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The Heavy and Light Hole properties studied by a Novel Potential Model for Cd1−xZnxS Quantum Dot Superlattices

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Abstract: This paper presents a theoretical investigation of chains based on Cd1−xZnxS quantum dots inserted in an insulating material. This system, assumed 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 fundamental mini band and the coupling between QDs, in the case of heavy and light holes, have been studied versus the inter-quantum dot separation for different zinc compositions. The obtained results showed that the ZnS system is the most appropriate to ensure the maximum of coupling. Moreover, this study is of a great interest for designing a new class of devices such as the nonvolatile memories.

Keywords: Quantum dots, super lattices, $Cd_{1-x}Zn_xS$, novel potential model, heavy and light holes, nonvolatile memories.

I. INTRODUCTION

Since several decades, the potentiality of $Cd_{1-x}Zn_xS$ Films has evidenced in many works [1-10]. This is, essentially, due to the utility of $Cd_{1-x}Zn_xS$ as a window material in hetero junction solar cells [5-6]. Concerning $Cd_{1-x}Zn_xS$ quantum dots (QDs), their interest has been demonstrated in technological applications [11-14]. In this context, our actual defy is to use $Cd_{1-x}Zn_xS$ QDs grown on nominal and vicinal Si surfaces [15-17] to find adequate structures for novel nanodevices such as the non - volatile memories.

As for the fundamental view point, we can cite our work made on the $Cd_{1-x}Zn_xS$ QDs which considered the spherical geometry and an infinite potential model [18]. Our other investigations have used the spherical geometry with a finite potential to model the $Cd_{1-x}Zn_xS$ QDs [19-20]. However, the spherical geometry model is not commode to study the coupling between the QDs. Thus, the flattened cylindrical geometry with a finite potential model has been suggested [21-32]. We have achieved several investigations concerning the electronic band parameters of super lattices based on $Cd_{1-x}Zn_xS$ quantum dots inserted in a dielectric matrix [23-29].

In this context, our interest has been focused, in a recent study, on the computation of the electronic band parameters for the electrons [29]. Calculations have been made versus the composition for different super lattice periods with use a novel potential model. The goal of the present work is to extend the last study to the heavy and light holes. The paper is presented as follows: after a brief introduction, we present the theoretical formulation, the numerical results and discussions. The conclusions are presented at the end.

II. MODELING

In a practical depiction, $Cd_{1-x}Zn_xS$ QDs inserted in an insulating material have a spherical geometry. Fig. 1- a shows a chain of $Cd_{1-x}Zn_xS$ QDs in the common confined direction denoted by z. The inter-quantum dot separation is labelled d. Along the common direction, one can easily observe 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.* [4] and N. Safta *et al.* [21], 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. Consequently, D is higher than L and the quantum confinement along transversal directions can be disregarded. Thus, the $Cd_{1-x}Zn_xS$ system under investigation can be considered as a QDs super lattice along the z direction. More precisely, the system to study is a $Cd_{1-x}Zn_xS$ QD super lattice (SL) 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 U0. In this study, we neglect the electron - hole interaction and we should solve the problem of one particle. Moreover, we consider the one-dimensional potential depicted in figure 1- b. The latter can be expressed as:

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

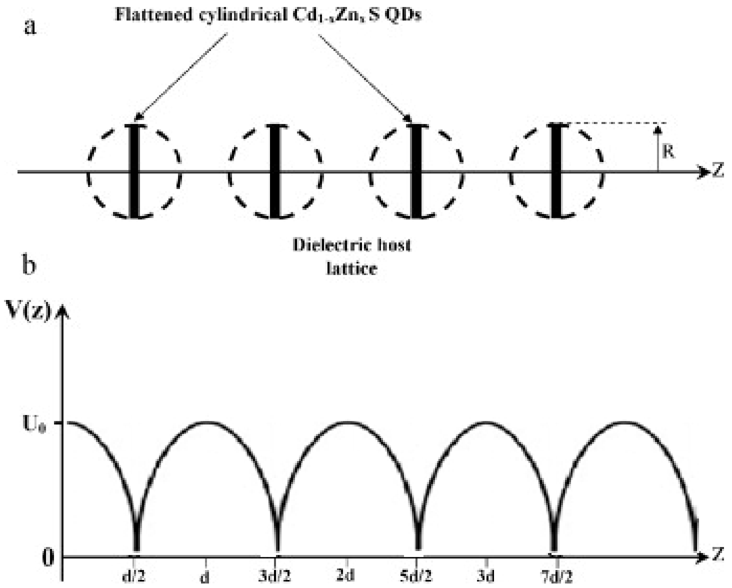

Figure-1(a): A schematic diagram of $Cd_{1-x}Zn_xS$ QD super lattices according to the flattened cylindrical geometry – (b) The barrier potential in the framework of the novel potential model.

