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Effect of Temperature on Exciton Binding Energy in ZnSe/ $Zn_{1-x}Mg_xSe$ Quantum Well with Poschl-Teller Potential

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Abstract : Exciton binding energies with temperature in a quantum well with Poschl-Teller Potential formed by $ZnSe/Zn_{1-x}Mg_xSe$ are calculated theoretically. Using the temperature dependent value of the effective mass and barrier height, the sub-band energies of the electron, heavy hole and light hole are calculated by variational method. Binding Energy of light hole exciton and heavy hole exciton are calculated as a function of the wellwidth for different temperatures. We have obtained the result that the binding energy of exciton decreases with enhancing the temperature and increases with reducing the wellwidth upto 12 nm for heavy hole exciton and 10 nm for light hole exciton, beyond this wellwidth the exciton binding energy decreases.

Keywords : Quantum well, Exciton, Binding energy, Poschl-Teller Potential, Temperature.

Introduction

In the last two decades, the low dimensional semiconducting systems have received much attention due to their potential application in optoelectronic devices such as displays[1], light emitting diodes[2], solar cells[3] and photovoltaic devices[4]. Elabsy[5] displays the variation of the binding energy of shallow donor in $GaAs/Ga_{1-x}Al_xAs$ superlattice with respect to temperature. Abraham and John Peter[6] have studied the exciton binding energy, interband emission energy and nonlinear optical properties in ZnMgSe quantum well with the effect of dielectric constant mismatch. Cingolani *et al.*[7] have investigated the excitonic states in $Zn_{1-x}Cd_xSe/ZnSe$ as a function of wellwidth and composition of Cd experimentally. Krystek *et al*[8] have reported the variation of energy and broadening parameter of the fundamental bandgap of ZnSe with different temperatures in the range 27 K to 370 K. Stachow *et al.*[9] have showed that the energy gap of CdMnTe epilayers depends upon the temperature. Several authors[10-11] have studied the effect of hydrostatic pressure on the binding energy of donor and acceptor in GaAs/GaAlAs quantum wells. Morales *et al*[12] have made theoretical studies on simultaneous effect of hydrostatic stress and electric field on donor binding energy in GaAs/GaAlAs. Arulmozhi[13] has studied the influence of temperature and pressure on the binding energy of hydrogenic donor in parabolic quantum well. Tevosyan *et al*[14] have computed the energy levels and direct interband absorption in a spherical quantum dot with Poschl-Teller potential. Mora-Ramos *et al*[15] have calculated the exciton binding energy in a cylindrical quantum dot with Poschl-Teller potential profile variationally. Effect of magnetic field on exciton binding energy in near triangular quantum well has been studied by Anitha and Arulmozhi[16]. II-VI semiconductors are extensively studied at nanoscale experimentally without doping[17-19], with doping[20-22] and with external perturbations[23, 24]. The purpose of the present work is to report the effect of temperature on binding energy of light and heavy hole exciton in quantum well with Poschl-Teller confining potential profile composed of $ZnSe/Zn_{1-x}Mg_xSe$ as a function of wellwidth.

Theory

The Hamiltonian of an exciton in effective mass approximation is given by[25]

$$\mathcal{H} = -\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}\right] - \frac{\mu_{hi}^*}{m_e^*}\frac{\partial^2}{\partial z_e^2} - \frac{\mu_{hi}^*}{m_{hi}^*}\frac{\partial^2}{\partial z_h^2} + V(z_e) + V(z_h) - \frac{2}{r} \tag{1}$$

The subscripts h and e represent the hole and electron respectively. μ_{hi}^* is the reduced effective mass of the heavy hole (i = h) or light hole (i = l) and the electron, $r = \sqrt{\rho^2 + |z_e - z_h|^2}$. The reduced effective mass of the exciton is

$$\frac{1}{\mu_{hi}^*} = \frac{1}{m_e^*} + \frac{1}{m_{hi}^*} \tag{2}$$

The potential profile for the electron and hole in Poschl-Teller potential[15] are given by

$$V(z_i) = \begin{cases} V_0 \dfrac{\mu_i \eta^2}{m^*_i}\left(\dfrac{\chi(\chi-1)}{\sin^2(\eta z_i)} + \dfrac{\lambda(\lambda-1)}{\cos^2(\eta z_i)}\right) & |z_i| < \dfrac{L}{2} \\ V_0 & |z_i| > \dfrac{L}{2} \end{cases} \tag{3}$$

