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The Electronic Band Parameters Calculated by a Novel Potential Model for $Cd_{1-x}Zn_xS$ Quantum Dot Super lattices

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Abstract

In this paper, our interest is focused on a theoretical investigation of chains based on $Cd_{1-x}Zn_xS$ quantum dots inserted in an insulating material. This system, supposed as a succession of flattened cylindrical quantum dots with a finite barrier height at the boundary, is treated with use a novel potential model. The super lattice band structure, the electron effective mass of the fundamental mini band and the coupling have been studied versus the inter-quantum dot separation for different zinc contents. The obtained results showed that the CdS system is the most adapted to have a super lattice behavior. Moreover, this study is of a great interest and can be considered as a helpful support for designing a new class of devices.

Keywords: Quantum dots, super lattices, $Cd_{1-x}Zn_xS$, novel potential model, non volatile memories.

Introduction

Films of $Cd_{1-x}Zn_xS$ are technologically useful materials[1-10]. This is due to the fact that $Cd_{1-x}Zn_xS$ plays the role of a window material in hetero junction solar cells[11]. $Cd_{1-x}Zn_xS$ is also used in devices based on quaternary compounds such as $CuIn_xGa_{1-x}Se_2$ or $CuSnS_zSe_{1-z}$ [12].

On the subject of $Cd_{1-x}Zn_xS$ quantum dots (QDs), their interest has been demonstrated in both fundamental and applied research. Concerning the technological applications of $Cd_{1-x}Zn_xS$ QDs, we can cite light-emitting diodes (LEDs) based on CdSe/ $Cd_{1-x}Zn_xS$ QDs [13], liquid laser achieved by CdZnS/ZnS alloyed-core/shell QDs [14], fluorescent CdS QDs [15] and low-threshold Optical Gain in CdSe/CdS QDs[16]. Recently, $Cd_{1-x}Zn_xS$ QDs become as one of the most promising materials in solar cell production [17].

As for the fundamental view point, the first works made on the $Cd_{1-x}Zn_xS$ QDs considered the spherical geometry and an infinite potential model[11, 18-20]. The following studies have used the spherical geometry with a finite potential to model the $Cd_{1-x}Zn_xS$ QDs [21, 22]. Nevertheless, the spherical geometry model is extremely complicated to study the coupling between the QDs. In order to around this problem, the flattened cylindrical geometry with a finite potential model has been suggested [23-30]. In particular, the interest has been focused on the study of the electronic band parameters of super lattices based on $Cd_{1-x}Zn_xS$ quantum dots inserted in a dielectric matrix. For this purpose, several potential models and different methods (Kronig – Penney method, sinusoidal and triangular potentials, Tight Binding approximation) have been proposed[25-30].

The objective of this work is to study the electronic properties of super lattices prepared by $Cd_{1-x}Zn_xS$ QDs with a flattened cylindrical geometry and a finite potential barrier at the boundary. Calculations have been carried out versus Zn composition using a novel potential model. The paper is structured as follows: the introduction is given in the first section. Methodology, results and discussion are reported in the following. Conclusion is presented at the end.

Methodology

In a practical depiction, $Cd_{1-x}Zn_xS$ QDs inserted in an insulating material have a spherical geometry. Figure- 1- a shows a chain of $Cd_{1-x}Zn_xS$ QDs. The common confined direction is denoted by z. The inter-quantum dot separation is written off as d. Along a common direction of spherical $Cd_{1-x}Zn_xS$ QDs, one can remark that electrons and holes perceive a series of flattened cylinders of radius R and effective height L. According to that reported by B. Battacharjee et al.[11] and N. Safta et al. [23], the diameter D = 2 R varies from 9 nm to 4 nm for $Cd_{1-x}Zn_xS$ QDs and the height L is equal to 1 nm. Thus, D is higher than L and the quantum confinement along transversal directions can be ignored. Consequently, the $Cd_{1-x}Zn_xS$ system under investigation can be regarded as a QDs super lattice along the z direction. In another words, the system to study is a $Cd_{1-x}Zn_xS$ QD super lattice in such a way that the $Cd_{1-x}Zn_xS$ flattened cylinders QDs are associated with wells while the host dielectric lattice corresponds to a barrier of height U_0. Here, we neglect the electron - hole interaction. Thus, we have to solve the problem of one particle. In this work, we consider the one dimensional potential depicted in figure-1- b. The mathematical formula of this potential is:

$$V(z) = U_0\sqrt{\left|\cos\left(\frac{\pi z}{d}\right)\right|} \quad (1)$$

More precisely, we have to solve the following Hamiltonian:

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

Here, the subscripts e and h are associated with electrons and holes respectively, $m^*_{e,h}$ is the effective mass. The Hamiltonian $H_{e,h}$ is established within the effective mass theory (EMT) and the band parabolicity approximation (BPA). Moreover, the effective mass is considered the same in the well and in the barrier.

