American Journal of Nano Research and Applications
2017; 5(3): 32-36
http://www.sciencepublishinggroup.com/j/nano
doi: 10.11648/j.nano.20170503.11

The Energy Levels Splitting Calculated for the Heavy and Light Holes in a $Cd_{1-x}Zn_xS$ Double Quantum Dot

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To cite this article:

Zoubeida Khéfacha, Nabil Safta, Mohamed Dachraoui. The Energy Levels Splitting Calculated for the Heavy and Light Holes in a $Cd_{1-x}Zn_xS$ Double Quantum Dot. *American Journal of Nano Research and Applications*. Vol. 5, No. 3, 2017, pp. 32-36.
doi: 10.11648/j.nano.20170503.11

Received: March 23, 2017; **Accepted**: April 19, 2017; **Published**: June 14, 2017

Abstract: This work reports on a theoretical investigation of a double $Cd_{1-x}Zn_xS$ quantum dot embedded in an insulating material.The quantum dots are assumed to have a flattened cylindrical geometry with a finite barrier at the boundary.The energy levels splitting has been computed, using the tight binding approximation, in the case of the heavy and light holes, as a function of zinc composition for different inter-quantum dot separations. An analysis of the results shows that, for the light holes, the coupling is maximum when x=0.8. Moreover, it has been demonstrated the strong localization character of the heavy holes in this nanostructure.

Keywords: Double Quantum Dot, $Cd_{1-x}Zn_xS$, Heavy and Light Holes, Tight Binding Approximation, Non Volatile Memories

1. Introduction

In the last decades, the high potentialities of $Cd_{1-x}Zn_xS$ films do not cease to be proved in many useful devices [1-3]. This is principally due to their utility as window materials in heterojunction solar cells with a p-type absorber such as $CuInSe_2$, $CuIn_xGa_{1-x}Se_2$ or $CuSnS_z$ Se_{1-z} [4-9].

Concerning $Cd_{1-x}Zn_xS$ quantum dots (QDs), their considerable advantage has been demonstrated in both fundamental and applied research [10-24].

From a fundamental view point, $Cd_{1-x}Zn_xS$ QDs have particular properties like size quantization, zero – dimensional electronic states, non linear optical behaviour, coupling between QDs etc [10-20].

In technological applications, $Cd_{1-x}Zn_xS$ QDs are of great importance as well. We can evoke red-light-emitting diodes (LEDs) fabricated using CdSe/ $Cd_{1-x}Zn_xS$ quantum dots (QDs) [21], blue (~440 nm) liquid laser with an ultra-low threshold achieved by engineering unconventional ternary CdZnS/ZnS alloyed-core/shell QDs [22] and fluorescent CdS QDs utilized for the direct detection of fusion proteins [23]. Furthermore, $Cd_{1-x}Zn_xS$ QDs have become one of the most promising materials in solar cell area [24]. In this context, our actual defy is to use $Cd_{1-x}Zn_xS$ QDs grown on nominal and vicinal Si surfaces [25-27] in order to find adequate structures for novel nanodevices such as the non - volatile memories.

Concerning the growth of $Cd_{1-x}Zn_xS$ QDs, there are several methods like the inverted micelles [28], the selective area – growth technique [29], the single source molecular. precursors [30], the colloidal method [31] and the Sol gel technique [4].

To describe the $Cd_{1-x}Zn_xS$ QDs, we have considered, on a one hand, the spherical geometry and two types of potentials, a potential with an infinite barrier [32] and a potential with a finite barrier at the boundary[33, 34].

For the first case [32], by taking account on the excitonic binding energy, we have calculated the band gap energy as a function of radius. The obtained results showed a good agreement with several experimental data.

For the second case [33, 34], by restricting the study to the ground state for both electrons and holes, we have calculated, in a first step, the shape of the confinement potentials, the

quantized energies, their related envelope wave – functions and the QDs sizes [33]. In addition, we have computed the binding energy of bound excitons and the oscillator strength of interband transitions as well [33]. We have calculated, in a second step, for both electrons and holes, the excited bound states [34]. All these calculations have been made versus the zinc composition.

