking fault density of some 20%. The nanoparticles were modelled and size, shape, stacking fault density, positional and displacement parameters fitted to the powder pattern by means of the Debye formula as well as to the respective experimental Pair Distribution Function. The two methods give similar results of some 3.5 nm parallel [100] and 2.5 nm parallel [001] in size.

The CdSe nanoparticles and CdSe/ZnS core-shell nanoparticles show diffraction pattern that qualitatively fit to a wurtzite structure. The size of 3 nm as well as stacking fault density of 25% and distortions at a surface layer degrade the powder pattern. The pattern of the CdSe/ZnS core-shell nanoparticles are widened at the high 2θ side compared to the pure CdSe nanoparticles. The smaller metal-anion distance (Zn-X=0.235 nm, Cd-X=0.27 nm) cause a distortion of the whole particle.

Keywords: nanoparticle, pair distribution function, local structure