CdS Nanocrystals and their Optical Properties

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Abstract: In this paper CdS nanocrystals were researched, investigated the absorption and Raman scattering, calculated sizes of nanocrystalls relative shift of the fundamental band edge. Energy diagram was constructed on basis of second derivatives of optical density.
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Due to technical progress more and more attention is paid to nanoscale structures and materials based on them. The use of nanomaterials becomes enormous opportunities because of their fundamental differences from conventional materials and the purchase of new and fundamentally different properties from CdS monocrystalls.

We investigated the absorption spectra of nanocrystals of cadmium sulfide (CdS) in a dielectric matrix. Nanocrystals were formed by a chemical reaction:

$$H_2S + Cd(NO_3)_2 \rightarrow CdS + 2HNO_3 \quad (1)$$

For this purpose, into aqueous solution of cadmium nitrate were added water, saturated with hydrogen sulfide. As a stabilizer and a dielectric matrix served photogelatin (chemically pure gelatin). The reaction took place at a temperature of 60 ± 5 C °.

Measurements of the absorption spectra were performed for the visible and UV spectral regions. There was a shift of the absorption edge to shorter wavelengths with decreasing size of nanocrystals, shown at fig. 1:

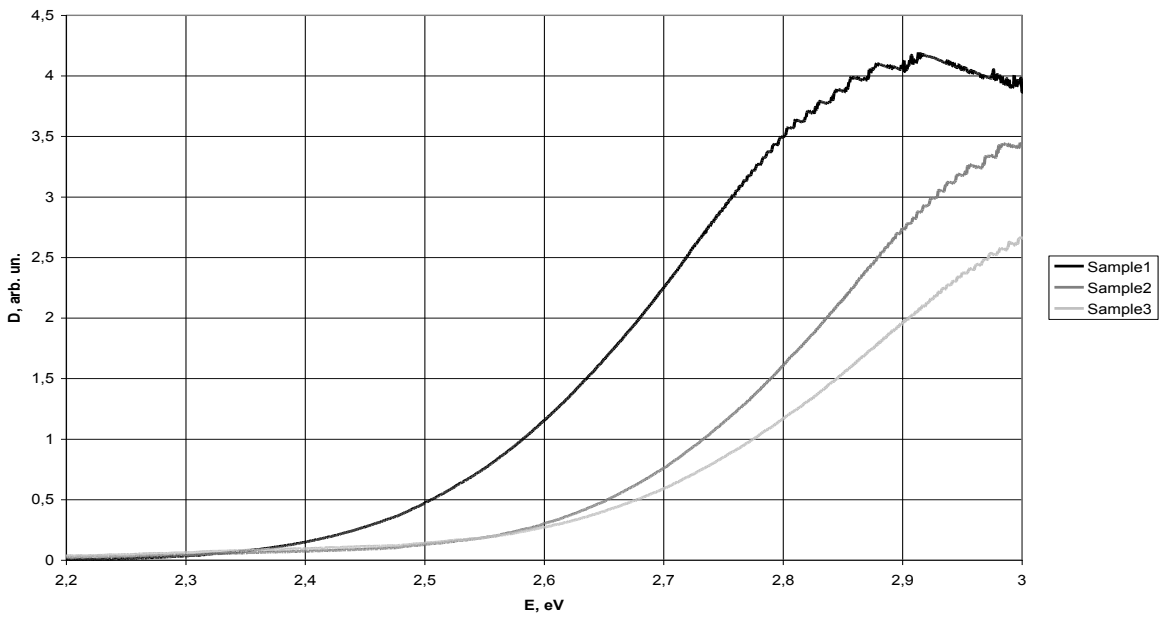

Fig.1. Absorption spectra of CdS nanocrystals in gelatin matrix (Sample1 – 2% of $Cd(NO_3)_2$, 9% of gelatin; Sample2 –1% of $Cd(NO_3)_2$, 9% of gelatin; Sample3 – 0.5% of $Cd(NO_3)_2$, 9% of gelatin)

Such a shift is predicted by the classical theory of size quantization, and confirms the assumption about the form of spherical nanocrystals as quantum dots. To determine the exact edge of the main absorption bands were constructed graphs of the first derivative of optical density [2] (the highest peak). Radii of the nanocrystals were calculated, based on eq.2:

$$E_{eff} = E_g + \frac{\hbar^2}{2\mu R^2}\varphi_{\ln}^2 \quad (2)$$

where E_{eff} is band gap of CdS nanocrystals, E_g - band gap of CdS monocrystalls, μ - reduced mass of effective electrons and holes, R – radius of CdS nanocrystal, $\varphi_{\ln}^2$ - roots of the Bessel function [1].

