Effects of Temperature and Hydrostatic Pressure on Binding Energy of an Exciton in a Spherical Quantum Dot

A. Rejo Jeice*
Department of Physics, Annai Velankannai College, Tholayarattam-629157 TamilNadu, India

K. S. Joseph Wilson
Department of Physics, Arul Anandar College, Karamathur, Madurai Dist.-625514, TamilNadu, India

(Received 16 December 2013; Accepted 16 May 2014; Published 2 August 2014)

The binding energies of the heavy-hole and light-hole exciton in a GaAs spherical quantum dot have been calculated using variational technique within effective mass approximation. The effect of pressure and temperature are also analyzed. Our result shows that exciton binding energy (i) decreases as the dot radius increases, (ii) further increases with increase in pressure and decreases with increase in temperature, and (iii) approaches zero as dot size approaches infinity. All the calculations have been carried out with finite models and results are compared with exciting literatures. [DOI: 10.1380/ejssnt.2014.358]

Keywords: Quantum effects; Photoluminescence; Semi-empirical models and model calculations; Quantum dots; Energy band edge; Valance and conduction band

I. INTRODUCTION

Low dimensional semiconductor systems (LDSS) show interesting behavior due to quantum confinement [1]. It has drawn considerable attention both experimentally and theoretically in the recent past. Most of the studies on semiconductor systems have been carried out on III-V semiconductor heterostructures and, in particular, in GaAs/Ga1-xAlxAs heterostructures. Of the quantum devices spherical quantum dot (SQD) plays an important role due to the quantum confinement of electron in all directions [2-4], in which exciton are of great importance for most of the optical and electrical properties of the semiconductors and devices [5]. Exciton is a quasiparticle which is formed due to the coulomb interaction between an electron and a hole. The coupled pair can propagate through the crystal as a single particle. They found in numerous applications [6]. The study of exciton was carried by many of the researchers.

M. Santhi et al. calculated the binding energy of excitons in a cylindrical quantum wire of the GaAs/GaAlAs under the influence of laser field intensity [7]. P. Le-long et al. calculated the binding energy of excitons of GaAs QD [8]. W. Heller et al. experimentally investigated the photoluminescence and photoluminescence excitation spectra of excitons in a GaAs/GaAlAs quantum dot [9]. E. M. Lopes et al. theoretical and experimental study of the excitonic binding energy in GaAs/AlGaAs single and coupled double quantum wells [10]. S. K. Lyo studied the Stark effect of optical properties of excitons in a quantum nanorod with parabolic confinement [11]. G. L. Miranda et al. studied the binding energies of the lowest four 1s-like exciton states in GaAs/AlGaAs coupled double quantum wells [12]. Kasapoglu et al. [13] have investigated the magnetic field induced ground state exciton binding energy in asymmetric and symmetric double quantum wells and showed the competition between the magnetic field and the geometric confinement on the exciton binding energy using a variational procedure for small well widths. Oyoko et al. [14] dealt with pressure- and temperature-dependent shallow impurity related optical absorption spectra in GaAs/GalAs single and double quantum wells. M. E. Mora-Ramos et al. studied the effect of hydrostatic pressure and temperature on excitons in cylindrical GaAs [15]. They found that exciton binding energy is a decreasing function of temperature for fixed pressure, and an increasing function of pressure for fixed temperature.

In the present work, we study the effects of hydrostatic pressure and temperature on the ground state of the binding energy of light- and heavy-hole exciton confined in GaAs/Ga1-xAlxAs spherical quantum dots with finite barrier model. We applied varational method to solve the problem within the effective mass approximation. We also computed the exciton binding energy as a function of the dot radius, pressure and temperature. Our result shows that the exciton binding energy increases with increase in pressure and decreases with increase in temperature for all dot radii.