where, V_0 is the barrier height, which depends on the composition x of Mg, $\eta = \frac{\pi}{2L}$.. The numerical values of χ and λ are chosen to be 1.0001. Since χ and λ are chosen to be same, a symmetric Poschl-Teller potential profile is considered. The trial wave function of the exciton in the Poschl-Teller potential[15] is taken to be

$$\Psi(\rho, \rho_e, \rho_h, z_e, z_h) = \Upsilon(\rho_e, \rho_h, z_e, z_h) e^{-\alpha\rho - \beta(z_e - z_h)^2} \tag{4}$$

where, $\Upsilon(\rho_e, \rho_h, z_e, z_h) = F(\rho_e)F(\rho_h)g(z_e)g(z_h)$ and $\rho = |\rho_e - \rho_h|$. Substituting the available values from Ref.15, the final trial wave function

$$\Psi = \{ \blacksquare (NAe^{\uparrow}(-\alpha_{\downarrow}e\,\rho - \beta_{\downarrow}e\;[\![(z_{\downarrow}e - z_{\downarrow}h)]\!]^{\uparrow}2\; e^{\uparrow}(-ar)) \qquad -L/2 < z_{\downarrow}e, z_{\downarrow}h < L/2 @ N_{\downarrow}1\; [\![\; e]\!]^{\uparrow}(-\beta_{\downarrow}e\; |z_{\downarrow}e|)\; [\![\; e]\!]^{\uparrow}(-\beta_{\downarrow}h\; |z_{\downarrow}h|)\; e^{\uparrow}(-ar) \tag{5}$$

where $A = J_0(\Theta_0\rho_e)J_0(\Theta_0\rho_h)\sin\left[\frac{\pi z_e}{2L}\right]^{\chi}\cos\left[\frac{\pi z_e}{2L}\right]^{\lambda} * \sin\left[\frac{\pi z_h}{2L}\right]^{\chi}\cos\left[\frac{\pi z_h}{2L}\right]^{\lambda}$. α_i, β_i and α are variational parameters, J_0 is the Bessel function of zeroth order with θ_0=2.40483 (Ref.15), N is the normalization constant. The continuity conditions at z_e = L/2 and z_h = L/2 relates the normalization constant N and N_1. We have computed expectation value of Hamiltonian as a function of the variational parameters using the Hamiltonian in (1) and the trial wave function in (5).

The binding energy of exciton is then given by

$$E_B = E_e + E_h - \langle\mathcal{H}\rangle_{\min} \tag{6}$$

where, E_e and E_h are the ground state energies of electron and hole in bare quantum well respectively obtained variationally. $\langle\mathcal{H}\rangle_{\min}$ is the minimized value of $\langle\mathcal{H}\rangle$ with respect to the variational parameters. By applying external temperature to the system, the band gap of the material changes, as[7]

$$E_g(T) = E_g(0) - \frac{\alpha T^2}{T + \beta} \tag{7}$$

where $E_g(0)$ is the energygap at T=0, α and β are Varshni coefficients, respectively.

The variation of effective mass, dielectric constant, barrier height according to the temperature is determined[12] by

$$\frac{1}{m*(T)} = 1 + E_p\left(\frac{2}{E_g(T)} + \frac{1}{E_g(T)+\Delta_0}\right) \quad (8)$$

In this equation E_p is an energy related to the momentum matrix element, Δ_0 is the spin-orbit splitting and $E_g(T)$ is the temperature dependence of the energy gap.

The variation of the barrier height with temperature is calculated by

$$V_0(T) = Q_c \Delta E_g(x,T) \quad (9)$$

Conduction band offset parameter Q_c is 0.70 eV and bandgap difference between quantum well and barrier layer material as a function of temperature and Mg concentration is given by

$$\Delta E_1 g\ (x,T) = \Delta E_1 g\ (x) + TC(x\ ) \quad (10)$$

Variation of dielectric constant with temperature is expressed as

$$\epsilon(T) = \epsilon(0)(1 + C(x)T) \quad (11)$$

The numerical values for this calculation is taken from the references (Ref. 6, 8).

Results and discussion

Table 1 represents the physical parameters of ZnSe, taken from references[6, 8, 27]. The difference of total band gap between $Zn_{1-x}Mg_xSe$ and ZnSe is determined[5] by the equation

$$\Delta E_g = 0.87x + 0.37x^2\ eV$$

The conduction band and valence band discontinuity is taken to be 70% and 30% of this band gap difference respectively.

