CHAPTER II
STRAIN INDUCED OPTICAL PROPERTIES OF EXCITON
IN A CdTe/ZnTe QUANTUM DOT

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2.1 Abstract

The influence of strain on the binding energies of heavy and light hole is obtained in a Zn$_x$Cd$_{1-x}$Te/ZnTe quantum dot taking into account the phonon confinement effect. The band offsets are calculated using model solid approach. The dielectric mismatch effect is introduced between the dielectric constants of dot and the barrier. The strain induced energies of excitonic transitions in a CdZnTe quantum dot with ZnTe barrier are brought out considering the internal electric field induced by the spontaneous and piezoelectric polarizations. Calculations are obtained using Bessel function as an orthonormal basis for different confinement potentials of barrier height, strain induced linear and third-order nonlinear optical absorption coefficients and the changes of refractive index with the incident photon energy are observed. The results show that the exciton binding energy is enhanced with the inclusion of potential taking into account the effects of dielectric mismatch and the geometry of quantum dot with various Zinc alloy content has a great influence on the optical properties of the dot.
2.2 Introduction

Quantum dots, among low dimensional semiconductors, are shown interests due to their discrete energy levels and the potential applications in fabricating devices such as opto-electronic devices, quantum information processing and terahertz devices [1]. Among all the materials, II-VI semiconductors are recently paid attention because they have large direct bandgaps throughout the visible spectrum further they have higher exciton binding energies and quantum efficiency which can be applied for opto-electronic devices in the middle regions of spectrum. CdTe/ZnTe material is considered to be an important semiconductor due to the lattice mismatch between its counter constitutes. Higher quality of ZnCdTe/ZnTe quantum dots are grown using latest advances in the growth technology [2-4]. Yellow and green laser diodes based on ZnCdTe materials are fabricated nowadays [5]. Photoluminescence (PL) spectra of various Zn$_{1-x}$Cd$_x$Te /ZnTe quantum dots grown by Molecular beam epitaxy were carried out by Bagaev et al, [6] who studied the influence of exciton level energy depth on the temperature dependences of integral PL in the quantum dots. Temperature-dependent photoluminescence measurements have been performed to investigate the optical properties and the enhancement mechanism of the activation energy in CdTe/ZnTe nanostructures [7,8]. The band offsets in strained ZnTe/Zn$_{1-x}$Cd$_x$Te/ZnTe and ZnSe/Zn$_{1-x}$Cd$_x$Se/ZnSe square quantum well structures were experimentally determined by the low-temperature cathodoluminescence and electrical current deep-level transient spectroscopy methods [9].

A detailed study of energy gaps, dielectric constants and the composition dependence in zinc-blende Cd$_{1-x}$Zn$_x$Te with the Zn alloy composition ranging from 0 to 1, using pseudo potential formalism, have
been recently carried out [10]. The influence of strain distribution in CdTe/ZnTe material is taken to be an interesting subject in order to carry out exotic optical and electrical properties. The effect of strain on the electronic energy band structure has been dealt in the strained ZnCdTe/ZnTe heterostructures [11]. Strain induced conduction and valence subband energies were carried out using $k.p$ Hamiltonian [12,13]. The composition of quantum dot (Zn in CdTe quantum dot) affects the linear and non-linear optical properties in any low dimensional semiconductor system. The electronic structure and optical properties of some III-V and II-VI semiconductor superlattices were investigated using superlattice-representation formalism on the basis of superlattice $k.p$ theory [14]. The wavelength dependence of refractive indices for some II–VI semiconductor alloys at wavelengths below their respective energy gaps were obtained using a combination of optical reflectivity and prism coupler technique [15].

In the present chapter, the exciton binding energies of heavy and light holes are investigated in a strained CdTe/ZnTe polar quantum dot nanostructure with the variation of Zn alloy content in the dot. The band offsets and the lattice mismatch effects are introduced between the dot and the barrier. Computations are carried out using Bessel function as an orthonormal basis for different confinement potentials considering the internal fields induced by the spontaneous and piezoelectric polarizations. Some nonlinear optical properties with the photon energies are investigated. The chapter is prepared as follows: the band offsets using Model-Solid theory, the strain induced exciton binding energy and the nonlinear optical properties are briefly discussed in Section 2.3. In Section 2.4, the numerical computations and the discussion are explained
in detail. Finally, a brief summary of this present work is presented in Section 2.5.

