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The Energy Levels Splitting Calculated for Electrons in a Double $Cd_{1-X}Zn_xs$ Quantum Dot

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Abstract. The present work is aimed to investigate theoretically the electronic properties 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. This system is studied using the tight binding approximation. The energy levels splitting has been computed, for the electrons, versus the Zn composition and the inter-quantum dot separation as well. An analysis of the results shows that the Zn compositions $x = 0.4$ and $x = 0.6$ are appropriate to ensure the best coupling for conduction electrons.

Keywords: Quantum dots, $Cd_{1-x}Zn_xS$, energy levels splitting, nanodevices.

1 Introduction

Since several decades, films of $Cd_{1-x}Zn_xS$ have been widely applied in many useful devices particularly as window materials for fabricating p-n junctions [1-10]. On the subject of $Cd_{1-x}Zn_xS$ quantum dots (QDs), their technological potentialities have been demonstrated. In this context, we can cite red-light-emitting diodes (LEDs) fabricated using CdSe/$Cd_{1-x}Zn_xS$ quantum dots (QDs)[11], blue liquid laser with an ultra-low threshold achieved by engineering unconventional ternary CdZnS/ZnS alloyed-core/shell QDs [12], fluorescent CdS QDs used for the direct detection of fusion proteins [13] and most promising materials in solar cell fabrication [14]. Our actual challenge is to use $Cd_{1-x}Zn_xS$ QDs grown on nominal and vicinal Si surfaces [15-17] in order to obtain reliable structures for novel nanotechnological applications such as nanomemories, nanolasers and nanodevices.

From a fundamental view point, to study the electronic properties of $Cd_{1-x}Zn_xS$ QDs, we have adopted, on the one hand, the spherical geometry and proposed to describe the potential energy, a potential with an infinite barrier [18] and a potential with a finite barrier at the boundary [19, 20]. The latter potential has the advantage to consider the coupling between QDs and opens a new way to use nanostructures involving tunneling-coupled $Cd_{1-x}Zn_xS$ QDs as an active element for nanodevices. But, the coupling study within the spherical geometry model is difficult. Consequently, we have proposed, on the other hand, the flattened cylindrical geometry with a finite potential barrier at the boundary to describe the QDs [21-31]. Particularly, we have studied the electronic properties of several structures based on $Cd_{1-x}Zn_xS$ such as the super lattices embedded in an insulating material [23-30].

The objective of this work is to study 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. Calculations have been carried as a function of the inter-QD separation for different Zn compositions. The paper is organized as follows: after an introduction, we report an outline on the modeling as well as the obtained results. 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. 1a depicts 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 correspond to wells of width L whereas the host dielectric lattice forms a barrier with a height U_0. For sake of simplicity, the electron and hole states are supposed to be uncorrelated. The problem to solve is, then, reduced to those of one particle in a one dimensional potential. In this work, we consider the potential $V(z)$ depicted in Fig. 1b.

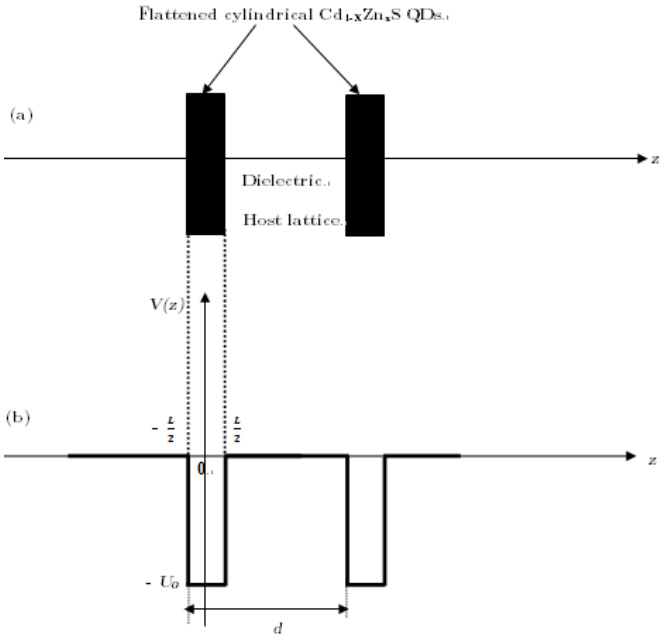

Figure 1. (a) A schematic diagram of $Cd_{1-x}Zn_xS$ QDs according to the flattened cylindrical geometry. (b) The potential V(z).

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

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

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.

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 as $\Delta E_{e,h}$. 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

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

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

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

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

By restricting this study to the electrons, we have computed the energy levels splitting as a function of the zinc composition, 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 Ref [21]. Values of the electron effective mass 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 for $Cd_{1-x}Zn_xS$ nanostructures.(m_0 is the free electron mass)

x	$\frac{m^*_e}{m_0}$	U_{0e}(eV)	L(nm)	$E_{1e}\left(\text{eV}\right)$
0.0	0.16	0.10	1.0	0.090
0.2		0.25	1.0	0.187
0.4		0.45	1.0	0.292
0.6		0.75	1.0	0.384
0.8		1.50	1.0	0.531
1.0	0.28	2.00	1.0	0.560

Typical results are depicted in Table 2. The analysis of the obtained results showed: (i) ΔE_e decreases as a function of d for all the compositions studied. Consequently, the coupling between QDs decreases as the inter – quantum dot separation increases. (ii) Concerning $x = 0$, ΔE_e is very low for all the inter – QD separations considered. In this case, $Cd_{1-x}Zn_xS$ QDs can be supposed as isolated, (iii) For $x = 0.2$, ΔE_e presents a small decline with d. The coupling between QDs remains low, (iv) For intermediate zinc compositions ($x = 0.4 - 0.6$), the order of magnitude of ΔE_e is important independently of the inter-quantum dot separation. In this composition range, the coupling between QDs is maximum. These results are, most probably, related to the barrier potential height U_{0e} and the energy E_{1e} values. Indeed, for all Zn compositions, the well width L being identical and the bulk effective mass m^*_e is practically the same. (v) For high zinc compositions ($x = 0.8 - 1.0$), the coupling decreases as the inter – quantum dot separation increases. For these compositions, the coupling between QDs is nearly absent at high d values.

Table 2. The energy levels splitting (eV) as calculated for electrons 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	0.028	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	0.147	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	0.008	0.004

4 Conclusion

We studied the coupling for a double $Cd_{1-x}Zn_xS$ quantum dot embedded in an insulating material. 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 calculated, for electrons, 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 evidenced that for intermediate zinc compositions ($x = 0.4 – 0.6$) the coupling between QDs is maximum. In the applied physics, this study opens a new way for designing nanodevices based on well controlled $Cd_{1-x}Zn_xS$ QDs.

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