II. MODEL AND CALCULATION

A. Energy and Wavefunction of exciton

In the effective mass approximation, the Hamiltonian of an exciton in a SQD under the influence of temperature and pressure is given by,

$$H = -\frac{\hbar^2}{2m_e^* (P,T)} \nabla_e^2 - \frac{\hbar^2}{2m_h^* (P,T)} \nabla_h^2 - \frac{e^2}{\varepsilon(P,T)|r_e - r_h|} + V_e(r,P,T) + V_h(r,P,T),$$  (1)

where $m_e^*(P,T)$ and $m_h^*(P,T)$ are the effective masses of the electron and hole respectively, $V_e(r,P,T)$ and $V_h(r,P,T)$ are the confinement potentials for the electron and the hole. $\varepsilon(P,T)$ is the dielectric constant which also

* Corresponding author: rejojeice@gmail.com
depends on pressure and temperature,

\[
V_e(r), V_h(r) = \begin{cases} 
0 & r < R(P,T), \\
V_e(r, P, T), V_h(r, P, T) & r > R(P,T),
\end{cases}
\]

where \(R(P,T)\) is the hydrostatic pressure and temperature dependent dot radius. \(V_e(r, P, T) = 0.658 \Delta E_g(x)\) is the barrier height of electron in the conduction band and \(V_h(r, P, T) = 0.34 \Delta E_g(x)\) is the barrier height of hole in the valence band when \(x = 0.2\) [16]. The band-gap difference [17] between the GaAs and Ga\(_{1-x}\)Al\(_x\)As is given by

\[
\Delta E_g(x) = 1.155 x + 0.37 x^2.
\]  

(3)

The wave function for the electron and hole in the ground state is chosen to be

\[
\psi = \begin{cases} 
N \frac{\sin(\alpha_1 r_e)}{r_e} \frac{\sin(\alpha_1 r_h)}{r_h} e^{-\beta_1 r_e} e^{-\beta_1 r_h} & r_e, r_h \leq R(P,T), \\
A \frac{\sin(\beta_1 r_e)}{r_e} \frac{\sin(\beta_1 r_h)}{r_h} e^{-\alpha_1 r_e} e^{-\alpha_1 r_h} & r_e, r_h \geq R(P,T),
\end{cases}
\]

(4)

where \(N\) and \(A\) are the normalization constant and \(\alpha_1 = \sqrt{2m^*_{P;T}} E\) and \(\beta_1 = \sqrt{2m^*_{e;V;p}} (V_e - E)\). Matching the wave function and their derivatives at the boundary \(r = R\) and imposing the boundary condition we obtain

\[
\alpha R + \beta R \tan(\alpha R) = 0.
\]

(5)

Solving this transcendental equation we obtain the lowest sub-band energy of the electron and hole. The trial wave function for the exciton ground state is was chosen to be [18]

\[
\psi = \begin{cases} 
N \frac{\sin(\alpha_1 r_e)}{r_e} \frac{\sin(\alpha_1 r_h)}{r_h} e^{-\lambda r} & r_e, r_h \leq R(P,T), \\
A \frac{\sin(\beta_1 r_e)}{r_e} \frac{\sin(\beta_1 r_h)}{r_h} e^{-\lambda r} & r_e, r_h \geq R(P,T),
\end{cases}
\]

(6)

where \(\lambda\) is the variational parameter. The binding of the exciton are given by \(E_{\text{ion}} = E_1 - \langle H_{\text{min}} \rangle\). The evaluation of \(\langle H_{\text{min}} \rangle\) in each case is straight forward. As the expression we obtained for \(\langle H_{\text{min}} \rangle\) is too lengthy, we refrain from giving here.

## B. Effect of temperature and pressure

The application of hydrostatic pressure and temperature effective masses, dielectric constants, barrier height and dot sizes is modified. We present the explicit expressions for these variables as a function of pressure is expressed in kbar and the temperature is in K [19]. The hydrostatic pressure and temperature dependent conduction-band-effective-mass of GaAs and Ga\(_{1-x}\)Al\(_x\)As can be written as [20, 21]

\[
\frac{m_e}{m^*(P,T)} = 1 + E \left\{ \frac{2}{E_g^b(P,T) + (E_g^b(P,T) + \Delta_0)^{-1}} \right\},
\]

