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Effect of Shell Thickness on Electron and Hole Transmission Probabilities of a ZnSe/ZnS Core- Shell Quantum Dot

Bashir Mohi Ud Din Bhat*[a], *Khurshed A. Shah*[b]

[a]Department of Physics, Govt. Degree College for Boys, Anantnag-192101, India
[b]Department of Physics, Sri Pratap College, Cluster University Srinagar, J&K-190001, India

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In this paper we report the effect of shell thickness on transmission probabilities of electrons and holes in the strained configuration of zinc-selenide/zinc-sulphide (ZnSe/ZnS) core-shell quantum dot. The transmission probabilities of electrons/holes were calculated within the frame work of effective mass approximation and quantum mechanical tunneling. In the first attempt, we introduced extra deposit shell thickness of ZnS in the range 0-5nm and calculated its size effects on the transmission of carriers from core to the shell. We observed that quantum dot of small size core show superb characteristics of possible transmissions and the transmission probability of the carriers across the potential barrier can be controlled by varying the shell thickness, which has practical significance for electron transport in quantum dots, electron transfer in bio-sensors and chemo-sensors etc. Moreover, it is also found that for higher values of electron/hole energies (greater than 0.7eV), the transmission probability oscillates, which too has practical significance for quantum oscillators.The study is important from both basic and applied point of view.

Keywords: *Core shell Quantum dot, Quantum tunneling, Transmission probability, Effective mass approximation, Quantum oscillators.*

1.Introduction

Recent advanced nanofabrication technology have made it possible to prepare three dimensionally confined quantum dot (QD)[1] and core-shell quantum dot (CSQD) structures whose characteristic dimensions are comparable with the exciton Bohr radius[2-4]. These structures exhibit opto-electronic properties due to the quantum mechanical nature of the electrons[5,6]. The superficial bonds on the surfaces of quantum dots can be coated with suitable organic materials or inorganic materials and the materials used for coating must possess desired band gap and lattice matching so as to give the quantum dot (QD) a structural continuity. The deposited layer is referred to as shell and the quantum dot as a whole is referred to as CSQDs. The confined electrons/ holes in CSQDs bear a strong barrier potential because of columbic interaction and extra deposited layer.In small QDs, the electrons/ holes confinement increases over the coulombic interaction due to which electrons/holes starts tunneling from core to shell takes place and the core structure exhibits a red shift in the absorption spectra[7]. Some of the examples of CSQDs include ZnSe/ZnSe, ZnS/CdS, CdSe/HgS etc[7,8].

In this study, we have chosen ZnSe/ZnS quantum dot because these CSQDs are considered novel nano-hetero-structures. As ZnS shell has higher band gap compared to ZnSe core. So by over coating the ZnSe core by higher band gap ZnS shell results in an enhancement in localization of the charge carriers which has a wide application in calculating spin polarized current in quantum dots. The extra deposited ZnS shell thickness strongly controls the function of the electron transfer in quantum dots, bio-sensor or chemo-sensorand the inclusion of tunneling property is of utmost importance to study the effect of shell thickness on the tunneling probabilities and energy level structures of the CSQDs[9].Moreover, the presence of shell results increase in exciton and biexciton energies and red shift in PL spectra in the CSQDs[10]. In the present work the barrier penetration (tunneling) probabilities have been theoretically calculated for ZnSe/ZnS core-shell quantum dots under strained configuration using varying potential barrier which depends on the conduction band offset of the QD. The results reveal that size of the core determines the potential barriers to carrier transmission. The smaller the core the more is the transmission and vice versa. The results have significant role in nano-devices using quantum dots, due to the fact that the controlled transmission probabilities of the particles could be utilized for the calculation of spin polarized current in CSQDs employing different types of semiconducting materials.Moreover, the results are consistent with the earlier reported results in the literature.

The paper is organized as follows:

Section 2 describes theoretical formulations and section 3 presents the results and discussions. The conclusion remarks are presented in section 4.