Results and Discussion

In a first step, we have computed, for electrons, the longitudinal dispersion relations which are the plots of eigen energies versus the k_z wave vector component. Values of parameters utilized in this computation are reported in Table-1. These parameters are given by N. Safta et al.[23]. The effective masses for different compositions have been calculated by the Vegard's law.

Table-1
Parameters used in the computation of the electron longitudinal dispersion relations for $Cd_{1-x}Zn_xS$ QD super lattices (m_0 is the free electron mass)

x	$\frac{m^*_e}{m_0}$	U_{0e}(eV)
0.0	0.16	0.10
0.2		0.25
0.4		0.45
0.6		0.75
0.8		1.50
1.0	0.28	2.00

Figure-2 and figure-3 depict the super lattice band structure in the cases of CdS and ZnS for d=1.5 and 2.5 nm. As can be deduced from the plots, the dispersion of the fundamental mini band (Γ_1 -mini band) is inferior to those of the excited mini bands for CdS and ZnS systems. An identical trend has been observed for all the zinc compositions. On the other hand, the dispersion of each mini band is found to decrease considerably with x and d separately.

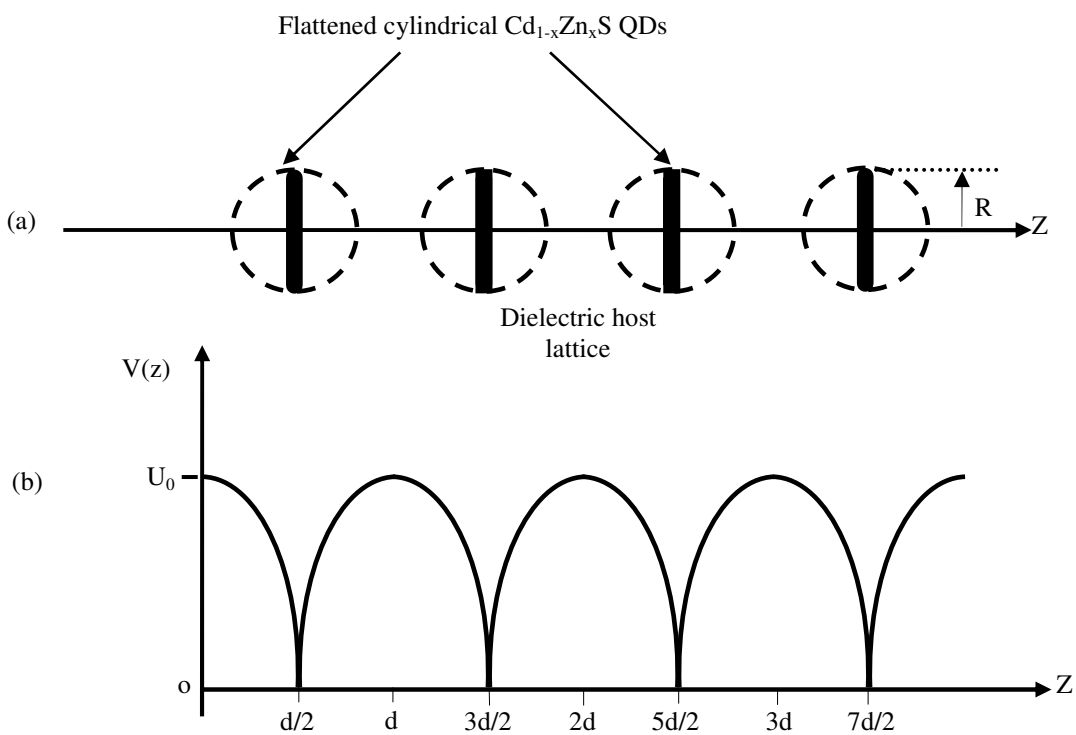

Figure-1
(a) A schematic diagram of $Cd_{1-x}Zn_xS$ QD chains – (b) The plot of the novel potential model