Table 1: Physical parameters of ZnSe

Physical parameters	Absolute values
Mass of Electron (m_e)	0.16 m_0
Mass of heavy hole (m_h)	0.6 m_0
Mass of light hole (m_l)	0.145 m_0
Dielectric Constant (ϵ)	8.8
Spin-Orbit splitting (Δ_0)	0.43 eV
Energy gap at 0 K ($E_g(0)$)	2.8 eV
Varshni co-efficient (α)	7.3×10^{-4} eV/^{0}K
Varshni co-efficient (β)	295^0K
Linear temperature co-efficient (C)	1.71×10^{-4} K^{-1}

where m_0 is the free electron mass.

Fig.1 shows that the variation of binding energy of heavy hole exciton as a function of well width L for different temperatures T for a barrier height corresponding to the Mg composition x = 0.3. When L is reduced, the binding energy increases. If the L is reduced further, they reach a maximum value and then start to decrease rapidly. The peak value of binding energy is observed at L = 12 nm, for all values of T.

The behavior of binding energy of light hole exciton as a function wellwidth L for different temperatures is shown in Fig. 2. The peak value of binding energy is observed at L = 10 nm, for all values of T. It is also noted that the binding energy of heavy hole exciton is more than that of the light hole exciton. So the hh-exciton is more bound than the lh-exciton, which is due to $m_{hh}^* > m_{lh}^*$. In both cases, the decrease in wellwidth produces a spreading of the wave function, which causes a lowering in the binding energy. The contribution of confinement is dominant for smaller wellwidth and make the electron unbound, and tunnels through the barrier. This behavior is similar to those reported in Ref. 15 for a quantum dot of same profile. But a decrease in binding energy for narrow wells is observed in quantum wells.

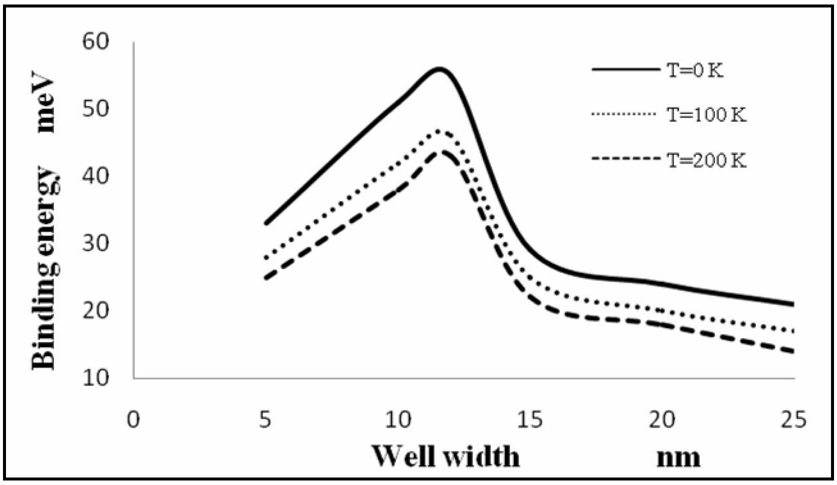

Fig.1. Variation of the binding energy of hh-exciton as a function of wellwidth for different temperatures

Fig.3 shows that the variation of binding energy of heavy hole exciton as a function of temperature for different wellwidths, for a barrier height corresponding to the Mg composition x = 0.3. As temperature increases, the binding energy decreases[4].

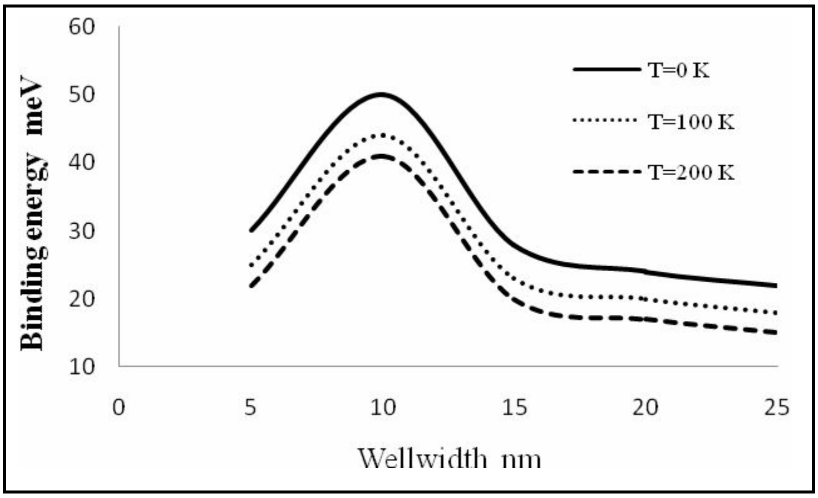

Fig.2. Variation of the binding energy of lh-exciton as a function of wellwidth for different temperatures

