Strain and electronic structure interactions in realisticallyscaled quantum dot stacks

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Strain and electronic structure interactions in realistically-scaled quantum dot stacks

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Abstract. Self-assembled quantum dots (DQ) can be grown as stacks where the QD distance can be controlled with atomic layer control. This distance determines the interaction of the artificial atom states to form artificial molecules. The design of QD stacks becomes complicated since the structures are subject to inhomogeneous, long-range strain and growth imperfections such as non-identical dots and inter-diffused interfaces. This study presents simulations of stacks consistent of three QDs in their resulting inhomogeneous strain field. The simulations are performed with NEMO 3-D which uses the valence force field method to compute the strain and the empirical $sp^3d^5s^*$ tight binding method to compute the electronic structure. Strain is shown to provide a very interesting mixing between states and preferred ordering of the ground state in the top-most or bottom most quantum dot subject to growth asymmetries.

Keywords: NEMO-3D, atomistic VFF model, Hamiltonian.
PACS: 73.21.La

INTRODUCTION AND APPROACH

Self-assembled quantum dots (QDs) in the InAs/GaAs material system like to grow on top of one another allowing for a simple creation of QD stacks [1]. Isolated atomic-like states are expected to transition into molecular-like states with decreasing QD distance. QD stacks therefore form a very interesting laboratory to explore basic quantum mechanics as well as a potential device structure for optical devices such as lasers and detectors.

The modeling and simulation of such QD stacks bears several difficulties. One should not assume that the devices are formed with perfect interfaces and perfect composition. Interface inter-diffusion and gradients in the composition are to be expected. Besides such imperfections, just crystal symmetry alone will determine some of the coupling mechanisms between the QD. Therefore it is not fundamentally sufficient to model the devices with jellium methods such as k.p or effective mass approaches.

The Nanoelectronic Modeling tool (NEMO 3-D) [2,3] was built to handle systems of large size with atomistic resolution. It has shown the capability to simulate strain in systems of up to 64 million atoms in an atomistic valence force field (VFF) method. A modified Keating potential that accounts for anharmonicity [4] is used in VFF. The electronic structure calculation is typically performed with the $sp^3d^5s^*$ empirical tight binding model which, due to its increased complexity compared to the VFF strain model, has only been demonstrated for systems up to 21 million atoms. The design space of a three dot quantum dot system and the physics of interaction of strain and wave function coupling is explored.

RESULTS

Quantum dot stacks consistent of three QD layers are simulated (see insets of Fig 1). The InAs quantum dots are disk shaped with height 1.5nm positioned on a 0.5nm thick wetting layer. Two QD stacks are considered: identical dots of width 5nm and a system of 5/6/7nm width, increasing in the growth direction. The substrate thickness under the first wetting layer is kept constant at 30nm and the cap layer on top of the topmost dot is kept at 10 nm for all simulations. The bottom-most atomic layer is fixed to GaAs lattice constant, periodic boundary conditions are assumed in the lateral dimensions and the topmost surface atoms are allowed to "breathe" freely. The largest system considered here requires the strain calculation of ~660,000 atoms. The electronic structure is computed

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in a smaller domain that just encompasses the central dots and a buffer region. To avoid the formation of surface states by the dangling bonds of the artificially cut simulation domain the resulting "numerical surface" atoms are passivated [5]. The largest electronic structure domain considered here is ~205,000 atoms. The lateral extent of the simulations is chosen very small here at 12nm for the very small QDs. Simulations with larger dots and larger lateral dimensions are under way.

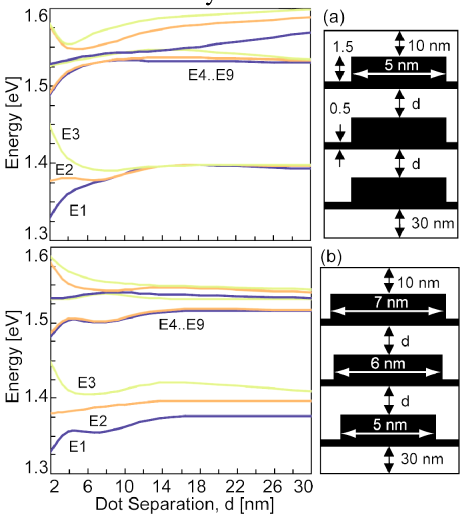

Fig 1: Electron state energies in the quantum dot molecule as a function interdot separation for two different QD stacks.