III. RESULTS AND DISCUSSION

We have computed, for heavy and light holes, the fundamental mini band (Γ_1 -mini band). More precisely, we have determined the Γ_1 -mini band width versus the inter-quantum dot separation for different zinc compositions. Values of parameters utilized in this computation are reported in Table-1. These parameters are given by Ref [21]. The effective masses for different compositions have been calculated by the Vegard's law. Fig. 2 and Fig. 3 depict the obtained result.

Table 1. Parameters used to calculate the Γ_1 -mini band widths for heavy holes and light holes in the case of $Cd_{1-x}Zn_xS$ QD super lattices. (m0 is the free electron mass)

x	$\frac{m^*_{hh}}{m_0}$	$\frac{m^*_{lh}}{m_0}$	$U_{0h}(eV)$
0.0	5.00	0.70	0.25
0.2	--	--	0.25
0.4	--	--	0.50
0.6	--	--	0.50
0.8	--	--	0.50
1.0	1.76	0.23	2.00

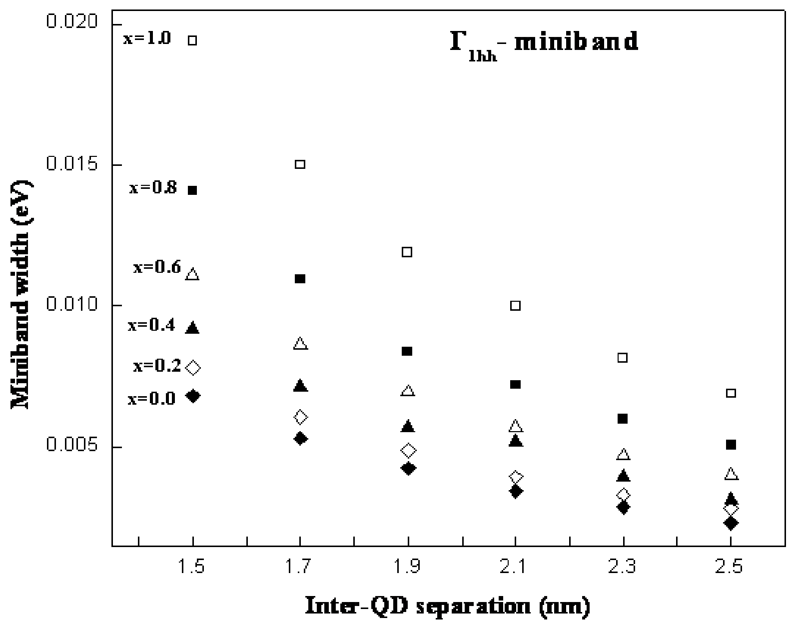

Figure 2. The Γ_1 - mini band width as calculated for the heavy holes versus the inter-QD separation for different Zn compositions.

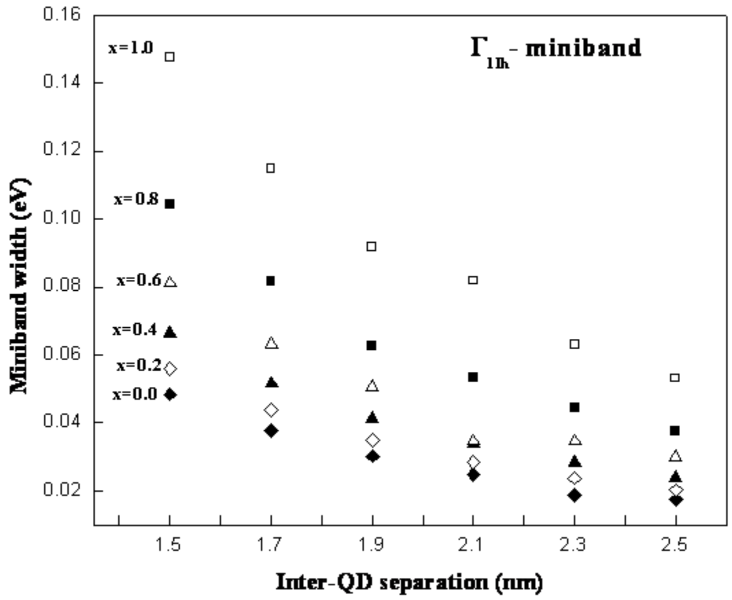

Figure 3. The Γ_1 - mini band width as calculated for the light holes versus the inter-QD separation for different Zn compositions.