2.3 Model and calculations

2.3.1 Band offsets – model-solid theory

The lattice mismatch (6.2%) between the dot (CdTe) and the barrier (ZnTe) leads a biaxial strain causing a split of the valence band degeneracy. This suggests that the heavy and light holes have different band edge positions. The heavy hole and light hole band offsets are calculated as the difference between the energies at the top of heavy hole and light hole bands in CdTe and ZnTe. Similarly, conduction band offset is calculated as the difference between the energies at the bottom of the conduction bands in CdTe and ZnTe. Thus, the valence band offset related to heavy holes in the CdTe/ZnTe heterostructure interface is given by

$$\Delta E_{v, hh} = \Delta E^B_{v, hh}(ZnTe) - \Delta E^D_{v, hh}(Cd_{1-x}Zn_xTe) + \delta E_{v, hh}$$  \hspace{1cm} (2.1)

where $\Delta E^B_{v, hh}(ZnTe)$ is the unstrained outer barrier material of the dot and the other values are linearly interpolated with other data taken from Table 2.1 $\Delta E^B_{v, hh}(Cd_{1-x}Zn_xTe)$ is the strained inner material of the dot and $\delta E_{v, hh}$, the shift in the heavy hole valence band energy due to strain, is expressed as

$$\delta E_{v, hh} = a_v (2\varepsilon + \varepsilon_{zz}) - b (\varepsilon_{zz} - \varepsilon)$$  \hspace{1cm} (2.2)

where $a_v$ is the hydrostatic deformation potential in the valence band, $b$ is the shear deformation potential and the strain tensors [16] are given by

$$\varepsilon = \frac{a_D - a_B}{a_B}.$$  \hspace{1cm} (2.3)
\[ \varepsilon_{zz} = -2 \frac{C_{12}}{C_{11}} \varepsilon \]  

(2.4)

where \( a_D \) and \( a_B \) are the lattice constants of \( CdTe \) dot material and \( ZnTe \) barrier material respectively. \( C_{11} \) and \( C_{12} \) are the elastic constants of the epitaxial layer material. Varying the alloy composition (Zn in CdTe) leads the variation in the lattice constants. This property tailors the electronic properties of the heterostructures. Similarly, the valence band offset for light hole is calculated as

\[ \Delta E_{v,\text{lh}} = \Delta E_{v,\text{lh}}^B (ZnTe) - \Delta E_{v,\text{lh}}^D (Cd_{1-x}Zn_xTe) + \delta E_{v,\text{lh}} \]  

(2.5)

where \( \delta E_{v,\text{lh}} \), the shift in the light hole valence band energy due to strain, is expressed as

\[ \delta E_{v,\text{lh}} = a_v (2\varepsilon + \varepsilon_{zz}) - \frac{1}{2} \Delta_0 + \frac{1}{4} b (\varepsilon_{zz} - \varepsilon) \]

\[ + \frac{1}{2} \sqrt{\frac{\Delta_0^2 + \Delta_0 b (\varepsilon_{zz} - \varepsilon) + \frac{9}{4} (b (\varepsilon_{zz} - \varepsilon))^2}{}} \]  

(2.6)

where \( \Delta_0 \) is the spin orbit splitting. The conduction band offset is given by

\[ \Delta E_e = \Delta E_e^B (ZnTe) - \Delta E_e^D (Cd_{1-x}Zn_xTe) + \Delta E_g + \delta E_e \]  

(2.7)

where \( \Delta E_g \) is bandgap energy of \( Zn_xCd_{1-x}Te \) inner dot material is given by [17]

\[ \Delta E_g(x) = 1.51 + 0.45x + 0.31x^2 \]  

(2.8)
The above expression of bandgap has been obtained by varying Zn concentration in ZnCdTe inner quantum dot. The quadratic term in Eq.(2.8) is correlated with the bowing of optical bandgap. And

$$\delta E_e = a_e (2\varepsilon + \varepsilon_{zz}) \quad (2.9)$$

The effects of band offsets and the lattice mismatch directly affect the electron and hole confinement potentials. Thus, the $V_e$ and $V_h$ are calculated using the following expression.

$$V_e = E_{e}^{ZnTe} - E_{e}^{Cd_{1-x}Zn_xTe} \quad (2.10)$$

$$V_h = E_{hh}^{ZnTe} - E_{v}^{Cd_{1-x}Zn_xTe} \quad (2.11)$$

where $E_{e}^{ZnTe}$ and $E_{hh}^{ZnTe}$ are the strain shifts of energies of conduction and heavy hole bands in the barrier dot, $E_{e}^{Zn_xCd_{1-x}Te}$ and $E_{v}^{Zn_xCd_{1-x}Te}$ are the strain shifts of energies of conduction and heavy hole bands in the inner dot.