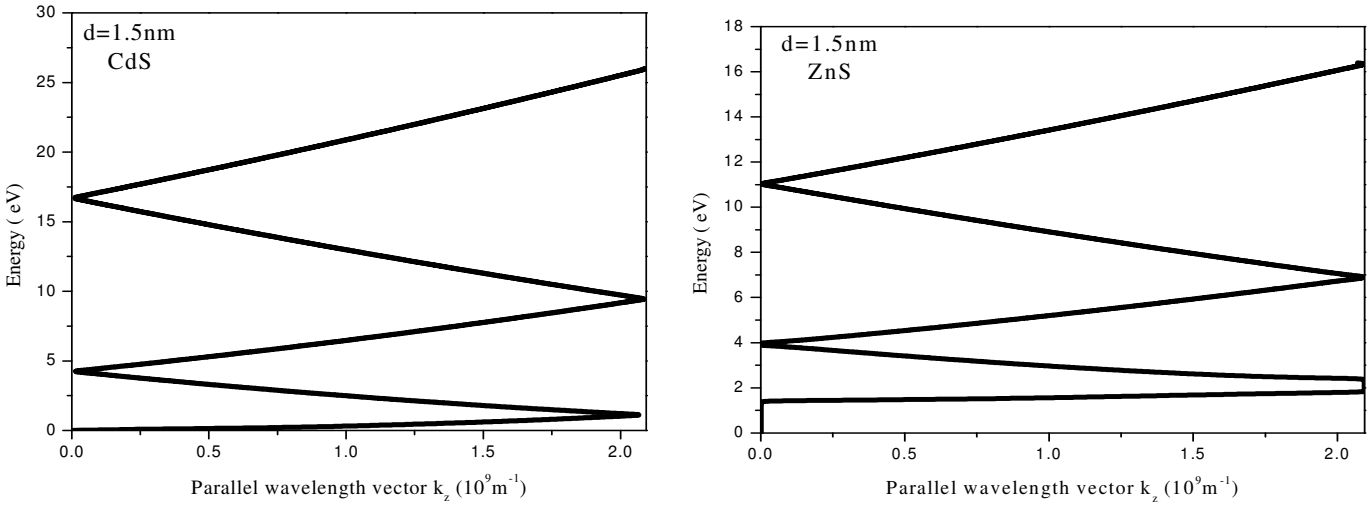

Figure-2
The super lattice band structure for CdS and ZnS QD systems in the case of d = 1.5 nm