2. Theoretical Formulations

The schematic representation of ZnSe/ZnS core-shell quantum dot (CSQD) is shown in Fig. 1. Here *a* is the radius

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*e-mail:drkhursheda@gmail.com

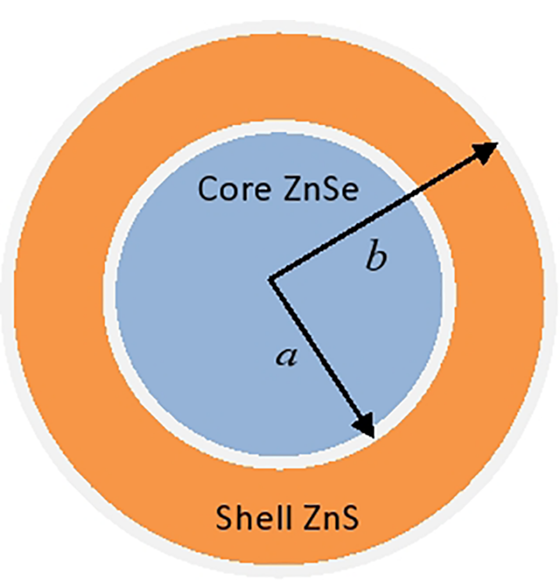

Figure 1. Schematic representation of ZnSe/ZnS core shell quantum dot

of the core and *b* is the radius of the CSQD as a whole. Henceforth, shell thickness is calculated as $t = (b - a)$.

To calculate the transmission probabilities in ZnSe/ZnS core-shell quantum dot, we have used arbitrary potential function $V_{e,h}(r)$, where the subscripts *e*, *h* denotes the electron and hole respectively and divided the potential barrier into thin square barriers each of width *dr* and varying height $V_{e,h}(r)$. The probability of tunneling *dp* through the barrier of height $V_{e,h}(r)$ (assumed constant in a length *dr*) and width *dr* can be written as[11]

$$dp = e^{-2\gamma d\tau} \tag{1}$$

Here in the above expression $d\tau$ is the volume element and parameter γ is defined in such a way, so as to make the above expression a positive real number and, is given by

$$\gamma = \sqrt{\frac{2m_{e,h}^{*}}{\hbar^2}\left[V_{e,h}(r) - E\right]}$$

This symbol is used when the total energy of electron/hole is less than barrier potential energy. After incorporating γ parameter, the equation (1) can be written as

$$dp = e^{-8\pi\sqrt{\frac{2m_{e,h}^{*}}{\hbar^2}[V_{e,h}(r)-E]}.r^2 dr} \tag{2}$$

In the above expression, $m_{e,h}^{*}$ is the effective mass of electron or of hole respectively. The single particle confinement potential $V_{e,h}(r)$ for our model is given by[11]

$$V_{e,h}(r) = \frac{V_{c,\nu}}{a^2}(r^2 - a^2) \quad a < r < b \tag{3}$$

Where the subscripts *c* and *h* denotes the conduction band and valence band for electrons (*e*) and holes (*h*) respectively. V_c and V_v is the conduction band and valance band offsets.

After multiplying equation (2) to all thin barriers each of width *dr* , the transmission probability (p) of the charge particles (electrons/holes) which tunnel through the given barrier becomes

$$p = e^{-8\pi\int_a^b\sqrt{\frac{2m_{e,h}^{*}}{\hbar^2}[V_{e,h}(r)-E]}.r^2 dr} \tag{4}$$

On solving the above expression (4), the final expression for transmission probabilities, is given by

$$p = \left(\frac{m_{e,h}^{*}}{2\hbar^2}\right)^{\frac{1}{2}}\left[\begin{array}{l}\sqrt{\frac{(t^2+2at)V_{c,\nu}}{a^2}}\sqrt{\frac{(t^2+2at)V_{c,\nu}-Ea^2}{a^2}} \\ -E\cos^{-1}h\left[\frac{\sqrt{(t^2+2at)V_{c,\nu}}}{Ea^2}\right]\end{array}\right] \tag{5}$$

Further, we investigate the distribution of energies of electrons/Holes in a quantum dot for that we choose the two dimensional potential for electrons (V_e) and holes V_h of the form

$$V_{e,h}(x) = \frac{V_{c,\nu}}{a^2}(x^2, y^2 - a^2) \tag{6}$$

The wave function can be found by solving Schrodinger equation for the quantum dot, and is of the form of

$$\psi(r,t) = [A\sin(kr) + B\cos(kr)]e^{-i\omega t} \tag{7}$$

Now using the wave function for the system, A and B being the normalization constants, the confinement energy of electrons/holes is calculated as:

$$E_{confinement} = \Delta E_g + \frac{h^2}{8a^2 m_{e,h}^{*}} \tag{8}$$

ΔE_g is the band gap energy of the semiconductor quantum dot, $m_{e,h}^{*}$ is the effective mass of electron and hole.