2.3.2 Strain induced exciton binding energy

An exciton located at the centre of a Zn$_x$Cd$_{1-x}$Te quantum dot confined by a potential barrier, ZnTe, is considered in this problem. The envelop wave functions are used based on the single band effective mass approximation as these materials are chemically related. The confining potential is assumed to be zero inside and $V$ outside. The Hamiltonian of the exciton with the effect of electron-LO phonon interaction in a Zn$_x$Cd$_{1-x}$Te/ZnTe strained semiconductor heterostructure is given by [18]
\[
\hat{H} = -\frac{\hbar^2}{2\mu_+ (x)} \frac{1}{\rho} \frac{\partial}{\partial \rho} \rho \frac{\partial}{\partial \rho} - \frac{\hbar^2}{2m^*_e (x)} \frac{\partial^2}{\partial z_e^2} - \frac{\hbar^2}{2m_+ (x)} \frac{\partial^2}{\partial z_h^2} - \frac{e^2}{\varepsilon(r)r} + \\
+ V_e (z_e, x) + V_h (z_h, x) + V_{PB} (r) + V_{KT} (r) + E_{self} 
\]

where \(m^*_e (x)\) is the Zn-dependent effective mass of electron and hole of \(Zn_xCd_{1-x}Te\), \(z_e\) and \(z_h\) are the electron and hole co-ordinates along the growth direction of the structure, \(V_{e,h} (z_{e,h}, x)\) are the Zn-dependent strain induced confined potentials for electrons and holes, \(V_{PB} (r)\) is the effective potential between an electron and a hole, \(V_{KT} (r)\) is the effective potential due to the effect of dielectric confinement in the image charge method [19], \(\varepsilon(r)\) is the size dependent dielectric function, \(e\) is the absolute value of the electronic charge, \(\mu_+\) is the reduced mass of the exciton given by [20] and \(r = \sqrt{\rho^2 + (z_e - z_h)^2}\). The expressions of effective masses of heavy hole and light hole are given by

\[
\frac{1}{m_+} = \frac{1}{m_0} (\gamma_1 - 2\gamma_2) \quad (2.13a)
\]

and

\[
\frac{1}{m_-} = \frac{1}{m_0} (\gamma_1 + 2\gamma_2) \quad (2.13b)
\]

respectively. Eq.(2.13a) and Eq.(2.13b) in which \(m_0\) is the free electron mass and \(\gamma_1\) and \(\gamma_2\) are Luttinger parameters. The size dependent dielectric function is given by [21, 22]
\[ \frac{1}{\varepsilon(r)} = \frac{1}{\varepsilon_{\infty}} - \left[ \frac{1}{\varepsilon_{\infty}} - \frac{1}{\varepsilon_0} \right] \times \left[ 1 - \frac{\exp(-r / \rho_e) + \exp(-r / \rho_h)}{2} \right] \]  

(2.14)

where \( r \) is the mean electron-hole distance, \( \varepsilon_0 \) and \( \varepsilon_{\infty} \) are the static and optical dielectric constants and \( \rho_{e,h} \) are given by [23]

\[ \rho_{e,h} = \left( \frac{\hbar}{2m_{e,h}^* \omega_{LO}} \right) \]  

(2.15)

where \( \hbar \omega_{LO} \) is the LO phonon energy.

The strain induced confinement potential is the combination of energy band offsets due to conduction, valence bands and the static electric potential related to the built-in internal fields. The strength of the built-in electric field \( F \) caused by the spontaneous and piezoelectric polarizations in the \( \text{Zn}_x\text{Cd}_{1-x}\text{Te} \) strained quantum dot is expressed as in Ref. [24]. The procedure for strain calculations are followed from the Ref. [25].

