Phonons Contribution to the Infrared and Visible Spectra of II-VI Semiconductor Nanoshells

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Abstract

We have investigated the phonons contribution in the infrared (IR) and visible (VIS) optical properties in II-VI semiconductor nanoshells of type I. For this, we use Mie scattering theory by defining appropriate dielectric functions for the constitutive materials of the nanoshells. Indeed, for the core we have considered dielectric function taking into account the spatial confinement of the charge carriers [1] along with the phonons contribution [2, 3]. In fact, to evaluate the exciton energy, we have considered the same treatment used previously in Ref. [4]; i.e., the Coulomb interaction is considered as a perturbative term in the Schrödinger equation in the framework of *"Effective Mass Approximation with Finite Barrier Potential"* for electrons and holes. For the shell, we have taken dielectric function similar to that used in bulk semiconductor [2, 3]. Independently of the core and shell sizes and the embedding medium, we obtain in the IR spectra, three resonant peaks ascribed to the Cd-S stretching vibration, the longitudinal optical (LO)-CdS and surface optical (SO)-ZnS phonon modes, respectively. The increase of core and shell sizes induces a red shift of the Cd-S stretching vibration and the SO ZnS branches, while a blue-shift is obtained for the LO CdS branch. In fact, figure 1 shows this behavior; i.e., we plot the wavenumber versus the geometrical parameter R_s / R_c; being R_c the core radius, while R_s is the total nanoshell size. If the phonons contribution is not considered in the IR spectrum, the Cd-S stretching vibration is dissapeared.

On the other hand, in the VIS spectra, we obtain one sharp resonant peak related to the $1s_e \rightarrow 1s_h$ optical transition, whose localization is characterized by the core size, essential parameter to evaluate the exciton energy. Phonons contribution in the VIS range yields information about the exciton-phonon coupling in II-VI semiconductor nanoshells. Indeed, we show in figures 2 and 3, the extinction versus the wavelength with and without phonons contribution for different nanoshell sizes. From the shifting of these two peaks (with and without phonons contribution), we estimate coupling energies of exciton-phonon in the range of 36 *meV* - 21 *meV*. This feature is in good agreement with the size-dependence of exciton-phonon coupling energy previously reported in the literature [5].

When the embedding medium is glass, where the dielectric constants at high frequency of core, shell and islanding materials are similar, we obtain two effects on the IR as well as the VIS optical properties: (i) the phonon peaks (IR range) or the exciton peak (VIS range) are red-shifted, and (ii) the peaks intensities are greater. Therefore, in the light of these results, it can be concluded that the phonons contribution is primordial if the optical properties are investigated in the low-dimensional systems.

References

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Figures

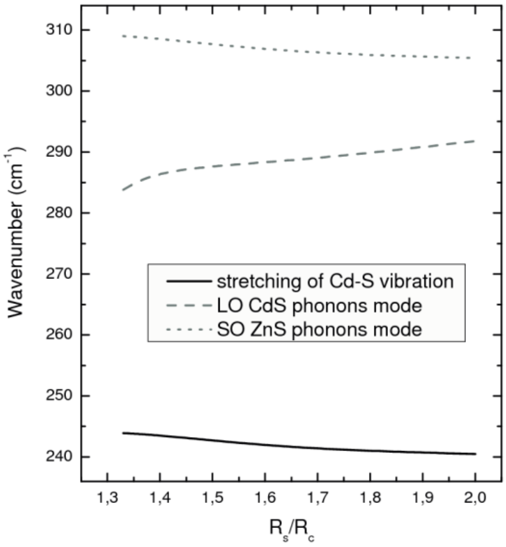

Figure 1. Dependence of the phonons branches for CdS/ZnS/polyethylene nanoshells with the ratio R_s/R_c.

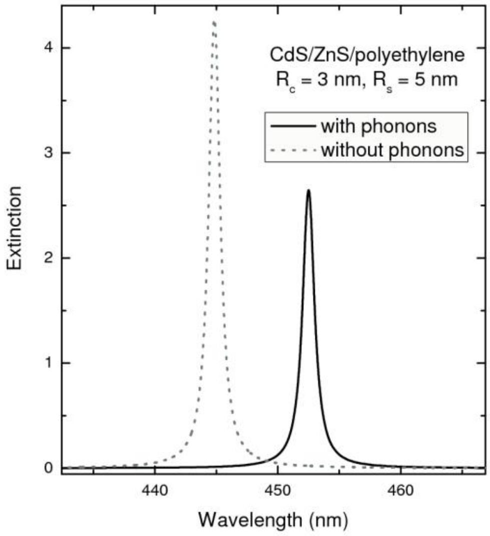

Figure 2. Extinction as a function of the wavelength, with (solid line) and without (dotted line) phonons contribution in the core dielectric function.

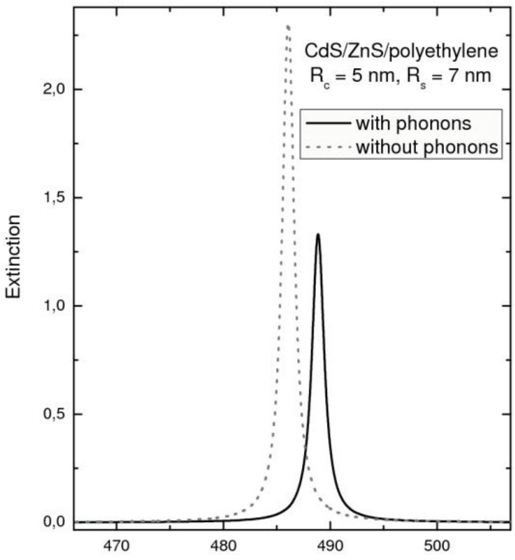

Figure 3. Extinction as a function of the wavelength, with (solid line) and without (dotted line) phonons contribution in the core dielectric function.