3. Results and Discussions

The material parameters used for numerical calculations are: $m_e^{*} = 0.17m_0$, $m_h^{*} = 0.60m_0$,where m_e^{*}, m_h^{*}, m_0 is the effective mass of electron, effective mass of hole and rest mass of the charge respectively[12-14]. Our theoretical model is similar to Sen et al[10], therefore in our calculations we used two different core radii 1.25nm and 2.25nm with varying shell thickness from 0 to 5nm, besides valence band offset V_v=0.58*eV* for core radius of 1.25nm, valence band offset V_v=0.14*eV* for core radius of 2.25nm, conduction band offset V_v=0.1*eV* for core radius of 1.25nm and conduction band offset V_v=0.03*eV* for core radius of 2.25nm.

In the first case, the electron transmission probability as a function of shell thickness has been determined. It is note worth from Fig. 2 that in both cases the transmission probability decreases as shell thickness increases. This is because the extra deposited shell thickness provides large confinement to carrier particles confined in the regime of ZnSe core. Moreover, it is also clear from Fig. 2 that the small size QD of radius 1.25nm provides greater possibilities of carriers for tunneling over the shell region as expected.

In next case, under the same conditions we calculated the transmission probability of holes as a function of shell thickness (Fig. 3). From Fig. 3 it is clear that the hole transmission probability decreases gradually as the shell thickness increases and for shell thickness of around 3nm and core radius of 2.25nm, the hole may remain in the core region and the electron tunnels to the shell region. Similar results were obtained for quantum dot of core radius 1.25nm (Fig. 3). Besides the decrease in transmission probability is more profound in case of core radius 2.25nm. Moreover, our results are in agreement with Kim et al[15].

In addition to the carrier transmission probability across the potential barrier, we have determined and plotted the transmission probability of electrons and holes as a function of their energies. It is clear from Fig. 4 and Fig. 5 that the transmission probability of carriers is dependent on their energies as previously reported in the reference[16].

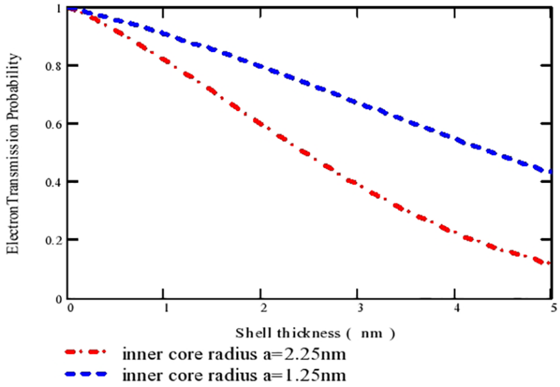

Figure 2. Variation of electron transmission probability as a function of shell thickness in ZnSe/ZnS Core shell quantum dot

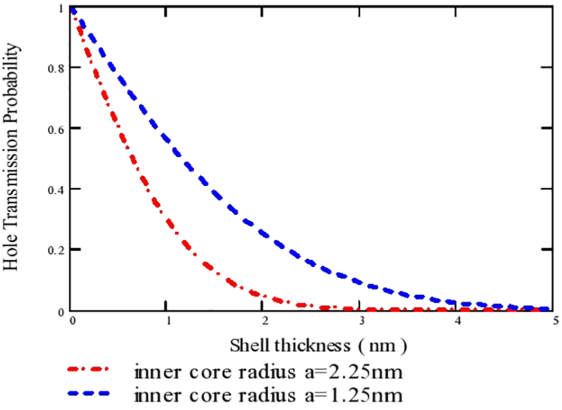

Figure 3. Variation of hole transmission probability as a function of shell thickness in ZnSe/ZnS core-shell quantum dot