The effect of exciton and the LO phonon interaction are derived by the effective potential \( (V_{PB}) \) between the electron and hole along with the self energy term \( (E_{\text{self}}) \) as given below. The quantum dot confinement effective potential of the electron and hole is given by [26]

\[ V_{PB}(r) = -\frac{\varepsilon^2}{\varepsilon^* r} \left[ \frac{C^4}{B^3} - \frac{m_{e}^* h_e}{\Delta m} \exp \left( -\frac{r A_e}{R_e} \right) + \frac{m_{h}^* h_h}{\Delta m} \exp \left( -\frac{r A_h}{R_h} \right) \right] \left\{ \frac{h + \frac{C^3 r}{2B^3 a_{ex}}}{R_p} \right\} \]  

(2.16)

where \( \varepsilon^* = (1/\varepsilon_{\infty} - 1/\varepsilon_s)^{-1} \), \( \varepsilon_{\infty} \) and \( \varepsilon_s \) are the optical and static dielectric constants of the CdTe material and \( \Delta m \) is the difference in
effective mass of electron and hole. When a dot material is embedded on a barrier material, the field effect caused by the charge distribution will enhance the Coulomb interaction.

The self energy term is given by [27]

$$E_{\text{self}} = - \left( \alpha_e g_e + \alpha_h g_h - \alpha_{\mu} g_{\mu} \right) \hbar \omega_{\text{LO}} \tag{2.17}$$

where $\hbar \omega_{\text{LO}}$ is the LO phonon energy. The calculations of other material parameters in Eq.(2.16) and Eq.(2.17) are followed from Ref. [20].

The effective potential due to the effect of dielectric confinement on the interaction between the electron and the hole is calculated below. The effect of electron–hole confinement in the image charge method is given by the effective potential as [19]

$$V_{KT}(r) = - \sum_{n=-\infty}^{\infty} \frac{\xi|p|}{\varepsilon_s \sqrt{\rho^2 + (z_z - (-1)^n z_h + nL)^2}} \tag{2.18}$$

where $\xi = (\varepsilon_s^w - \varepsilon_s^b)/ (\varepsilon_s^w + \varepsilon_s^b)$ and $\varepsilon_s^w$ and $\varepsilon_s^b$ are the static dielectric constants of the dot and the barrier material respectively. L is the height of the cylindrical quantum dot.

The variational formulism is followed for computing the binding energy of ground state exciton as a function of dot radius. The energy levels, wave functions of bound electron and hole states are computed as done in Ref.[25]. Ultimately, the exciton binding energy and the optical transition energy are given as

$$E_{\text{exc}}(x) = E_e + E_h - \langle H_{\text{exc}} \rangle_{\text{min}} \tag{2.19}$$
and

\[ E_{ph}(x) = E_e(x) + E_h(x) + E_{g}^\Gamma(x) - E_{exc}(x) \]  \hspace{1cm} (2.20)

where \( E_{e,h}(x) \) is the lowest binding energy of electron (hole) obtained by self-consistent calculation. \( E_{g}^\Gamma(x) \) the Zn dependent bandgap of the inner dot material.

The strain induced energies of excitonic transitions in the \( Zn_xCd_{1-x}Te/ZnTe \) quantum dot are given by

\[ E_{e,hh} = E_g(Zn_xCd_{1-x}Te) + \Delta E_{v,hh} + \Delta E_e + E_{e,h} - E_{exc} . \]  \hspace{1cm} (2.21)

The single band effective mass approximation is employed with the expansion of electron (hole) wave function in an appropriate set of orthonormal functions. And then, the nonlinear optical properties with the photon energies are calculated using compact density matrix approach.

### 2.3.3 Linear and non-linear optical absorption

The computation on optical absorption is based on the Fermi Golden rule. Consequently, the total absorption coefficient is given by [28]

\[ \alpha(\omega, I) = \alpha_1(\omega) + \alpha_3(\omega, I) \]  \hspace{1cm} (2.22)

The calculations are important to know the various optical properties taking into consideration of any electronic transitions system. The optical transition takes place between the initial and final states. However, the dipole transitions occur following the selection rules.
\( \Delta l = \pm 1 \) where \( l \) is the angular momentum quantum number. And, hence, the oscillator strength connected with the dipole transition, is given by

\[
P_{fi} = \frac{2m_e^*}{\hbar^2} \Delta E_{fi} |M_{fi}|^2
\]

