Band structures of laterally coupled quantum dots, accounting for electromechanical effects

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Band structures of laterally coupled quantum dots, accounting for electromechanical effects

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Abstract. In a series of recent papers we demonstrated that coupled electro-mechanical effects can lead to pronounced contributions in band structure calculations of low dimensional semiconductor nanostructures (LDSNs) such as quantum dots, wires, and even wells. Some such effects are essentially nonlinear. Both strain and piezoelectric effects have been used as tuning parameters for the optical response of LDSNs in photonics, band gap engineering and other applications. However, these effects have been largely neglected in literature while laterally coupled quantum dots (QDs) have been studied. The superposition of electron wave functions in these QDs become important in the design of optoelectronic devices as well in tayloring properties of QDs in other applications areas. At the same time, laterally grown QDs coupled with electric and mechanical fields are becoming increasingly important in many applications of LDSN-based systems, in particular where the tunneling of electron wave function through wetting layer (WL) becomes important and the distance between the dots is treated as a tuning parameter. Indeed, as electric and elastic effects are often significant in LDSNs, it is reasonable to expect that the separation between the QDs may also be used as a tuning parameter in the application of logic devices, for example, OR gates, AND gates and others. In this contribution, by using the fully coupled model of electroelasticity, we build on our previous results while analyzing the influence of these effects on optoelectronic properties of QDs. Results are reported for III-V type semiconductors with a major focus given to GaN/AlN based QD systems.

1. Introduction

Wide band gap semiconductor materials such as AlN/GaN QDs have attracted significant attention due to their current and potential applications in optical, optoelectronic and electronic devices used in nano- and bionano- technological applications. Strongly coupled self-assembled QDs are grown either in the same wetting layer or a vertically stack of closely spaced layers. Laterally coupled QDs in the same wetting layer are of special interest because of its potential applications in QDs lasers, light emitting diodes as qubits for quantum computation and other applications [1, 2, 3]. In this work, the coupled QDs have been considered as a wurtzite structure which can be easily grown on a sapphire substrate in c-direction (0001) by any conventional method such as MBE, MOCVD and others [4, 5]. Strain is induced due to the lattice mismatch at the interfaces between two different types of semiconductors which can be used as a tuning parameter in tailoring the electronic and optical properties of single and multiple self assembled quantum dots. Atomistic approach, pseudopotential approach and tight binding formalism have been applied to investigate the optical and electronic properties of such nano-objects [6, 7, 8].

