Effects of Internal Fields in Self-Assembled InN/GaN Quantum Dots: Multimillion-Atom Tight-Binding Simulations

Sasi Sundaresan (1), Muhammad Usman (2), and Shaikh Ahmed (1)

(1) Department of Electrical and Computer Engineering, Southern Illinois University at Carbondale, 1230 Lincoln Drive, Carbondale, IL 62901

Phone: (618) 453 7630, Fax: (618) 453 7972, E-mail: ahmed@siu.edu

(2) Network for Computational Nanotechnology, Purdue University, W Lafayette, IN 47907

Recent spectroscopic analyses of self-assembled quantum dots (QDs) demonstrate polarized transitions between confined hole and electron levels [1]. These observations suggest the existence of certain symmetry lowing internal fields that originate mainly from: (1) the fundamental atomicity and interfaces in the crystal, (2) atomistic strain relaxation, and (3) the piezoelectric and the pyroelectric polarization. Electronic and optical properties of these reduced-dimensional QDs, to a large extent, are determined by an intricate interplay between these competing fields. While continuum models (effective mass and k.p [2]) can reliably predict the single-particle energy states, they fail to capture the observed non-degeneracy and optical anisotropy of the excited states in the growth plane. These methods fail because they use a confinement potential which is assumed to have only the shape symmetry of the QDs ignoring the underlying true atomistic crystal symmetry. In this work, we study the origin and nature of various internal fields in InN/GaN quantum dots with different geometries and sizes. We then calculate the impact of the internal fields on the one-particle electronic states in terms of shift in the conduction band energy states, anisotropy and non-degeneracy in the P level, formation of mixed excited bound states, and interband light transition rates. While investigating the size and geometry dependence of optical transition rates, it has been found that local maximum transition rate can be

achieved through geometry engineering of QD fabrication. Our results clarify the physical picture and provide a qualitative and quantitative analysis to the experimentalists for the future design of optical devices based on InN/GaN QDs. This study has been carried out through fully atomistic simulations using the Nanoelectronic Modeling tool NEMO 3-D [3]. Based on the atomistic valence-force field (VFF) and a variety of tight-binding models (s, sp3s*, sp3d5s*), NEMO 3-D enables the computation of electronic structure for over 52 million atoms. Excellent parallel scaling up to 8192 cores has been demonstrated. Whereas, the piezoelectric and the pyroelectric fields arising from the off-diagonal components of the strain tensor is included in the Hamiltonian as an external potential by solving the 3-D Poisson equation on the QD atomistic lattice.

References:

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