(7)

where \(E = 7.51\) eV is the energy related to the momentum matrix element. \(\Delta_0 = 0.341\) eV is the spin-orbit splitting, \(m_e\) is the free electron mass and \(E_g^b(P,T)\) is the pressure and temperature dependent energy gap for the GaAs QD at the \(\Gamma\)-point and is given by [22, 23]

\[
E_g^b(P,T) = E_g^b(0,T) + bP + CP^2,
\]

(8)

where

\[
b = 1.26 \times 10^{-2} \text{ eV bar}^{-1},
\]

(9)

\[
C = 3.77 \times 10^{-5} \text{ eV bar}^{-2},
\]

(10)

\[
E_g^b(0,T) = 1.519 - \frac{5.405 \times 10^{-4} \ T^2}{T + 204}.
\]

(11)

The effective mass of Ga\(_{1-x}\)Al\(_x\)As is given by [24]

\[
m^*_e(P,T) = m^*_e(P,T) + 0.083 \ x,
\]

(12)

where \(x\) is the aluminum composition. The hydrostatic pressure and temperature dependent valance band effective mass of GaAs and Ga\(_{1-x}\)Al\(_x\)As can be written as

\[
m^*_v(P) = \frac{m^*_v}{m_0} = x + 2P + x_3P^2,
\]

(13)

where \(x_1 = 0.30242, x_2 = -0.1 \times 10^{-3} \text{ K bar}^{-1}\) and \(x_3 = 5.56 \times 10^{-6} \text{ K bar}^{-2}\). The variation of dielectric constant with pressure and temperature is given as [25]

\[
\frac{\Delta \varepsilon_{b,d}(P,T)}{\Delta \varepsilon_{b,d}(P,T)} = \begin{cases} 
12.74 e^{-1.73 \times 10^{-3} \ P + 9.4 \times 10^{-5} \ (T - 75.6)} & T \leq 200 \ [K], \\
13.18 e^{-1.73 \times 10^{-3} \ P + 2.4 \times 10^{-4} \ (T - 300)} & T \geq 200 \ [K].
\end{cases}
\]

(14)

The corresponding dielectric constant of Ga\(_{1-x}\)Al\(_x\)As is given as

\[
\varepsilon_{b,d}(P,T) = \varepsilon_{d}(P,T) + 3.12 \ x.
\]

(15)

From eq. (2), the pressure-and-temperature-dependent barrier height, the band-gap difference is given by

\[
E_g(x, P, T) = E_g(x) + D(x) P + G(x) T,
\]

(16)

where

\[
D(x) = -1.3 \times 10^{-3} \ [\text{eV/kbar}],
\]

(17)

\[
G(x) = -1.15 \times 10^{-4} \ [\text{eV/K}].
\]

(18)

The variation of dot size with pressure is given [26] by

\[
R(P) = R_0(1 - 1.5082 \times 10^{-3} \ P),
\]

(19)

where \(R_0\) is the zero-pressure dot radius. In the numerical work, the pressure used was 0-4 GPa, which corresponds to 40 kbar. We have not considered pressures beyond 4 GPa, because of a direct to indirect band-gap transition of GaAs at about 4 GPa [27, 28].

## III. RESULTS AND DISCUSSION

The results obtained are shown in Figs. 1-5. We have computed the combined effect of hydrostatic pressure and temperature effects on heavy-hole and light-hole excitons
in the SQD. For the light-hole exciton and heavy-hole exciton the effective mass of GaAs is 0.50 and 0.07 respectively [6]. We find that the increase in temperature will decreases the values of both the effective mass and the barrier height and increase the value of dielectric constant of GaAs and Ga$_{1-x}$Al$_x$As. Similarly increase in pressure will increase the effective mass and decrease the dielectric constant and barrier height. This effect will affect the exciton binding-energy.

Figure 1 shows the variation of binding energy of an exciton quantum dot as a function of dot radius for different pressures. We found that in all cases the exciton binding-energy increases reaches the maximum value and then decreases as the dot radius increases except for the heavy-hole exciton of pressure 4 GPa. The above results are due to the tunneling effect as $R$ tends to zero. When $R$ tends to infinity the system behaves like a bulk with no confinement, a feature that is well known in literature [7]. We have also seen that the heavy-hole exciton have less binding energy as compares to the light-hole exciton binding energy. This is due to the variation of exciton effective mass. When the pressure increases the exciton binding energy also increases. Also the pressure effect is more in the light exciton than in heavy exciton. There is no bound state for the dot radii less than 25 Å for the exciton in a SQD. This result is contract to the quantum-well case. There for every well size a bound state is assured in the quantum well [6].