Nevertheless, the spherical geometry does not lend simply to calculate the band edges of coupled QDs, especially along different quantization directions. Thus, we have suggested, on another hand, the flattened cylindrical geometry with a finite potential barrier at the boundary [35-45]. Using this model, we have investigated, in a first step, the electronic properties of a single $Cd_{1-x}Zn_xS$ quantum dot [35]. More precisely, we have calculated the shape of the confining potential, the subband energies and their eigen envelope wave functions.

We have studied, in a second step, the electronic properties of the super lattices based on $Cd_{1-x}Zn_xS$ embedded in an insulating material with use of several potential models and different methods (Kronig – Penney method, sinusoidal and triangular potentials, Tight Binding approximation…) [36-43]. Thus, our interest has especially been focused on the computation of the ground miniband width and the longitudinal effective mass for the carriers.

On the other hand, we have recently studied the coupling effect in the case of a double $Cd_{1-x}Zn_xS$ quantum dot embedded in an insulating material. More precisely, our interest has been focused on the investigation of the energy levels splitting in the case of electrons. This study has evidenced that for intermediate zinc compositions (x = 0.4 – 0.6) the coupling between QDs is maximum [45].

The purpose of the present work is to extend the last study to the heavy and light holes. The paper is organized as follows: after an introduction, we present the modeling, the obtained results and discussions. The conclusion derived from this study is presented in the last section.

2. Modeling

The system under investigation is a double $Cd_{1-x}Zn_xS$ quantum dot (DQD) inserted in an insulating material. Every QD is assumed to have a flattened cylindrical geometry of height L in such a way that the quantum confinement along transversal directions can be ignored. The inter-QD separation is labeled d. Fig. 1. a represents the geometry used to describe this system. The common confined direction is denoted by z. Here, the $Cd_{1-x}Zn_xS$ flattened cylinders QDs behave as wells of width L while the host dielectric lattice corresponds to a barrier with a height U_0. For sake of simplicity, the electron and hole states are assumed to be uncorrelated. The problem to solve is, then, reduced to those of one particle in a one dimensional potential. In this work, we adopt the potential $V(z)$ depicted in Fig. 1. b.

For this potential, the electron and hole states can be calculated using the effective Hamiltonian:

$$H_{e,h} = \frac{-\hbar^2}{2m^*_{e,h}}\frac{d^2}{dz^2_{e,h}} + V_{e,h}\left(z_{e,h}\right) \quad (1)$$

where $\hbar$ is the Plank's constant and m^* is the effective mass of carriers. The subscripts e and h refer to electrons and holes respectively. In deriving the Hamiltonian $H_{e,h}$, we have considered the effective mass theory (EMT) and the band parabolicity approximation (BPA). The difference of the effective mass between the well and the barrier has been disregarded.