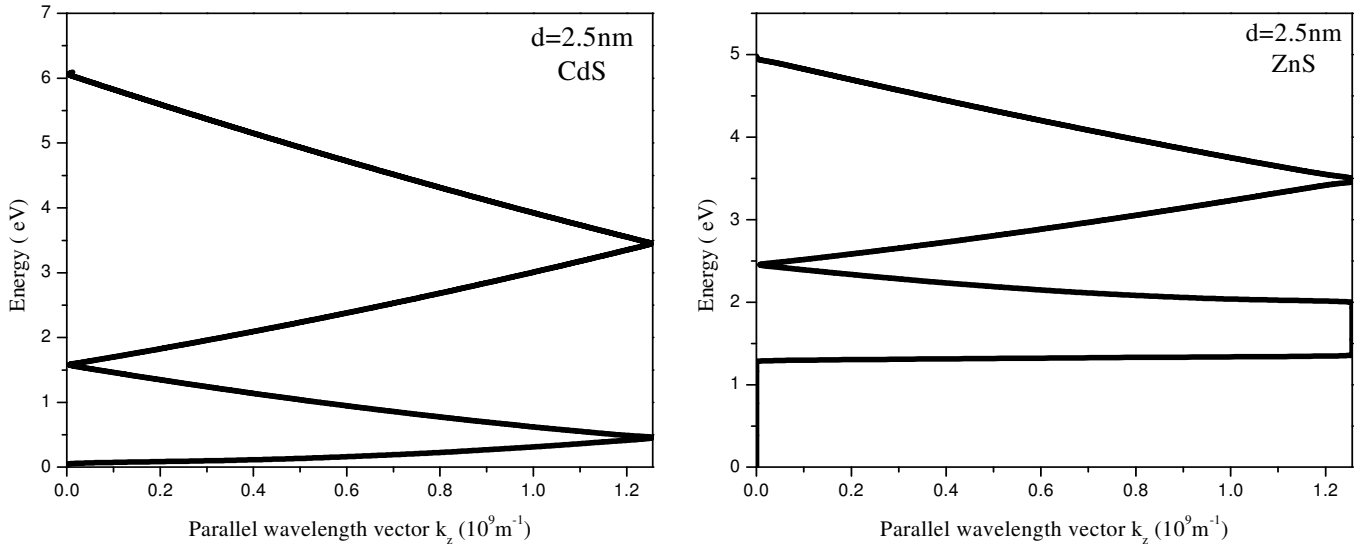

Figure-3
The super lattice band structure for CdS and ZnS QD systems in the case of d = 2.5 nm

From the Γ_1 -mini band dispersion curve, we can deduce the longitudinal electron effective mass m^*_{e,Γ_1} for the $Cd_{1-x}Zn_xS$ QDs studied. In fact, we consider this curve at the neighborhood of the minima. The longitudinal effective mass has been deduced from the second derivative of the band energy as a function of the wave vector k_z. Typical results are reported in Table-2. The fit of the calculated Γ_1 - mini band versus the inter-QD separation for different Zn compositions is presented in Table-3. One can observe that, for all the inter-QD separation, m^*_{e,Γ_1} increases as a function of x. This result can be explained in terms of the barrier potential height U_{0e} which is found to increase with x [23]. For $Cd_{1-x}Zn_xS$ QDs with low zinc compositions, m^*_{e,Γ_1} is weak. Moreover, this parameter is, practically, not affected by the super lattice (SL) period d. The electron mobility is significant in this composition range. For intermediate zinc contents, m^*_{e,Γ_1} slowly varies with the (SL) period. As a consequence, the electron mobility in SL QD $Cd_{1-x}Zn_xS$ systems becomes weaker for large inter - QD separations. However, for high zinc compositions, the magnitude order of the electron mobility is low especially when the inter-QD separation is high. In this case, the super lattice behavior is nearly absent.

Table-2

The longitudinal electron effective masses $\frac{m^*_{e,r1}}{m_0}$ versus the inter -QD separation for $Cd_{1-x}Zn_xS$ QD super lattices

d (nm) x	1.5	1.7	1.9	2.1	2.3	2.5
0.0	0.2890	0.2893	0.2896	0.3105	0.3107	0.3117
0.2	0. 3157	0.3175	0.3180	0.3220	0.3235	0.3377
0.4	0.3350	0.3398	0.4439	0.4494	0.4545	0.4749
0.6	0.3592	0.3704	0.5761	0.5783	0.5881	0.5932
0.8	0.3649	0.3992	0.7676	0.7998	0.8522	0.9582
1.0	0.4696	0.5959	0.8135	1.1533	1.6756	2.0833

Table-3

The fit of the calculated Γ_{1e} - mini band as a function of the inter-QD separation for different Zn compositions

Zinc composition x	Γ_{1e} - mini band
0.0	$1.341-1.400d+0.542d^2-0.074d^3$
0.2	$1.098-1.108d+0.414d^2-0.054d^3$
0.4	$1.080-1.150d+0.452d^2-0.062d^3$
0.6	$0.964-1.030d+0.407d^2-0.056d^3$
0.8	$0.798-0.807d+0.304d^2-0.040d^3$
1.0	$0.697-0.681d+0.243d^2-0.030d^3$

From the longitudinal dispersion relation curve, one can obtain the Γ_1 - mini band width ΔE_{1e}. Thus, we have calculated this parameter for all the compositions and super lattice periods studied. Typical results are illustrated in figure-4. One can deduce: (i) for any composition x, ΔE_{1e} decreases as a function of the inter-QD separation d. (ii) The Γ_1 - mini band width decreases with the composition x for all the super lattice periods. Besides, for $Cd_{1-x}Zn_xS$ QDs with low zinc contents, ΔE_{1e} is important and reflects the high coupling between the QDs. At high zinc compositions, ΔE_{1e} is lesser and the QDs are nearly isolated. On the other hand, the difference between the Γ_1 - mini band widths for CdS QDs is of 0.091eV whereas those for the ZnS QDs is equal to 0.032 eV. For the other compositions, this difference takes intermediate values.

