Size-dependent structural phase transitions and their correlation with photoluminescence and optical absorption behavior of annealed Zn$_{0.45}$Cd$_{0.55}$S quantum dots

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Abstract:

In this paper, we investigate the effect of thermally induced structural phase transitions on the photoluminescence (PL) and optical absorption behaviour of Zn$_{0.45}$Cd$_{0.55}$S nanoparticles (NPs). Analysis of X-ray diffraction (XRD) patterns and high-resolution electron microscope (HRTEM) images reveal that the as-synthesized sample possesses zinc-blende-type cubic structure. In addition, at annealing temperature (Ta) 400 °C, the cubic structure transforms completely into the wurtzite-type hexagonal structure. Furthermore, the second phase transition of the as-synthesized sample has observed at 700 °C, where the cubic structure has transformed into mixed polycrystalline phases of hexagonal ZnO, cubic CdO, monoclinic CdSO$_3$, and orthorhombic ZnSO$_4$ structures. These new phases have also confirmed from the analysis of Raman and FTIR spectra. Analysis of UV–visible optical absorption spectra demonstrates that Increasing Ta results in the decrease of optical band gap due the improvement in crystallinity accompanied by the increase in the particle size. The PL emission bands at an excitation energy of 3.818 eV exhibit redshift and a decrease in the intensity with increasing Ta up to 500 °C. Meanwhile, further increase in Ta up to 700 °C results in the enhancement of green emission intensity. On the other hand, PL emission spectra at 3.354 eV and Ta 700 °C, reveal a dramatic increase in the emission intensity nearly by one-order of magnitude with respect to its value of the as-synthesized sample. This behaviour is ascribed to the incorporation of oxygen-related defects via thermal annealing in air, which act as additive radiative centers. Also, we have interpreted the observed spectral blue shift of PL emission spectrum with increasing excitation energy.

Keywords: Structural phase transitions Optical gap tuning PL quenching FTIR and Raman spectroscopy High-resolution TEM

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