In Fig. 2, we plot the variation of binding energy of an exciton quantum dot as a function of dot radius for constant temperature with different pressure. We found that due to the application of temperature the exciton binding energy decreases. This result is in comparable with that of Ref. [15] of Fig. 1 where they have studied the effects in exciton binding energy in a cylindrical quantum dot with Pöschl-Teller confining potential. The physical reason for the behavior is that the pressure goes up the wave function is very confined for the dot and the effective mass and dielectric constant increases. Thus at higher temperature also for larger dot radii the exciton binding energy reaches the bulk value. Unlike in other system when GaAs dot is embedded in Ga$_{1-x}$Al$_x$As matrix, the dielectric mismatch becomes insignificant, especially when $x$ is small.

In Fig. 3, we have presented the variation of binding energy of an exciton quantum dot as a function of dot radius for different pressure and temperature. It clearly explains the effect of temperature on the exciton binding energy for the constant pressure. For dot radii in between 25 Å and 60 Å range, the spatial confinement on electron and hole becomes the most important effect. In this region, the excitonic binding energy increases smoothly with decreasing dot radius. For even smaller values of dot radius (< 30 Å for heavy hole and < 40 Å for light hole), the exciton binding energy strongly depends on the variation of the dot radius. This means that spatial confinement is much more important relative to confinement effects at

![FIG. 1. The variation of binding energy of an exciton quantum dot as a function of dot radius for different pressures.](image1)

![FIG. 2. The variation of binding energy of an exciton quantum dot as a function of dot radius for constant temperature with different pressure.](image2)

![FIG. 3. The variation of binding energy of an exciton quantum dot as a function of dot radius for a given pressure and temperature.](image3)
FIG. 4. The variation of binding energy of an exciton quantum dot as a function of temperature for dot radius of 30 Å.

FIG. 5. The variation of binding energy of an exciton quantum dot as a function of pressure for dot radius of 30 Å.

the binding energy maxima. This effect can be explained by squeezing the particles even stronger for smaller dot radii results in leakage of the electronic wave functions of both electrons and holes to the barrier. After particles have leaked outside the barrier, the spatial confinement effect is weakened so the particles are no more close to each other resulting a sharp decrease in excitonic binding energies. The above results are well agreement with N. Elmeshad et al. who have studied the effect of hydrostatic pressure and temperature dependence of exciton binding energy inside a cylindrical quantum dot [29]. The physical origin of this result is related to the effect of the existence of the Coulomb repulsion in an exciton-donor complex system. Moreover, we observed that the influence of pressure on the binding energy is more obvious than temperature.

Figure 4 shows the variation of binding energy of an exciton quantum dot as a function of dot radii 30 Å for different temperature. The exciton binding energy decreases linearly with increases temperature. This is due to increase in effective mass and dielectric constant and barrier height. The linearity of the curve tells us that a system operates under hydrostatic pressure and temperature may be used to tune the output of the optoelectronic devices without modifying the physical size of the SQD.

In Fig. 5, we display the variation of binding energy as a function of dot radii of 30 Å for different pressure. The exciton binding energy increases linearly with increase in pressure. From this it follows the pressure and temperature have opposite effect on the exciton binding energy. Liang et al. found the ground state binding energy of the neutral donor in a QD increased as hydrostatic pressure increased [30]. The physical origin of the result is related to the effect of the existence of the Coulomb repulsion in an exciton-donor complex system. Moreover, we observed that the influence of pressure on the exciton binding energy is more obvious than temperature which is also due to columbic repulsion. The effect of temperature and pressure can be tuned the bandgap of the exciton in SQD. Tunability of bandgap of the SQD play an important role in luminescent and photovoltaic devices.