(2.23)

where \( \Delta E_{fi} = E_f - E_i \) is the difference of the energy between the lower and upper states. The matrix element \( M_{fi} = 2\langle f | e r | i \rangle \) is calculated from the electric dipole moment of the transition from \( i \) state to \( f \) state in the quantum dot. The optical absorption coefficient is given by

\[
\alpha_1(\omega) = \frac{4\pi\alpha_f \sigma_s}{n_r e^2} \hbar \omega |M_{fi}|^2 \delta(E_f - E_i - \hbar \omega)
\]

(2.24)

and

\[
\alpha_3(\omega, I) = -\frac{32\pi^2\alpha_f \sigma_s I}{n_r^2 e^2 \hbar \Gamma_{fi}} \hbar \omega |M_{fi}|^2 \delta(E_f - E_i - \hbar \omega)
\]

\[
\left\{ 1 - \frac{|M_{ff} - M_{fi}|^2}{4|M_{fi}|^2} \times \left\{ \frac{[(\hbar \omega - E_{fi})^2 - (\hbar \Gamma_{fi})^2 + 2E_{fi}(E_{fi} - \hbar \omega)]}{E_{fi}^2 + (\hbar \Gamma_{fi})^2} \right\} \right\}
\]

(2.25)

where \( n_r \) is the refractive index of the material, \( \sigma_s \) is electron density of the quantum dot, \( \omega \) the angular frequency of the incident photon energy, \( \alpha_f \) is the fine structure constant and \( E_i \) and \( E_f \) denote the confinement energy levels for ground and the first excited state, respectively [29].

The two equations (Eq.(2.24) and Eq.(2.25)) are linear and third order nonlinear optical absorption coefficients respectively.
The energy-conserving delta function by the Lorentzian is given by
\[
\delta(E_f - E_i - \hbar \omega) = \lim_{\Gamma \to 0} \pi \frac{\Gamma}{(E_f - E_i - \hbar \omega)^2 + \Gamma^2}
\] (2.26)
where \( \Gamma \) is the line width of the exciton for which the value, \( \Gamma = 0.1 \) meV, is taken into consideration. In addition, the homogeneous spectral width due to the finite coherence time between the two energy levels is also taken into account for calculating the absorption coefficients.

The optical susceptibilities which are related to the refractive index changes are given by
\[
\frac{\Delta n(\omega)}{n_r} = Re \left[ \frac{\chi(\omega)}{2n_r^2} \right]
\] (2.27)
where \( n_r \) is the refractive index of the given material. The linear and nonlinear changes of refractive index are expressed as
\[
\frac{\Delta n_{(i1)}(\omega)}{n_r} = \frac{\sigma_s e^2}{2e_r} |M_{fi}|^2 \frac{\hbar \omega_{fi} - \hbar \omega}{(E_{fi} - \hbar \omega)^2 - (\hbar \Gamma_{fi})^2}
\] (2.28)
and
\[
\frac{\Delta n_{(i3)}(\omega)}{n_r} = -\frac{\mu_0 c I}{4e_r n_r^2} \frac{\sigma_s e^4 |M_{fi}|^4}{[(E_{fi} - \hbar \omega)^2 + (\hbar \Gamma_{fi})^2]^{3/2}} \left[ -\left( |M_{fi} - M_{\alpha i}|^2 \times \frac{[(E_{fi} - \hbar \omega_{\alpha i})^2 - (\hbar \Gamma_{\alpha i})^2 + (3(E_{\beta i} - 2\hbar \omega))]^{1/2}}{E_{\beta i} + (\hbar \Gamma_{\beta i})^2} \right) \right]
\] (2.29)
Hence the total changes of refractive index are given by
\[
\frac{\Delta n(\omega)}{n_r} = \frac{\Delta n_{(i1)}(\omega)}{n_r} + \frac{\Delta n_{(i3)}(\omega)}{n_r}
\] (2.30)
2.4 Results and discussion