Radii of CdS nanocrystals were $2 \div 4$ nm. Also, the graphs of the second derivative of the optical density at the inflection points were determined energy levels of the occurrence of optically allowed transitions, as it's show at fig.2:

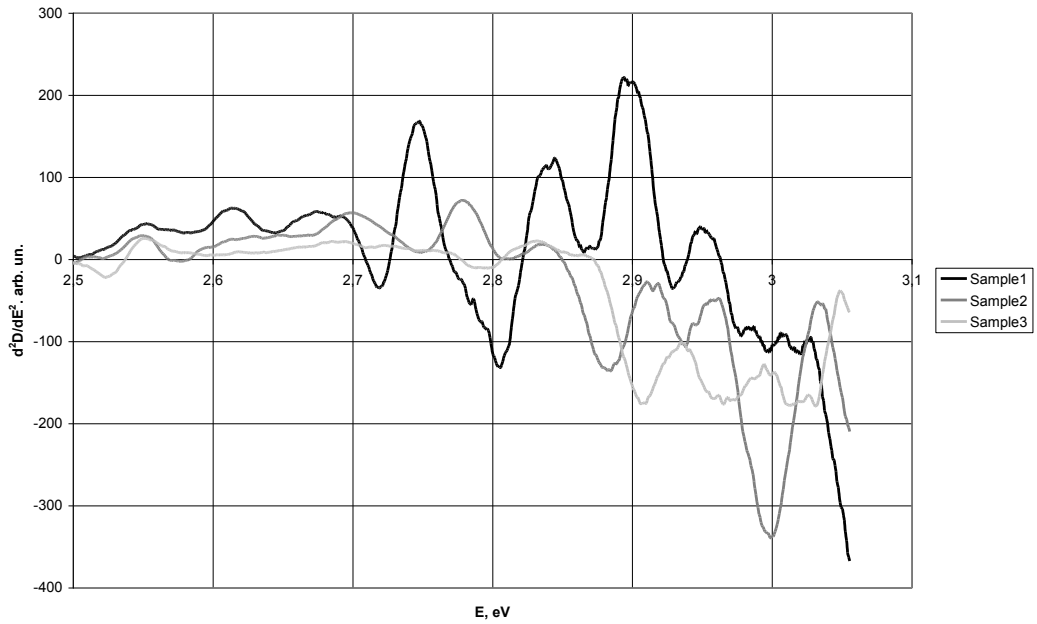

Fig.2. Second derivates of absorption spectra of CdS nanocrystals in gelatin matrix ((Sample1 – 2% of $Cd(NO_3)_2$, 9% of gelatin; Sample2 –1% of $Cd(NO_3)_2$, 9% of gelatin; Sample3 – 0.5% of $Cd(NO_3)_2$, 9% of gelatin)

Energy diagram of optically allowed transitions was built based on eq. 2:

$$E_{eff} = E_g + \frac{\hbar^2}{2\mu R^2}\phi_{\ln}^2 \qquad (2)$$

where E_{eff} is band gap of CdS nanocrystals, E_g - band gap of CdS monocrystalls, μ - reduced mass of effective electrons and holes, R – radius of CdS nanocrystal, $\varphi_{\ln}^2$ - roots of the Bessel function [1].

Thanks to second derivates of absorption spectra of CdS nanocrystals and eq.2 the corresponding energy diagram is constructed. The experimental data correlate well with the calculated values obtained using a model based on the classical theory of quantum nanocrystals of spherical shape and indicate the possibility of receiving sensors of light in visible and UV spectra with predetermined properties [3].

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