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Dielectric Confinement on Exciton Binding Energy in a II-VI Semiconductor

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ABSTRACT

Exciton binding energy is obtained in a $Zn_xCd_{1-x}Te/ZnTe$ strained quantum dot taking into account the phonon confinement effect. The effect of mismatch between the dielectric constants of the dot and the barrier (dielectric mismatch effect) is taken into account in our calculation. The calculations include the effect of exciton and the LO phonon interaction is derived by the effective potential (V_{PB}) between the electron and hole along with the self energy term (E_{self}). It is observed that the potential taking into account the effects of phonon makes the exciton binding energies more than the obtained results using a Coulomb potential screened by a static dielectric constant and the optical properties of exciton in a quantum dot are strongly affected by the confining potential and the quantum size.

Introduction

Generally, II–VI semiconducting materials have recently attracted increasing attention due to their large band gaps and their potential applications in short-wavelength optoelectronic devices such as blue and ultra violet LEDs. When a wide bandgap semiconductor is optically excited, the electrons and photogenerated holes are bound strongly together within the band gap as excitons by the Coulombic interaction. Strong interactions between excitons and longitudinal optical (LO) phonons usually lead to the dissociation of the excitons at room temperature. Hence, the study of suppression of the exciton-LO phonon scattering is imperative in low dimensional semiconductor systems. Dissociation of the excitons should not be allowed in these systems wherein the excitons have a higher binding energy than the LO phonons [1]. These large excitonic binding energies can be achieved by geometrical confinement and the proper composition.

Model and calculations

We consider an exciton located at the centre of a $Zn_xCd_{1-x}Te$ spherical dot confined by a spherical potential barrier (ZnTe). The confining potential is assumed to be zero inside and V outside. Within the framework of single band effective mass approximation, the Fröhlich interaction Hamiltonian of the system, a strained $Zn_xCd_{1-x}Te/ZnTe$ quantum dot with the radius R, can be written as,

$$H = H_{exc} + H_{ph} + H_{exc-ph} \tag{1}$$

where

$$\hat{H}_{exc} = -\frac{\hbar^2}{2\mu}\left(\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r}\right) - \frac{\hbar^2}{2m_e^*}\frac{\partial^2}{\partial z_e^2} - \frac{\hbar^2}{2m_h^*}\frac{\partial^2}{\partial z_h^2} - \frac{e^2}{\varepsilon(r)r} + V_e(z_e) + V_h(z_h) + V_{PB}(r) + V_{KT}(r) + E_{self} \tag{2}$$

where $V_z(z_z)$ and $V_h(z_h)$ are the strain induced conduction and valence band offsets respectively and $V_{PB}(r)$ is the effective potential between an electron and a hole. $V_{KT}(r)$ is the correction term with the inclusion of image charge effect [2].

The electron longitudinal-optical phonon interaction is an important factor determining the physical properties of any polar crystal. The binding energies will be enhanced when a screened Coulomb potential is considered. The quantum well confinement effective potential of the electron and hole is given by [3]

$$V_{PB}(r) = -\frac{e^2}{\varepsilon^* r}\left[\frac{C^4}{B^4} - \frac{m_e^* h_e}{\Delta m}\exp\left(-\frac{rA_e}{R_e}\right) + \frac{m_h^* h_h}{\Delta m}\exp\left(-\frac{rA_h}{R_h}\right)\right] - \left(h_\mu + \frac{C^3 r}{2B^3 a_{ex}}\right)\exp\left(-\frac{rB}{R_\mu}\right) \tag{3}$$

where $\varepsilon^* = (1/\varepsilon_\infty - 1/\varepsilon_s)^{-1}$, ε_∞ and ε_s are the optical and static dielectric constants of the ZnSe material and Δm is the difference in effective mass of electron and hole. The calculation of other material parameters is followed from Ref.3. when a well material is sandwiched between two barrier materials, the field effect caused by the charge distribution will enhance the Coulomb interaction. The effect of electron –hole confinement in the image charge method is given by the effective potential,

$$V_{KT}(r) = -\sum_{n=-\infty}^{\infty}\frac{\xi^{|n|}}{\varepsilon_s\sqrt{\rho^2 + (z_z - (-1)^n z_h + nL_W)^2}} \tag{4}$$

where $\xi = (\varepsilon_s^w - \varepsilon_s^b)/(\varepsilon_s^w + \varepsilon_s^b)$ and ε_s^w and ε_s^b are the static dielectric constants of the well and the barrier material respectively.