IV. CONCLUSION

In conclusion, we investigated the effect of pressure and temperature on heavy-hole and light-hole exciton in a SQD. We found that the exciton binding energy increases as the pressure increases and decreases as temperature increases. The effect of high temperature is quite significant in small dot radii due to the thermal broadening in the mixed quantum state. The effect of pressure influence is more than that of temperature for an exciton in a SQD. The important conclusion that emerges from Figures 1-5 is that the pressure and temperature effects are important for smaller dot radii and should be consider in the studies of LDSS.

ACKNOWLEDGMENTS

The authors would like to thank Prof. K. Navaneethakrishnan, School of Physics, Madurai Kamaraj University, Madurai, India for his valuable and useful suggestions.

[1] S. Smith, A. Mascarenhas, and J. M. Olson, Phys. Rev. B 68, 153202 (2003).
[2] U. Banin, Y. Cao, D. Katz, and O. Millo, Nature 400, 542 (1999).
[3] A. R. Jeice and K. Navaneethakrishnan, Braz. J. Phys. 39, 526 (2009).
[4] A. Sivakami, A. R. Jeice, and K. Navaneethakrishnan, Int. J. Mod. Phys. B 24, 5561 (2010).
[5] B. P. Zhang, N. T. Binh, K. Wakatsuki, C. Y. Liu, Y. Segawa, and N. Usami, Appl. Phys. Lett. 86, 032105 (2005).
[6] V. V. Mitin, V. A. Kochelap, and M. A. Stroscio, *Micro Electronics and Optoelectronics* (Cambridge University Press, Cambridge, 1999).

[7] M. Santhi and A. J. Peter, Physica E 42, 1643 (2010).

[8] P. Lelong and G. Bastard, Solid State Commun. 98, 819 (1996).

[9] W. Heller, U. Bockelmann and G. Abstreiter, Physica E 2, 623 (1998).

[10] E. M. Lopes et al., J. Lumin. 144, 98 (2013).

[11] S. K. Lyo, J. Lumin. 145, 98 (2014).

[12] G. L. Miranda, M. E. M. Ramos, and C. A. Duque, J. Lumin. 132, 2525 (2012).

[13] E. Kasapoglu, H. Sari, N. Balkan, I. Sokmen, and Y. Ergun, Semicond. Sci. Technol. 15, 219 (2000).

[14] H. O. Oyoko, C. A. Duque, N. P. Montenegro, and L. E. Olivieria, Physics B 371, 153 (2006).

[15] M. E. M. Ramos, M. G. Barseghyan, and C. A. Duque, Physica E 43, 338 (2010).

[16] E. H. Li, Physica E 5, 552 (2000).

[17] R. S. D. Bellia and K. Navaneethakrishnan, Solid State Commun. 130, 773 (2004).

[18] A. Sivakami and K. Navaneethakrishnan, Physica E 40, 649 (2008).

[19] A. M. Elabey, J. Phys.: Condens. Matter 6, 10025 (1994).

[20] Y. Li, O. Voskoboynikov, J. L. Li, C. P. Lee, and S. M. Sze, Nanotechnology 1, 562 (2001).

[21] H. J. Ehrenreich, J. Appl. Phys. 32, 2155 (1961).

[22] B. Welber, M. Cardona, C. K. Kim, and S. Rodriguez, Phys. Rev. B 12, 5729 (1975).

[23] D. E. Aspnes, Phys. Rev. B 14, 53319 (1976).

[24] A. Sivakami and V. Gayathri, Superlatt. Microstr. 58, 218 (2013).

[25] A. J. Peter and K. Navaneethakrishnan Superlatt. Microstru. 43, 63 (2008).

[26] S. Adachi, *GaAs and Related Materials* (World Scientific, Singapore, 1994).

[27] Sr. G. Jeyam and K. Navaneethakrishnan, Solid State Commun. 126, 681 (2003).

[28] S. Adachi, J. Appl. Phys. 58, R1 (1985).

[29] N. Elmeshad, H. Abdelhamid, H. Hassanein, S. Abdelmola, and S. Said, Chin. J. Phys. 47, 1 (2009).