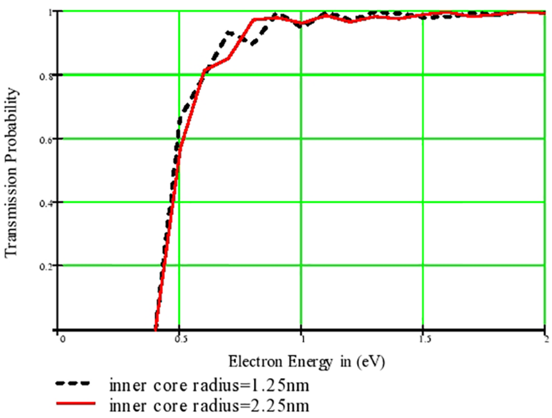

Figure 4. Dependence of electrons transmission probability on energy

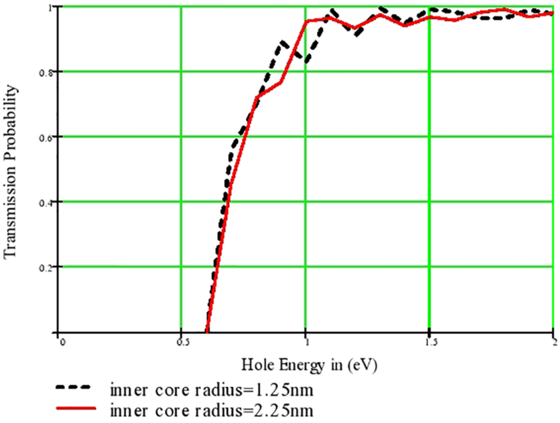

Figure 5. Dependence of holes transmission probability on energy

From the Fig. 4, for electron energy ≤0.4 > *eV*, the transmission probabilities of electrons remains zero due to extra deposit shell of ZnS, henceforth the transmission probability increases almost to unity at 0.7 *eV*. Furthermore, at higher values of energy (>0.7 *eV*) the transmission coefficient oscillates. On the other hand for a given core radius, the transmission probability of holes increases with increasing hole energy (Fig. 5) and the transmission coefficient oscillates for an energy value greater than the electron transmission energy. These results are of great importance in designing of futuristic CSQD sensors and other electronic devices.

To investigate the effect of shell thickness on spatial distributions of electrons and holes, we carried out calculations for the radial probabilities of electrons/holes in the lowest energy state for ZnSe/ZnS core shell quantum dot at core radius 2nm. Fig, 6 shows the radial probabilities of electron/hole as a function of shell thickness in which the ZnS shell thickness is varied from 1.8nm to 4.3nm.

From Fig. 6 we note that the probability of electron/hole at the core region is slightly affected by the ZnS shell thickness and the electron/hole probability remains unconcerned to the shell thickness at core regime. As the shell thickness increases continuously, the electron and hole remain confined

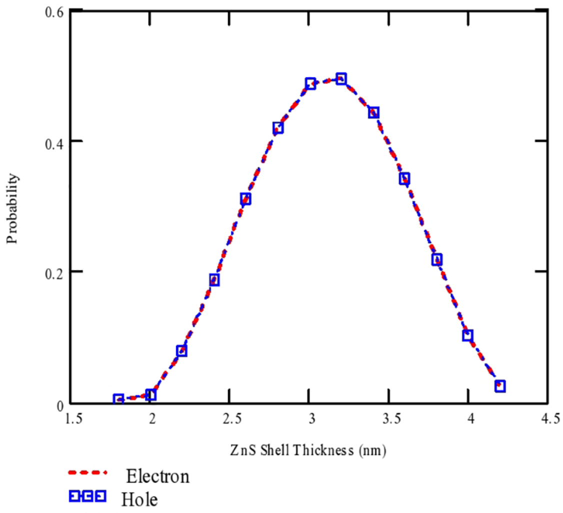

Figure 6. Electron and hole probability distribution in the lowest energy state in ZnSe/ZnS CSQD as a function of ZnS shell thickness

in the core region as they haven't enough energy to cross the barrier due to extra deposited shell thickness. The lowest energy of electron/hole is increasing gradually but due to the barrier height with increasing shell thickness the energy of electrons/holes does not exceed the confinement ability of the barrier height. The infinite potential due to extra deposited ZnS shell confines the charge carriers in the core region, as such the probability distribution of electron/holes decreases as shown in Fig. 6.