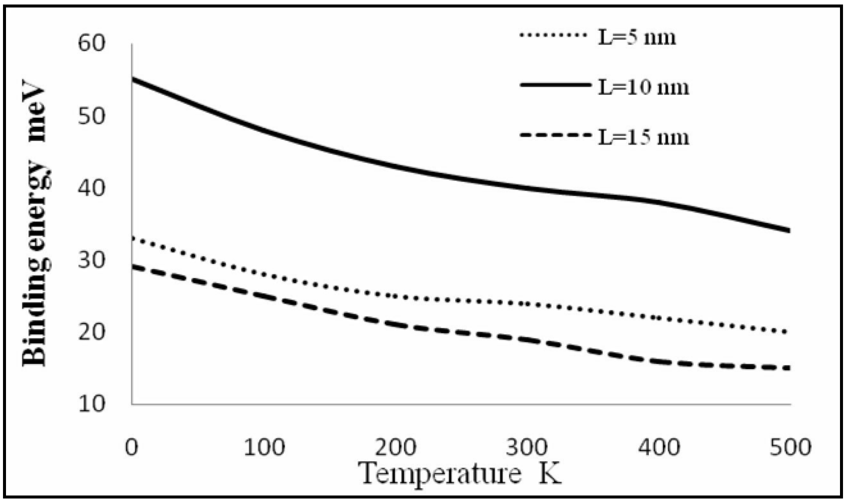

Fig.3. Variation of the binding energy of hh-exciton as a function of temperature for different wellwidths

The behavior of binding energy of light hole exciton as a function of temperature for different wellwidths is shown in Fig. 4. For a given quantum well thickness, there is a decrease in the binding energy of the exciton, when the temperature is increased, because increasing the temperature, decreases the values of both the effective mass and the barrier height.

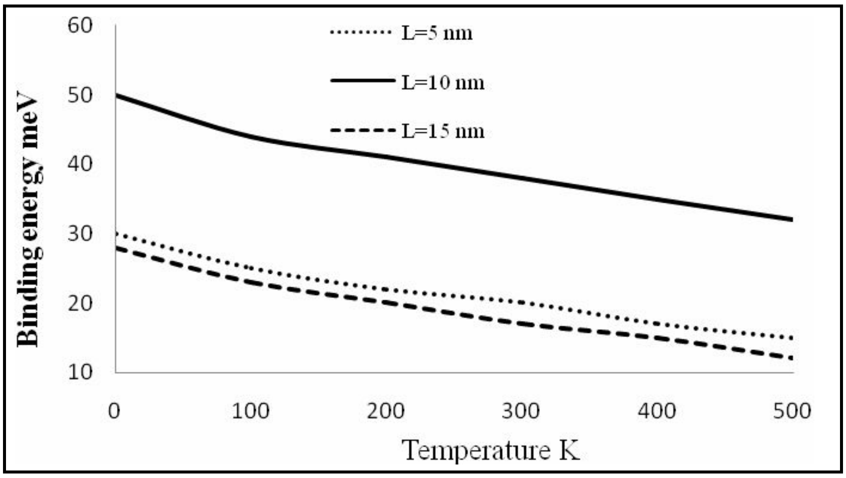

Fig.4. Variation of the binding energy of lh-exciton as a function of temperature for different wellwidths

Conclusions

Binding energies of hh-exciton and lh-exciton in the presence of temperature in a quantum well with Poschl-Teller potential are calculated variationally. A maximum value of binding energy occurs at a critical well width (12 nm for hh-exciton and 10 nm for lh-exciton), same for all values of temperature. For a fixed wellwidth, the binding energy decreases as temperature increases. For same wellwidth and temperature, the binding energy of hh-exciton is more than that of lh-exciton.

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