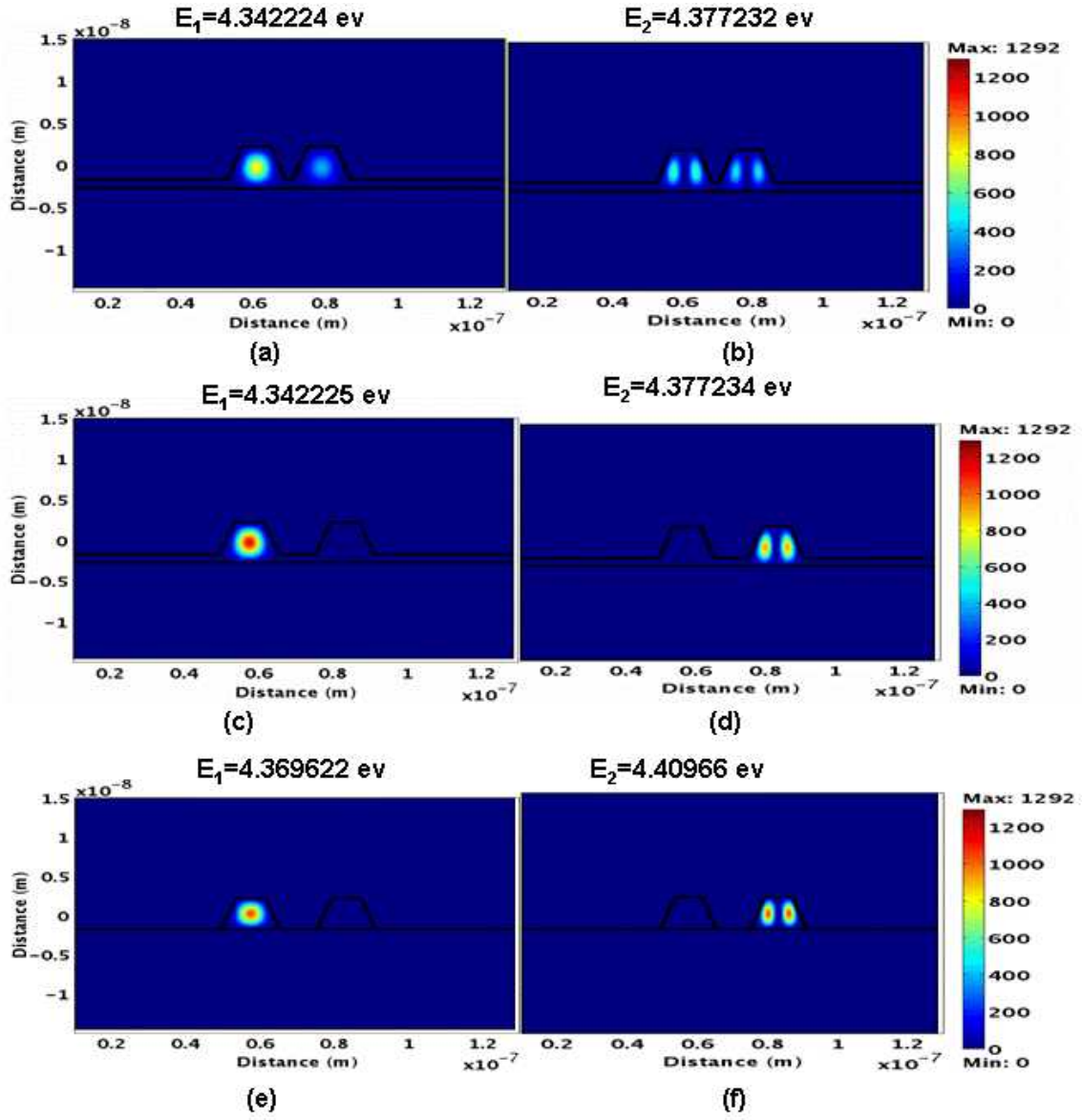

Figure 1. The influence of electromechanical effects on the band structure of two laterally coupled truncated pyramidal GaN/AlN QDs (a) ground state energy E_1 and (b) first excited state energy E_2 when the lateral QD separation is 2 nm with WL, (c) ground state energy E_1 and (d) first excited state energy E_2 when the lateral QD separation is 10 nm with WL, (e) ground state energy E_1 and (d) first excited state energy E_2 when the lateral QD separation is 10 nm without WL.

In this paper, we present a numerical analysis of the band structure of two coupled truncated GaN/AlN QDs under the influence of electroelasticity. By using the Finite Element Method (FEM), we study the effect of elasticity on the electronic properties of the two coupled truncated GaN/AlN QDs in the presence of WLs based on the 8×8 $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian. Several parameters such as electromechanical fields, eigenvalues and electron wave functions in the two coupled truncated GaN/AlN QDs are compared to the previously reported results for single GaN/AlN truncated QDs [1].

2. Mathematical model for coupling classical and quantum mechanical parts

Based on boundary conditions and geometry of the system, we conclude that the electromechanical balance equations for wurtzite (WZ) structures are axisymmetric. Therefore, the original 3D problem can be reduced to a 2D problem. The coupled equations of WZ structure in the presence of electromechanical effects in cylindrical coordinates can be written as [10]

$$\frac{\partial \sigma_{rr}}{\partial r}+\frac{\partial \sigma_{rz}}{\partial z}+\frac{\sigma_{rr}-\sigma_{\theta\theta}}{r}=0,\ \frac{\partial \sigma_{rz}}{\partial r}+\frac{\partial \sigma_{zz}}{\partial z}+\frac{1}{r}\sigma_{rz}=0,\ \frac{\partial D_r}{\partial r}+\frac{\partial D_z}{\partial z}+\frac{1}{r}D_r=0. \quad (1)$$

The stress tensor components and the electric displacement vector components can be written as

$$\sigma_{rr}=C_{11}\varepsilon_{rr}+C_{12}\varepsilon_{\theta\theta}+C_{13}\varepsilon_{zz}-e_{31}E_z,\ \sigma_{rz}=C_{44}\varepsilon_{rz}-e_{15}E_r, \quad (2)$$

$$\sigma_{zz}=C_{13}\varepsilon_{rr}+C_{13}\varepsilon_{\theta\theta}+C_{33}\varepsilon_{zz}-e_{33}E_z,\ D_r=e_{15}\varepsilon_{rz}+\epsilon_1 E_r. \quad (3)$$

