Nanocomposites and nanomaterials

Role of interfacial centers in the emission of CdS-containing nanocomposites

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The steadily increasing interest to nanoobjects is caused by their attractive size-dependent properties which open vast possibilities for applications in electronics, optoelectronics, biology and medicine. The properties and, correspondingly, the applications of nanomaterials crucially depend on the surface and interfacial states. The role of interface is especially important for colloidal nanoparticles (NPs) because surface termination with various types of capping agents is an inherent feature of the colloidal synthesis. However, the analysis of the interfaces is still a challenge for the researchers. Here we use the optically detected magnetic resonance (ODMR) method for identification of paramagnetic centers that participate in the emission of nanocomposite.

We have studied the ODMR of two types of CdS NPs obtained by colloidal synthesis. The capping agents used during the synthesis of the particles were either the macromolecules of polyvinyl alcohol (PVA) or the molecules of polyethylene imine (PEI). The most important difference between these two capping materials is the content of oxygen. PVA is an oxygen-containing substance, its structural formula is $(C_2H_4O)_x$. PEI, $(C_2H_5N)_n$, does not contain oxygen by itself; thus, oxygen can be present in the CdS/PEI samples only as an uncontrolled impurity.

Another important difference between the samples is either the excess or deficiency of sulfur ions during the synthesis. Namely, nano-CdS/PVA samples were grown under the conditions of sulfur excess while nano-CdS/PEI – under the conditions of sulfur deficiency which, naturally, produces different interfacial conditions between the particles and capping molecules.

The measured ODMR spectra of the two types of samples are complex and the overlapping signals are predominantly positive while the PEI-terminated NPs exhibit also a weak negative signal. The experimental spectra of the two types of samples demonstrate the differences. By comparing our data for different NPs and pure capping materials with the literature data on paramagnetic centers in single crystalline CdS (both on the surface and in the bulk) we have identified the signals with interfacial oxygen centers and sulfur vacancies.