The ground state exciton binding energies of an exciton located at the centre of a strained Zn$_x$Cd$_{1-x}$Te/ZnTe quantum dot are computed with various Zn content with and without the dielectric confinement due to the image charge potential. The effect of z-confinement has been calculated through a finite quantum dot model with the confinement potential determined by the band offsets and strain effects. All the computations have been carried out using Bessel function as an orthonormal basis for various Zn alloy content in the inner quantum dot which ultimately has the impact of changing the confinement potentials of barrier height. The atomic units are followed for the determination of electronic charges and wave functions and assume the electronic charge and the Planck’s constant as unity. The effective masses of heavy and light holes are $m_+ = 1/(\gamma_1 - 2\gamma_2)$ and $m_- = 1/(\gamma_1 + 2\gamma_2)$ respectively. $T(Zn_xCd_{1-x}Te) = (1-x)TCdTe + xTznTe$, where T refers various physical parameters used in our calculations. All the values of material parameters of Cd$_{1-x}$Zn$_x$Te used in the present numerical calculations have been obtained by interpolating the binary data referred in the Table 2.1.
Table 2.1 Material parameters* used in the calculations (all the other parameters are linearly interpolated)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>CdTe</th>
<th>ZnTe</th>
<th>Zn\textsubscript{x}Cd\textsubscript{1-x}Te</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m^*_e$</td>
<td>0.11</td>
<td>0.2</td>
<td>0.11+0.091x</td>
</tr>
<tr>
<td>\varepsilon</td>
<td>10.4</td>
<td>9.4</td>
<td>10.4-1.0x</td>
</tr>
<tr>
<td>$a$ (nm)</td>
<td>0.6481</td>
<td>0.61037</td>
<td>0.6481-0.03773x</td>
</tr>
<tr>
<td>$C_{11}$ (GPa)</td>
<td>53.8</td>
<td>72.2</td>
<td>53.8+18.397x</td>
</tr>
<tr>
<td>$C_{12}$ (GPa)</td>
<td>37.4</td>
<td>40.9</td>
<td>37.4 + 3.471x</td>
</tr>
<tr>
<td>$e_{14}$ (C/m\textsuperscript{2})</td>
<td>0.91</td>
<td>0.028</td>
<td>0.91 – 0.88x</td>
</tr>
<tr>
<td>$E_g^r$ (eV)</td>
<td>1.51</td>
<td>2.27</td>
<td>1.51 + 0.45x +0.31x\textsuperscript{2}</td>
</tr>
<tr>
<td>$\Delta$ (eV)</td>
<td>4.67</td>
<td>4.789</td>
<td>4.67-0.119</td>
</tr>
<tr>
<td>$\gamma_1$</td>
<td>4.14</td>
<td>3.96</td>
<td>4.14-0.18x</td>
</tr>
<tr>
<td>$\gamma_2$</td>
<td>1.019</td>
<td>0.86</td>
<td>1.019-0.159x</td>
</tr>
<tr>
<td>$a_c$ (eV)</td>
<td>-3.96</td>
<td>-5.83</td>
<td>-3.96-1.87x</td>
</tr>
<tr>
<td>$a_v$ (eV)</td>
<td>0.55</td>
<td>0.79</td>
<td>0.55+0.24x</td>
</tr>
<tr>
<td>$b$ (eV)</td>
<td>-1.0</td>
<td>-1.4</td>
<td>-1.0-0.4x</td>
</tr>
</tbody>
</table>