Figure 1a shows the electron state energy as a function of inter-dot separation for nominally identical dots. In a system without inhomogeneous strain one would expect the identical dots to have degenerate eigenstate energies for large dot separations. Strain breaks the degeneracy even for large systems. The strain field clearly extends over the distance of 30nm quantum dot separation. As the dot separation is narrowed the dots interact with each other mechanically through the strain field as well as quantum mechanically through wavefunction overlaps. The set of lowest states E1-3 as well as the excited states E4-9 clearly show the state repulsion of bonding and anti-bonding molecular states for short inter-dot distances.

Figure 1b shows the corresponding trace of eigen energies for the stack of non-identical dots. The states are non-degenerate for all inter-dot distances, however the formation of molecular states can be seen in the separation of the eigen states as the distance decreases. The set of E4-9 excited states show a slightly different admixture of states compared to Figure 1a.

Figure 2 shows cross-sectional cuts in the growth direction and one lateral direction through the middle of the 3D wavefunctions. The wavefunctions are quite clearly separated into the individual dots with little overlap across the dots for dot separations of 30 and 15nm. For 2nm and 4nm, wavefunction overlap can be observed.

Whether or not the coupled dot system favors the top-most or bottom-most QD to peak the ground state wavefunction is a complicated interplay of strain, QD size, and wavefunction overlap. Only a detailed simulation can reveal that interplay.

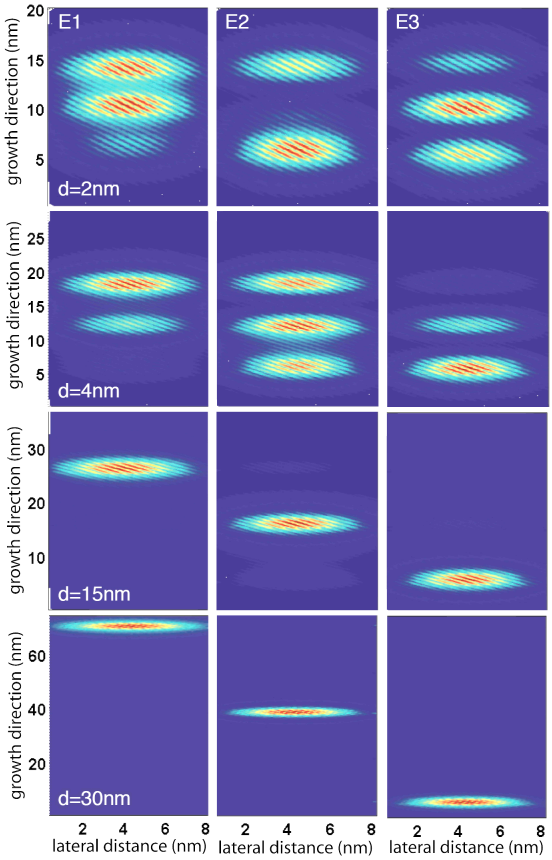

Fig 2: First three electron states wavefunction magnitudes (columns) with QD 2, 4, 15 and 30nm separation (rows) for non-identical dots (Figure 1 b).

CONCLUSIONS

QD stacks consistent of three QDs are analyzed. Non-trivial strain and electronic structure coupling is revealed with an analysis of the eigen energies and eigen states of the artificial molecule system. More detailed analysis on the strain distribution is needed to fully explain the movement of the electron states as a function of quantum dot distance.

REFERENCES

[1] Michler, P, Ed., Springer, Berlin, (2003).
[2] Klimeck, G, et al, Comp. Mod. in Eng. and Sci., 3, 601 (2002).
[3] OL Lazarenkova, et al, Appl. Phys. Lett. 85, 4193 (2004).
[4] Oyafuso, F, et al, J of Computational Electronics, 1, 317,(2002).
[5] Seungwon Lee, et al, Phys. Rev. B 69, 045316 (2004)