Concerning the light holes, some distinctive features were revealed: (i) the miniband width ( ) shows a increasing tendency with increased zinc composition independently to the inter-QD separation. For $Cd_{1-x}Zn_xS$ QDs with high zinc contents, the order of magnitude of the width is important and reflects the strong degree of coupling between the QDs. At low zinc compositions, however, is very low (ii) for any composition x, the width of the miniband decreases with the increase of the SL period d. The difference between the miniband widths for CdS QDs is approximately equal to 3 10-2 eV while that of the ZnS-related QDs is nearly equal to of 0.1 eV. For intermediate compositions, this difference is situated between the two extreme values. About $Cd_{1-x}Zn_xS$ QDs with high zinc compositions, the coupling between QDs exhibits a significant decline as the inter – quantum dot separation increases. All these results are most probably related to the effective mass of the light holes which decreases as a function of x.

For the heavy holes, the same trend has been observed except that the miniband width (□E〗 _1hh^) remains insignificant, which denotes that the strong localization character of these carriers in the studied nanostructures is always maintained.

Let us now compare the results obtained for light holes with those found for electrons [29] (Fig. 4). As can be seen, the magnitude order of the miniband width is practically the same. Nevertheless, for electrons, this parameter decreases with the zinc composition independently to the inter-QD separation.

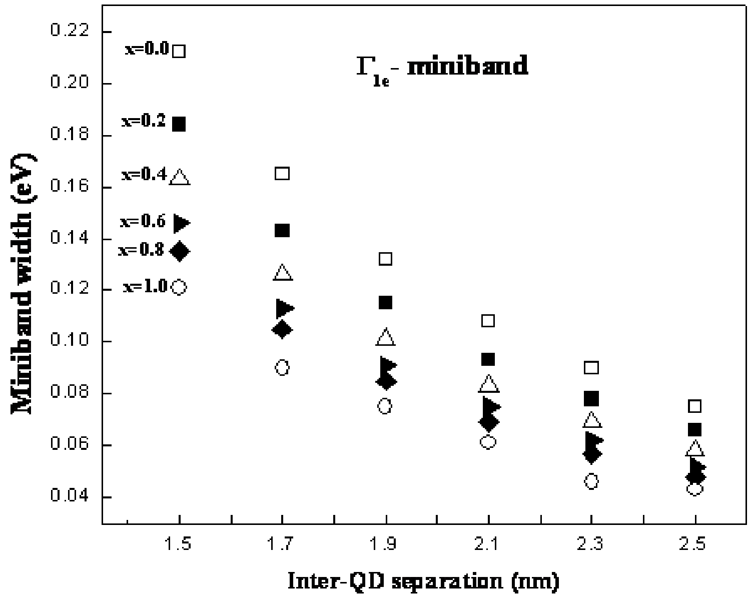

Figure 4. The Γ_1 -mini band width, as calculated for electrons versus the inter-QD separation for different zinc compositions [29].

IV. CONCLUSION

We investigated the electronic properties of super lattices based on $Cd_{1-x}Zn_xS$ embedded in a dielectric matrix. To describe the QDs, we have suggested the flattened cylindrical geometry with a finite potential barrier at the boundary. Using a novel sinusoidal potential model, we have calculated the fundamental miniband width for heavy holes and light holes. Calculations have been made as a function of inter-QD separation for different Zn composition. An analysis of the results has evidenced that (i) for these two types of carriers, the coupling between QDs is found to be increasing with x (ii) the magnitude order of the miniband width in the case of heavy holes is very low and reflects their localization nature. In the applied physics, one could use theses nanostructures as basic components in several devices, particularly the non – volatile memories.

Conflict of interest: The authors declare that they have no conflict of interest.

Ethical statement: The authors declare that they have followed ethical responsibilities.

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