The self energy term is given by [4]

$$E_{self} = -(\alpha_e g_e + \alpha_h g_h - \alpha_\mu g_\mu)\hbar\omega_{LO} \tag{5}$$

where $\eta\omega_{LO}$ is the LO phonon energy. The exciton wave function is given by

$$\psi(r) = \begin{cases} N_0 e^{\pm i\theta} J_0(r_{0l} r)\exp(-\gamma r) & r < R \\ N_1 \dfrac{J_0(r_{0l}R)}{K_0(b_{0l}R)} e^{\pm i\theta} K_0(b_{0l} r)\exp(-\gamma r) & r \geq R \end{cases} \tag{6}$$

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where N_1 is the normalization constant, η are the variational parameters and The exciton binding energy E_b is calculated using the following equation

$$E_b = E_{e,h} - \langle H_{\min} \rangle \quad (7)$$

where $E_{e,h}$ is the sum of the free electron and the free hole self-energies in the same quantum well. For this purpose, we use the single band effective mass approximation and expand the electron wave function in an appropriate set of orthonormal functions. The atomic units have been followed in the determination of electronic charges and wave functions in which the electronic charge and the Planck's constant have been assumed as unity. All the other values of $Cd_{1-x}Zn_xTe$ parameters which are interpolated from the data mentioned in the Table.1.

Results and discussion

Table 1. Material parameters* used in the calculations

Parameter	CdTe	ZnTe
m_e^*	0.11	0.2
ε	9.6	9.81
a (nm)	0.6481	6.466
C_{11}(GPa)	5.66	5.315
C_{12} (GPa)	3.96	1.87
$E_g^{\Gamma}(eV)$	1.606	2.394

Fig.1 displays the variation of binding energy as a function of dot radius in a $Zn_xCd_{1-x}Te/ZnTe$ quantum dot. The curve (1) represents the binding energy with the inclusion of PB potential using Eq.(3) and the dielectric mismatch, the curve (2) represents using PB potential and the curve (3) is obtained using bare screened Coulomb potential. It is observed that the enhancement of the binding energy due to electron-phonon interaction is larger for all the dot radii but we notice that the binding energy is more influence for smaller dot radii than the larger dot radii due to the confinement. It is important to notice that the polaronic effect is small for heterostructures with weak ionic structure whereas it is appreciable for all the polar heterostructures when the effect of polaron is included [5]. The electron-phonon interaction enhances the electron effective mass (polaron mass) and diminishes the electrostatic screening. Both the effects give rise to the enhancement of the binding energy when the effect of the polaron is included. Further we notice that the decrease of screening due to the less value of dielectric constant in CdTe material increases the binding energy. It is because the larger the polaron mass increases the effective Rydberg energy ultimately increases the binding energy.

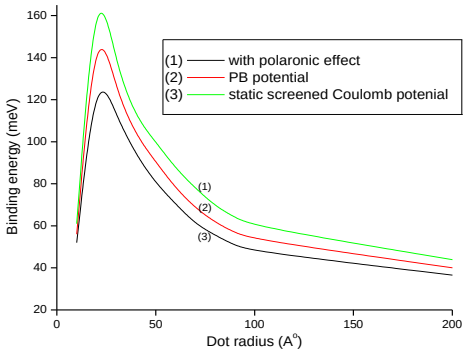

Fig.1 Variation of binding energy as a function of dot radius in $aZn_xCd_{1-x}Te/ZnTe$ quantum dot; the curve (1) represents the binding energy with the inclusion of PB potential) and the dielectric mismatch, the curve (2) represents using PB potential and the curve (3) is obtained using bare screened Coulomb potential.

Conclusion

It is investigated that the potential with the inclusion of phonon will make the hydrogenic binding energies more than the obtained results using a Coulomb potential screened by a bare static dielectric constant and the optical properties of hydrogenic impurity in a quantum dot are strongly affected by the confining potential, dot radii and the Zn composition. We hope that our results would explore new findings in experimental sides on electro-optical devices.

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