MS40-P12 | NANOCRYSTALLINE CDS AND (CD,MN)S PARTICLES: STRUCTURE AND MORPHOLOGY

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Defect structure and morphology of CdS and (Cd,Mn)S nanocrystalline samples synthesized by hydrothermal synthesis at temperatures of 80, 100, 120, and 140° C were investigated. The full-profile analysis by the Rietveld method showed that the experimental X-ray diffraction patterns do not correspond to either the cubic structure of the sphalerite or the hexagonal structure of wurtzite, which are characteristic of well-crystalline CdS. In addition, X-ray diffraction patterns are not fitted by scattering on a mixture of these two modifications. Simulation of X-ray diffraction patterns with use of Debye scattering equation [1] showed that CdS and (Cd,Mn)S nanoparticles contain high consentraition of stacking faults (SFs). Optimization of the structural models using the genetic algorithm showed that the probability of SFs (relative to the wurtzite structure) decreases for CdS from 0.55 to 0.46, and for (Cd,Mn)S from 0.47 to 0.36. Therefore, the structure of nanoparticles in both series gradually approaches the structure of wurtzite. It was also shown that at all synthesis temperatures the CdS and (Cd,Mn)S particles have an ellipsoidal shape, with the ellipsoids stretched along the direction perpendicular to the SFs. With an increase in the synthesis temperature, the average particle size increases. Ellipsoidal shape of particles was confirmed by TEM data.

[1] Proffen, Th., Neder, R.B. DISCUS: A program for diffuse scattering and defect-structure simulation (1997) Journal of Applied Crystallography, 30 (2), pp. 171-175