*Ref. [17]
The valence band and conduction band offsets in a Zn\textsubscript{x}Cd\textsubscript{1-x}Te/ZnTe quantum dot are shown in Fig. 2.1. The variation of conduction band offset ($V_c$), heavy-hole ($V_{hh}$) and light hole band offsets ($V_{lh}$) and the energy splitting between light and heavy hole bands ($E_{hh-lh}$) as a function of Zn alloy content is taken in a strained Zn\textsubscript{x}Cd\textsubscript{1-x}Te/ZnTe quantum dot of a constant radius, 100 Å. It is observed that both $V_c$ and $V_h$ increase linearly with Zn alloy composition. It is because the bandgap of the dot material increases in turn the barrier height also increases. $V_{lh}$ is found to be greater than $V_{hh}$ due to the increase in induced tensile strain. Further, it is observed that the lattice constant of the outer material ($Zn_xCd_{1-x}Te$) is greater than that of the inner dot ($ZnTe$). Hence, the tensile strain will be induced in the dot material. Also, the energy splitting between heavy and light hole bands increases with increasing Zn alloy content due to the increase in induced compressive strain [30].
Fig. 2.1 Variation of conduction band offset ($V_e$), heavy-hole ($V_{hh}$) and light hole band offsets ($V_{lh}$) and the energy splitting between light and heavy hole bands ($E_{hh-lh}$) as a function of Zn alloy content in a strained Zn$_x$Cd$_{1-x}$Te/ZnTe quantum dot with a dot radius (100Å).
The variation of exciton binding energies related to the heavy holes and light holes as a function of dot radius for various confinement potentials in a strained Cd$_{1-x}$Zn$_x$Te/ZnTe quantum dot with the inclusion of dielectric confinement due to image charge potential is shown in Fig. 2.2. Enhancement of binding energy with the reduction of dot radius is observed for all the cases of Zn incorporation in CdTe material. However, the exciton binding energy decreases below the critical radius of the quantum dot. Spreading of wave functions with the larger dot radius are the cause for the reduction of exciton binding energy and the contribution of confinement is dominant for smaller dot radii which makes the exciton unbound and ultimately tunnels through the barrier. Eventually, the electron and hole wave functions penetrate into the barrier for narrow dots. Moreover, the contribution of confinement is dominant for smaller dot radii making the electron unbound with the spread of the wave function through the barrier [25]. The light hole exciton binding energies seem to be higher than the heavy hole exciton binding energy for all the dot radii. The behaviour of binding energy with the decrease in dot radius has the same trend as reported earlier [31]. The variation in Zn composition causes the increase in the barrier height of the quantum dot and hence, the exciton binding energy increases with the Zn composition whereas the enhancement of exciton energy with the reduction of dot radius is due to the spatial confinement. All our calculations include the effect of dielectric confinement and the size dependent dielectric function. It is found that the barrier height increases as the Zn alloy concentration is increased due to the enhancement of the bandgap with the concentration. Hence, the binding energies increase with the composition of Zn in CdZnTe quantum dot.
Fig.2.2 Variation of exciton binding energies due to heavy and light holes as a function of cylinder dot radius for a Cd$_{1-x}$Zn$_x$Te/ZnTe quantum dot for various Zn content
Fig. 2.3 shows the variation of heavy and light hole exciton binding energies as a function of dot radius in a Zn$_{0.8}$Cd$_{0.2}$Te/ZnTe quantum dot and the solid curve represents the binding energy with the inclusion of PB potential (Eq.(2.16)) and the dielectric mismatch and the dashed curve represents without the PB potential. It is observed that the enhancement of the binding energy due to electron-phonon interaction is larger for all the dot radii but it is noticed that the binding energy is more influence for smaller dot radii than the larger dot radii due to the geometrical confinement. It shows the effect of PB potential which includes dielectric mismatch term. It is found that the exciton binding energy obtained using static screened Coulomb potential is lower than the exciton binding energy with the inclusion of effective potential. It is observed that the effect of dielectric mismatch enhances the exciton binding energy. The results bring out that the effect of dielectric mismatch on the exciton binding energy is very important in low dimensional semiconductor heterostructures. Hence, it is concluded that dielectric confinement due to image charge potential enhances the exciton binding energy [32].
Fig. 2.3 Variation of heavy and light hole exciton binding energies as a function of dot radius in a $\text{Zn}_{0.8}\text{Cd}_{0.2}\text{Te}/\text{ZnTe}$ cylindrical quantum dot; the solid curve represents the binding energy with the inclusion of PB potential (Eq.(2.16)) and the dielectric mismatch and the dashed curve represents without the PB potential.
Fig. 2.4 represents the variation of free exciton energies ($e_{1h_1}$ and $e_{1l_1}$) as a function of dot radius in a strained Cd$_{1-x}$Zn$_x$Te/ZnTe quantum dot. It is noted that the energies of free excitons are increased as the radius of dot decreases. It is found that this effect is more pronounced for smaller dots. It is because the confinement of electron-hole with respect to z-plane for smaller dot radii. The geometrical confinement of electron-hole increases when the dot radius is decreased. Further, it is found that this energy increases with the addition of Zn alloy content in inner dot for all the dot radii. It is clearly shown that the effect of bound exciton has a great significant on the excitonic transition energy. This demonstration illustrates the quantum size effect.
Fig. 2.4 Variation of free exciton energies (e₁h₁ and e₁l₁) as a function of dot radius in a strained Cd₁₋ₓZnₓTe/ZnTe cylindrical quantum dot.
Variation of absorption coefficients in the strained Zn$_x$Cd$_{1-x}$Te/ZnTe quantum dot with the radius 40Å as a function of photon energy and $I = 10\text{MW/m}^2$ for different Zn concentration is shown in Fig.2.5. It is noticed that the magnitude of the absorption coefficients becomes higher and shifts towards the higher photon energy when the Zn alloy composition in CdTe inner dot increases. It is because the increase of Coulomb interaction energy leads to the increase of the energy difference between the initial and final states. Moreover, it is obvious that the size of the quantum dot depends on the transition matrix element, the electron density and ultimately on the absorption coefficients. Moreover, it is notified the binding energy is more for when the Zn composition is increased for all the dot radii due to the enhancement of binding energy when the Hamiltonian is included with the dielectric confinement. Hence, it is concluded that intensity dependent nonlinear absorption coefficients near the resonant frequencies are important and it should be taken into account in studying the optical properties of exciton in the low dimensional hetero-system.