The strain tensor components due to lattice mismatch in a semiconductor can be written as [10] $\varepsilon_{rr}=\frac{\partial u_r}{\partial r}-\varepsilon_a^\star$, $\varepsilon_{zz}=\frac{\partial u_z}{\partial z}-\varepsilon_c^\star$, $\varepsilon_{\theta\theta}=\frac{u_r}{r}-\varepsilon_a^\star$, $\varepsilon_{rz}=\frac{1}{2}\left(\frac{\partial u_r}{\partial z}+\frac{\partial u_z}{\partial r}\right)$. Here $\varepsilon_a^\star=\frac{a_m-a_{QD}}{c_{QD}}$ and $\varepsilon_c^\star=\frac{a_m-a_{QD}}{c_{QD}}$ are the local intrinsic strains along a and c directions, respectively. Also, a_m, c_m and a_{QD}, c_{QD} are the lattice constants of the matrix and the QD, respectively.

We analyze the band structures of QDs with an 8 band $\mathbf{k}\cdot\mathbf{p}$ model. Here we consider two conduction bands coupled with six valence bands including heavy hole, light hole and spin orbit bands [9, 11]. The 8×8 Hamiltonian can be written as

$$H=\begin{pmatrix} H_e^k+H_e^\varepsilon+E_c & & & & 0 & \\ & H_h^k+H_h^\varepsilon+E_v & & & & \\ & & H_e^k+H_e^\varepsilon+E_c & & & \\ 0 & & & H_h^k+H_h^\varepsilon+E_v & & \end{pmatrix}, \quad (4)$$

where H_e^k and H_e^ε are the kinetic and strain dependent parts of the electron Hamiltonian, respectively, whereas H_h^k and H_h^ε are the 3×3 matrix of the kinetic and strain dependent parts of the hole Hamiltonian respectively. E_c and E_v are the energies of unstrained conduction and valence band edges respectively. The physical parameters were chosen as in [10].

3. Results and Discussions

We have observed and quantified the electron wave functions overlap in the laterally grown coupled pyramidal shape quantum dots. The wave functions for the ground state and the first excited state for two laterally coupled truncated pyramidal shape of GaN/AlN QDs with and without WL have been calculated by applying the model described in section 2 (see [12] and [13] for more details on the influence of the WL. Here we include the coupled equations of electroelasticity (see (1)) into the 8-band $\mathbf{k}.\mathbf{p}$ model to account for the influence in electron wave functions with and without wetting layers. These results are presented in Figure 1. Here we observe the ground state energy E_1 at 4.342224 eV in Fig. 1(a)and first excited state at 4.377232 eV in Fig. 1(b) when the lateral separation between the dots are 2 nm and $E_1 = 4.342225$ eV in Fig. 1(c), $E_2 = 4.377234$ eV in Fig. 1(d) when the lateral separation between the dots are 10 nm with WL. These reported values for ground and first excited states are consistent with the results published in [1]. However, here we consider the distance between the two coupled lateral QDs as a tuning parameter.

We observe that electron wave functions are localized in both QDs when the separation between them is approximately 4 nm and are restricted to a single quantum dot when the separation between the dots exceeds about 5 nm in presence of wetting layers. The electron

wave functions are localized in one QD in the absence of wetting layers for any distance of lateral separation of the QDs. We compared the magnitude of the electron wave function to the previously reported results of [1] single QDs of identical geometry in both cases and found that the magnitude is approximately one order higher which is likely due to the electron wave functions overlap between the two QDs.

In addition, we also carried out a series of comparison studies of ground and first excited states eigenvalues with and without WL as shown in Figure 1. We found that the localization of electron wave functions is pushed down by approximately 3 meV.

4. Conclusions

Combined contributions of electromechanical effects in the band structure of two laterally coupled GaN/AlN QDs have been analyzed for the first time with and without wetting layer. The magnitude of the electron wave functions in ground and first excited states for two laterally coupled QDs is approximately one order higher than that of a single QD of identical geometry in both cases, pointing out to the evidence of electron wave functions overlap. Localization of electron wave functions changes significantly from one QD to the other QD or it spreads out into both QDs with the variation of lateral distance between the two QDs. Thus in addition to the electromechanical tuning, the distance between the QDs can also provide an additional tuning parameter in the design of QDs-based systems.

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