4.Conclusions

In this paper we reported the impact of shell thickness on barrier transmission penetration probabilities of electrons and holes in ZnSe/ZnS core- shell quantum dot. In the proposed technique, we introduced extra deposited shell thickness of ZnS and analyzed its size effects on the transmission of electrons/holes across the potential barrier between the core and the shell. We observed that small size QDs (< 1.25nm) shows characteristics of probability of transmission. Therefore it is concluded that the transmission probability of electrons as well as holes of ZnSe/ZnS CSQD can be controlled by varying the shell thickness. In addition, our theoretical results determined that at higher values of electron/hole energies, the transmission coefficient oscillates.In future the findings of this article may find various practical applications particularly for the calculation of spin polarized current in different types of core shell quantum dots (CSQDs).

5. References

1. Jang YD, Lee H, Lee D, Hong SU, Oh DK. Dependence of the Carrier Life Time on the Level Spacing in Semiconductor Quantum Dots. *Journal of the Korean Physical Society*. 2005;47(2):328-330.
2. György E, Pérez del Pino A, Roqueta J, Ballesteros B, Miguel AS, Maycock C et al. Synthesis and characterization of CdSe/ZnS core-shell quantum dots immobilized on solid substrates through laser irradiation. *Physica Status Solidi A*. 2012;209(11):2201-2207.
3. Soni U, Arora V, Singh G, Hussain M, Sapra S. Synthesis of core-Shell Quantum Dots and their Potential Application. Advanced Nanomaterials and Nanotechnology. *Springer Proceedings in Physics*. 2013;143:85-93.
4. Song KK, Lee S. Highly luminescent (ZnSe)ZnS core-shell quantum dots for blue to UV emission: synthesis and characterization. *Current Applied Physics*. 2001;1(2-3):169-173.
5. Bimberg D. Quantum dots: Paradigm changes in semiconductor physics. *Semiconductor*. 1999;33(9):951-955.
6. Vivas-Moreno JJ, Porras-Montenegro N. The Effects of Quantum Confinement and Magnetic Fields on the Binding Energy of Hydrogenic Impurities in low-Dimensional Systems. *Physica Status Solidi B*. 1998;210(2):723-729.
7. Goswami B, Pal S, Sarkar P. A Theoretical Study on the Electronic Structure of ZnSe/ZnS and ZnS/ZnSe Core/Shell Nanoparticles. *Journal of Physical Chemistry C*. 2008;112(31):11630-11636.
8. Lad AD, Mahamuni S. Effect of ZnS shell formation on the confined energy levels of ZnSe quantum dots. *Physics Review B*. 2008;78(12):125421.
9. Callan JF, Raymo FM, eds. *Quantum Dot Sensors*. Singapore: Pan Stanford Publishing; 2013.
10. Sen P, Chattopadhyay S, Andrews JT, Sen PK. Impact of shell thickness on exciton and biexciton binding energies of ZnSe/ZnS core-shell quantum dot. *Journal of Physics and Chemistry of Solids*. 2010;71(9):1201-1205.
11. Ghatak A, Lokanathan S. *Quantum Mechanics: Theory and Applications*. 5thed. New Delhi: Macmillan India; 2004.
12. Nikesh VV, Mahamuni S. Highly photoluminescent ZnSe/ZnS quantum dots. *Semiconductor Science and Technology*. 2001;16(8):687-690.
13. Marple DTF. Refractive Index of ZnSe, ZnTe and CdTe. *Journal of Applied Physics*. 1964;35(3):539-541.
14. Berger LI. *Semiconductor Materials*. Boca Raton: CRC Press; 1997.
15. Kim S, Fisher B, Eisler HJ, Bawendi M. Type-II Quantum Dots: CdTe/CdSe (Core/Shell) and CdSe/ZnTe (Core/Shell) Heterostructures. *Journal of the American Chemical Society*. 2003;125(38):11466-11467.
16. Bird JP. *Electron Transport in Quantum Dots*. New York: Springer Science;2003.