However, the contribution from the nonlinear optical absorption coefficient should be considered provided the optical intensity is very strong. The intensity of the total absorption spectra increases for the transition between higher levels due to the increase of electronic dipolar matrix element. When the effect of Zn composition is included the optical absorption peak increases remarkably due to the increase of electronic dipolar matrix element with the strong confinement potential. The phonons in strong ionic crystals involve the relative motion of positive and negative ions occurring polarization with a strong interaction of electromagnetic waves. Thus, the LO phonon has a significant influence on the optical properties of polar crystals. Moreover, phonon
has an important effect due to the electron transition between the intersubband when the system is irradiated with the photon. Hence, the total optical absorption magnitude, with the inclusion of the electron-phonon interaction, increases by a factor of 2–3 [33].
Fig. 2.5 Variation of absorption coefficients of a heavy hole exciton in the strained Zn$_x$Cd$_{1-x}$Te/ZnTe cylindrical quantum dot for the radius 40Å, as a function of photon energy and $I = 10$ MW/m$^2$ for three different Zn concentration.
Fig. 2.6 shows the variation of changes of refractive index for a heavy hole exciton in the strained Zn$_x$Cd$_{1-x}$Te/ZnTe quantum dot with the radius 40Å, as a function of photon energy and I = 10MW/m$^2$ for different Zn alloy composition. The linear and nonlinear components of refractive index are included in all the calculations to obtain the total changes of refractive index which have been studied with the incident photon energy and with increasing Zn content in CdTe dot. It is observed that the total refractive index changes shift towards the higher values and the magnitude of total refractive index increases as the Zn incorporation increases. This is because the increase in exciton binding energy with the Zn-composition. Also, it is noticed from the Eq.(2.28) and Eq.(2.29) that the linear relative change in refractive index depends on photon intensity but the third order relative change in refractive index changes with photon intensity and it varies quadratically with the matrix element of the electric dipole moment of the transition [25, 34]. Thus, the nonlinear term must be considered when calculating the refractive index changes of low dimensional semiconductor systems in which the incident light propagates along the z-axis [35]. Thus, the nonlinear term must be considered when calculating the refractive index changes in any low dimensional semiconductor systems.
Fig. 2.6 Variation of changes of refractive index for a heavy hole exciton in the strained Zn$_x$Cd$_{1-x}$Te/ZnTe cylindrical quantum dot with the radius 40Å, as a function of photon energy and I = 10MW/m$^2$ for three different Zn concentration.
2.5 Conclusion

The ground state exciton binding energies of heavy and light holes have been investigated in a strained $\text{Zn}_x\text{Cd}_{1-x}\text{Te}/\text{ZnTe}$ polar quantum dot nanostructure and the influence of strain on the optical properties of heavy hole exciton for various Zn composition has been studied. Calculations have been obtained using Bessel function as an orthonormal basis for different confinement potentials of barrier height considering the internal electric field induced by the spontaneous and piezoelectric polarizations. The magnitude of the absorption coefficients and the refractive index changes have been found to increase for transitions between higher levels with the inclusion of phonon effect. The results of free exciton energies have been presented for various dot sizes, Zn content and confining potentials. Moreover, the studied non-linear absorption coefficients and the changes of refractive near the resonant frequencies are important and it should be taken into account in studying the optical properties of exciton in the low dimensional heterosystem. It is hoped that there results would explore new findings on experimental research works using II-VI semiconductors in optoelectronic and terahertz devices.
References