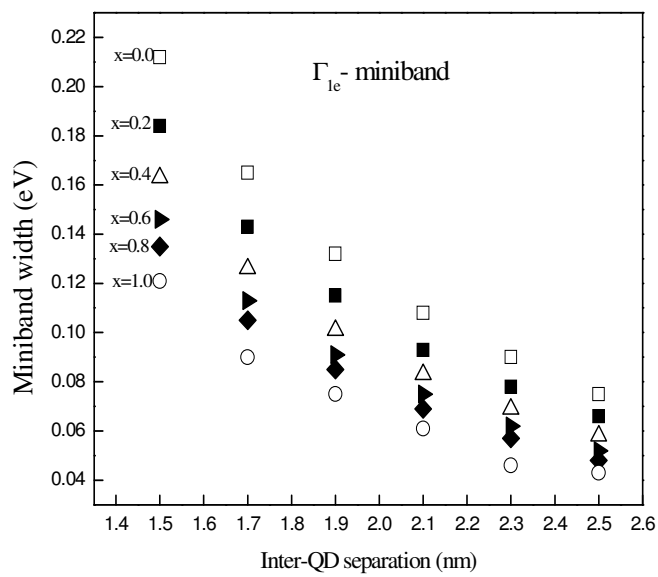

Figure-4

The Γ_1 -mini band width, for electrons, as a function of the inter-QD separation for different zinc compositions

Let us now compare these results with those found by using the sinusoidal potential given by A. Sakly et al. [26] and expressed as: $V(z)=\frac{U_0}{2}\left(\cos\frac{2\pi\pi}{d}+1\right)$. We report in table-4, widths of Γ_1 - mini band associated with this work and those obtained by A. Sakly et al. [26]. As can be seen, practically, for all the cases studied, the mini band widths of this work are inferior. This result means that the potential used in this work accounts for the coupling less than the sinusoidal potential model suggested by A. Sakly et al. [26].

Table-4

Widths of the Γ_1 –mini band (eV) for the present work (a) and those obtained by the sinusoidal potential expressed by:

$$V(z) = \frac{U_0}{2}\left(\cos\frac{2\pi\pi}{d} + 1\right) \text{ (b)}$$

d (nm) x	1.5	1.7	1.9	2.1	2.3	2.5
0.0	0.212(a) 0.711(b)	0.165(a) 0.523(b)	0.132(a) 0.449(b)	0.108(a) 0.345(b)	0.090(a) 0.276(b)	0.075(a) 0.230(b)
0.2	0.184(a) 0.587(b)	0.143(a) 0.450(b)	0.115(a) 0.335(b	0.093(a) 0.281(b)	0.078(a) 0.226(b)	0.066(a) 0.190(b)
0.4	0.163(a) 0.511(b)	0.126(a) 0.379(b)	0.101(a) 0.292(b)	0.083(a) 0.223(b)	0.062(a) 0.178(b)	0.058(a) 0.136(b)
0.6	0.146(a) 0.420(b)	0.113(a) 0.307(b)	0.091(a) 0.230(b)	0.075(a) 0.165(b)	0.062(a) 0.120(b)	0.052(a) 0.085(b)
0.8	0.135(a) 0.229(b)	0.105(a) 0.148(b)	0.085(a) 0.091(b)	0.069(a) 0.064(b)	0.057(a) 0.044(b)	0.048(a) 0.023(b)
1.0	0.121(a) 0.162(b)	0.090(a) 0.105(b)	0.075(a) 0.055(b)	0.061(a) 0.034(b	0.046(a) 0.023(b)	0.043(a) 0.009(b)

Conclusion

The electronic band parameters of super lattices based on $Cd_{1-x}Zn_xS$ QDs implanted in an insulating material for compositions varying from CdS to ZnS have been investigated. The QDs have been described by the flattened cylindrical geometry with a finite potential barrier at the boundary. Using a novel sinusoidal potential, we have calculated, for electrons, the super lattice band structure. Calculations have been carried out versus the inter-QD separation for different Zn contents. The obtained results have shown that: i. the Γ_1 -mini band dispersion is lower than those of the excited mini bands for $Cd_{1-x}Zn_xS$ systems, ii. the electron mobility and the coupling between QDs are found to be decreasing with x and d separately, iii. the potential used in this work accounts for the coupling less than the sinusoidal potential model studied in a previous work.

In the applied physics, these nanostructures based on $Cd_{1-x}Zn_xS$ QDs could be used as basic components in a new class of devices such as the non – volatile memories.

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