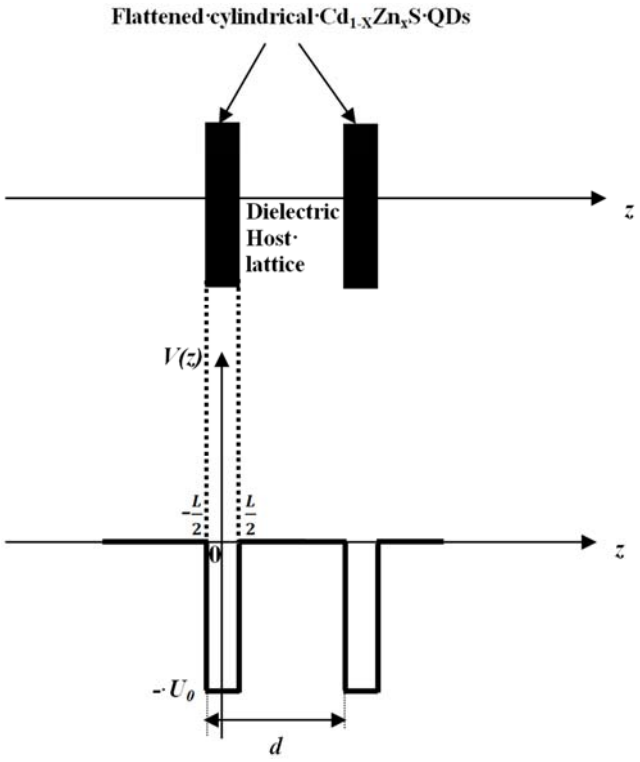

Figure 1. *(a)A schematic diagram of a double $Cd_{1-x}Zn_xS$ QD according to the flattened cylindrical geometry–(b) The potential used in this work.*

We have resolved the Schrodinger equation using the Tight Binding Approximation. Our interest is focused on the energy levels splitting in the case of the ground state. This parameter will be noted $\Delta E_{e,h}$. If we neglect the wave function overlap, our calculation shows that:

$$\Delta E_{e,h} = 2\beta_{e,h}$$

where

$$\beta_{e,h} = -\frac{2U_{0e,h}\,A_{e,h}B_{e,h}\,e^{-\rho_{e,h}\left(d-\frac{L}{2}\right)}}{\rho_{e,h}^{\,2}+k_{e,h}^{\,2}}\left(\rho_{e,h}\cos\left(\frac{k_{e,h}L}{2}\right)sh\left(\frac{\rho_{e,h}L}{2}\right)+k_{e,h}\sin\left(\frac{k_{e,h}L}{2}\right)ch\left(\frac{\rho_{e,h}L}{2}\right)\right)$$

with

$$A_{e,h} = \left[\frac{L}{2} + \frac{\cos^2\left(\frac{k_{e,h}L}{2}\right)}{\rho_{e,h}} + \frac{\sin\left(k_{e,h}L\right)}{2k_{e,h}} \right]^{-\frac{1}{2}}$$

$$B_{e,h} = A_{e,h}\cos\left(\frac{k_{e,h}L}{2}\right)$$

$$k_{e,h} = \sqrt{\frac{2m^*_{e,h}E_{1e,h}}{\hbar^2}}; \quad \rho_{e,h} = \sqrt{\frac{2m^*_{e,h}\left(U_{0e,h} - E_{1e,h}\right)}{\hbar^2}}$$

E_1 corresponds to the ground state energy associated with an isolated flattened cylindrical quantum dot of $Cd_{1-x}Zn_xS$. E_1 is calculated in such a way that the zero energy is taken at the bottom of the QD well.

3. Results and Discussion

We have computed, for the heavy holes and light holes, the energy levels splitting as a function of the ZnS molar fraction, for inter quantum dot separations going from d = 1.5 nm to d= 2.5 nm. Values of parameters used in this computation are summarized in Table 1. All these parameters are taken from the Ref [35]. Values of the effective masses of the heavy and light holes for $Cd_{1-x}Zn_xS$ with different Zn compositions have been deduced using the Vegard's law.

Table 1. *Parameters used to calculate the energy levels splitting in the case of the heavy and light holes for a double $Cd_{1-x}Zn_xS$ QD.(m_0 is the free electron mass).*

x	$\frac{m^*_{hh}}{m_0}$	$\frac{m^*_{lh}}{m_0}$	U_{0h}(eV)	L(nm)	E_{1hh}(eV)	E_{1lh}(eV)
0.0	5.00	0.70	0.25	1.00	0.040	0.129
0.2			0.25	1.00	0.049	0.136
0.4			0.50	1.00	0.060	0.216
0.6			0.50	1.00	0.070	0.238
0.8			0.50	1.00	0.083	0.266
1.0	1.76	0.23	2.00	1.00	0.145	0.538

Typical results are reported in Table 2 and Table 3.

