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Symmetry Breaking and Fine Structure Splitting in Zincblende Quantum Dots: Atomistic Simulations of Long-Range Strain and Piezoelectric Field

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Abstract. Electrons and holes captured in self-assembled quantum dots (QDs) are subject to symmetry breaking that cannot be represented in with continuum material representations. Atomistic calculations reveal symmetry lowering due to effects of strain and piezo-electric fields. These effects are fundamentally based on the crystal topology in the quantum dots. This work studies these two competing effects and demonstrates the fine structure splitting that has been demonstrated experimentally can be attributed to the underlying atomistic structure of the quantum dots.

Keywords: Quantum dots, Strain, Piezoelectricity, Crystal Symmetry.
PACS: 73.21.La

INTRODUCTION

Existing nanofabrication techniques create QDs in a variety of types and sizes. Among them, semiconductor QDs grown by self-assembly (SADs), trapping electrons as well as holes, are of particular importance in quantum optics, since they can be used as detectors of infrared radiation, optical memories, single photon sources, and lasers. At device sizes of tens of nanometers effects of atomistic granularity cannot be neglected. Surface roughness, unintentional doping, or distortions of the crystal lattice, if not taken into account, can have a deleterious impact on the device design.

Spectroscopic analysis of self-assembled quantum dots demonstrates polarized transitions between confined hole and electron levels. While the continuum models (effective mass or ***k.p***) can reliably predict aspects of the single-particle energy states, they fail to capture the non-degeneracy and optical polarization anisotropy of the energy states in the (001) plane [1]. The symmetry in quantum dots realized from III-V materials is lowered due to two fundamental symmetry breaking mechanisms: 1) the underlying crystal, which lacks inversion symmetry, and 2) the presence of strain which induces piezoelectric charges. Strain in self-assembled quantum dots is a long-range phenomenon and the dot states depend strongly on both the size of the strain domain and the boundary conditions. Both sources of symmetry breaking influence the fine structure splitting (splitting of the bright exciton) in self-assembled quantum dots. In this work, the impact of various factors on the symmetry breaking/lowering and fine structure splitting in atomistally represented self-assembled zincblende quantum dots is studied.

SIMULATION APPROACH

The study has been carried out through atomistic simulations using the Nanoelectronic Modeling tool NEMO-3D [2] capturing both the fundamental quantum character of charge carriers and the classical, long-distance strain effects on equal footing. Since the strain is long-ranged, its realistic determination requires a large computational domain. To tackle this problem for an embedded InAs quantum dot NEMO-3D uses the atomistic VFF Keating model containing up to 64 million atoms or $(110\text{nm})^3$. Interatomic distance changes obtained are used to influence the $sp^3d^5s^*$ tight-binding electronic Hamiltonian defined in a subdomain containing up to 21 million atoms or $(78\text{nm})^3$ (matrix size of order of 4×10^8). Such system

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sizes require use of parallel clusters or other HPC resources.

The dome-shaped QDs in this study (schematic shown in Fig. 1) have diameters and height within a range of 4.0 − 20.0 nm and 1.7 − 8.0 nm respectively, and are positioned on a 0.6-nm-thick wetting layer (dark regions). The simulation of strain is carried out in the large computational box (width D and height H), while the electronic structure computation is usually restricted to the smaller domain (width d and height h). All the strain simulations fix the atom positions on the bottom plane to the GaAs lattice constant, assume periodic boundary conditions in the lateral dimensions, and open boundary conditions on the top surface. The inner electronic box assumes closed boundary conditions with passivated dangling bonds.

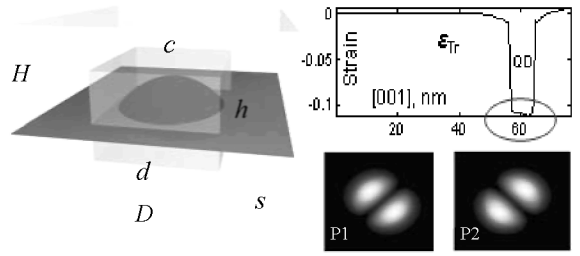

Fig 1. (Left) Schematic view of the QD nanostructure, with two simulation domains: central for electronic structure, and larger for strain calculations. (Right) Strain distribution along [001] and the introduced optical anisotropy in the first set of excited electron states P_1/P_2.

RESULTS AND DISCUSSION

Atomistic strain and relaxation modifies the effective confinement volume in the device and hence modulates the energy states. Fig. 1 (right panel) shows the net strain distribution along the [001] direction in a typical dome shaped quantum dot. The presence of the gradient in the strain profile introduces unequal stress in the zinc-blende lattice structure along the depth, breaks the equivalence of the [110] and [1$\underline{1}$0] directions, and breaks the degeneracy of the P_1/P_2 first excited states.

The simulation results also show a significant dependence of the dot states and magnitude of fine-splitting on the substrate layer thickness (underneath the dot) and the cap layer (above the dot). The strain in the QD system therefore penetrates *deeply* into the substrate and *cannot be neglected*. Fig. 2 shows such observed dependency where *E0* is the ground state energy and *dE* is the magnitude of the fine structure splitting in the *P* electronic states due to the inclusion of atomistic strain and relaxation. The wavefunction orientation remains unchanged irrespective of the included substrate depth.

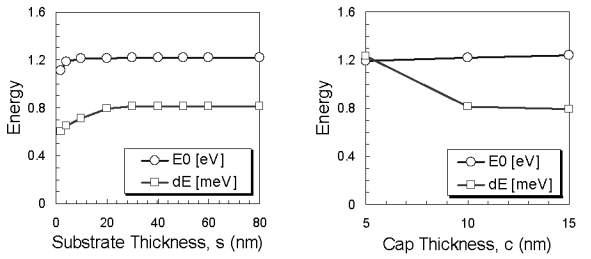

Fig 2. (Left) Substrate thickness dependence of the ground state and the P_1/P_2 energy splitting. Other structural parameters remain constant (h = 4 nm, d = 20 nm, c = 10 nm). (Right) The impact of cap layer thickness (with deep substrate thickness, s = 50nm).

The presence of off-diagonal strain tensor elements leads to the generation of a piezoelectric field, which is incorporated in the simulations as an external potential by solving the Poisson equation on the zincblende lattice. The relevant parameters for the piezoelectric calculation are taken from ref [1]. The piezoelectric potential has been found to introduce a global shift in the energy spectrum potentially strong enough to flip the optical orientation in certain sized quantum dots. In those cases the piezoelectric potential dominates over that resulting from the inclusion of atomistic strain in the simulations.

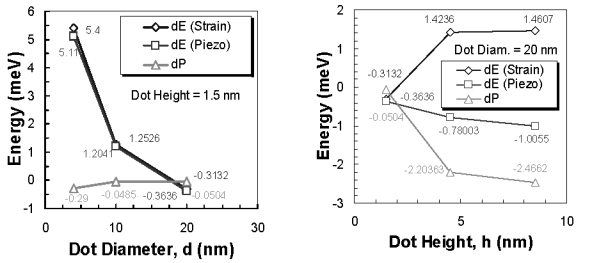

Fig 3. Influence of strain and piezoelectricity as a function of dot diameter (left) and dot height (right) on the fine-splitting and polarization of states.

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