Concerning the light holes, this study showed: (i) ΔE_{lh} decreases when d increases independently of the Zn composition. Consequently, the coupling decreases with the inter – quantum dot separation (ii) for $Cd_{1-x}Zn_xS$ QDs with x = 0; 0.2 and 0.4, ΔE_{lh} is low especially when d is high. Thus, the coupling is weak at high values of d (iii) for x = 0.8, ΔE_{lh} is maximum for all the inter-quantum dot separations studied. In this case, the coupling between the QDs is highest. These results are probably due to the barrier potential height U_{0h}, the bulk effective mass m^*_{lh} and the energy E_{1lh} values (iv) For $Cd_{1-x}Zn_xS$ QDs with x = 0.6, the magnitude order of ΔE_{lh} is not far from the one of x = 0.8(v) concerning x = 1.0, ΔE_{lh} significantly declines as a function of the inter – quantum dot separation.

As for the heavy holes, we can make the following observations: (i) The energy levels splitting decreases with d for all the compositions studied,

(ii) ΔE_{hh} is very low in all the cases studied.

These results can be explained in terms of the effective mass. Indeed, there is a large difference between the light hole and heavy hole effective masses in CdS, ZnS and in their alloys.

This reflects the strong localization character of the heavy holes for all the inter – quantum dot separations and independently to the composition.

Table 2. *The energy levels splitting (10^{-3} eV), as calculated for the heavy holes versus the zinc composition for different inter-QD separations.*

d(nm)	1.5	1.7	1.9	2.1	2.3	2.5
x						
0.0	2.732	0.957	0.185	0.117	0.041	0.144
0.2	3.814	1.529	0.585	2.253	0.086	0.033
0.4	1.798	0.486	0.131	0.035	0.096	0.002
0.6	3.266	1.010	3.124	0.096	0.029	0.009
0.8	8.155	2.156	0.773	0.277	0.099	0.035
1.0	0.943	0.014	0.023	0.018	0.001	0.001

Table 3. *The energy levels splitting (eV), as calculated for the light holes versus the zinc composition for different inter-QD separations.*

d(nm)	1.5	1.7	1.9	2.1	2.3	2.5
x						
0.0	0.067	0.050	0.035	0.027	0.020	0.015
0.2	0.095	0.057	0.044	0.033	0.026	0.019
0.4	0.093	0.063	0.042	0.029	0.019	0.013
0.6	0.118	0.087	0.585	0.041	0.029	0.021
0.8	0.156	0.108	0.082	0.061	0.045	0.035
1.0	0.150	0.086	0.047	0.026	0.014	0.008

The comparison with results obtained for electrons [45] shows that the ΔE_{lh} values are not far from those of electrons (Table 4).

Table 4. *The energy levels splitting (eV), as calculated for the electrons versus the zinc composition for different inter-QD separations[41].*

d(nm)	1.5	1.7	1.9	2.1	2.3	2.5
x						
0.0	0.023	0.027	0.026	0.025	0.024	0.023
0.2	0.105	0.094	0.084	0.075	0.067	0.060
0.4	0.176	0.145	0.121	0.100	0.083	0.069
0.6	0.203	0.151	0.112	0.083	0.061	0.045
0.8	0.172	0.104	0.062	0.038	0.022	0.013
1.0	0.120	0.063	0.032	0.017	0.085	0.004

4. Conclusion

We studied the coupling in a double quantum dot made by $Cd_{1-x}Zn_xS$. To describe the QDs, we have suggested the flattened cylindrical geometry with a finite potential barrier at the boundary. Using the Tight Binding Approximation, we

have computed for the heavy and light holes the energy levels splitting. Calculations have been made as a function of Zn composition for different inter – quantum dot separations.

An analysis of the obtained results has showed that, for the light holes, the Zn composition x = 0.8 is appropriate to ensure the maximum of coupling between QDs. As for the heavy holes, the results indicated the strong localization character of theses carriers in all the cases studied.

In the applied physics, this study is of a great interest for designing novel devices based on $Cd_{1-x}Zn_xS$ QDs particularly the non – volatile memories.

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