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Computational Methods for Electromechanical Fields in Self-Assembled Quantum Dots

D. Barettin, S. Madsen, B. Lassen* and M. Willatzen

Alsion 2, Mads Clausen Institute, University of Southern Denmark, DK-6400 Sønderborg, Denmark.

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Abstract. A detailed comparison of continuum and valence force field strain calculations in quantum-dot structures is presented with particular emphasis to boundary conditions, their implementation in the finite-element method, and associated implications for electronic states. The first part of this work provides the equation framework for the elastic continuum model including piezoelectric effects in crystal structures as well as detailing the Keating model equations used in the atomistic valence force field calculations. Given the variety of possible structure shapes, a choice of pyramidal, spherical and cubic-dot shapes is made having in mind their pronounced shape differences and practical relevance. In this part boundary conditions are also considered; in particular the relevance of imposing different types of boundary conditions is highlighted and discussed. In the final part, quantum dots with inhomogeneous indium concentration profiles are studied in order to highlight the importance of taking into account the exact In concentration profile for real quantum dots. The influence of strain, electric-field distributions, and material inhomogeneity of spherical quantum dots on electronic wavefunctions is briefly discussed.

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1 Introduction

The understanding of electromechanical fields in nanostructures and their coupling is a topic of ever-increasing interest. Semiconductor nanocrystals serve as an ideal platform for investigating quantum-physics interactions between conduction and valence

*Corresponding author. *Email addresses:* daniele@mci.sdu.dk (D. Barettin), sma@mci.sdu.dk (S. Madsen), benny@mci.sdu.dk (B. Lassen), willatzen@mci.sdu.dk (M. Willatzen)

electrons, phonons, and photons [1,2]. The possibility to control nanostructure geometry (size and shape), material parameters, charge transport, impurities, external fields etc. allows tailoring of device properties towards specific applications [2–11]. Optimization of the latter process (tailoring towards specific device applications) requires determination of coupled strain and electric-field distributions including, in some cases, piezoelectric and electrostrictive effects [12–21]. Eventually, having obtained electromechanical field distributions, properties related to, e.g., quantum computing and optoelectronic devices can be evaluated.

Two routes are traditionally followed in addressing electromechanical field effects based on either atomistic [22–26] or continuum methods [27, 29–31]. While the former are computationally more demanding they provide details on inter-atomic (i.e., lattice constant) scales automatically accounting for the full crystal lattice structure as well as the (location of) specific atoms associated with a lattice point. Evidently, it is expected that these details become increasingly important as nanostructure dimensions approach lattice-constant values. Continuum models, however, are known to provide computationally fast and accurate results for nanostructures with dimensions much larger than a lattice constant. The benefit in using continuum models in terms of reduced computation times makes them preferable (and often unavoidable) for many device calculations where, typically, multiphysics effects such as electromechanical field interactions become important.

To computationally bridge the two regimes of small- or large nanostructures [32], it is necessary to know if atomistic and continuum models can be practically combined for certain applications and to assess qualitatively and quantitatively the level of inaccuracy obtained in using continuum models to evaluate physical properties of smaller nanostructures. Furthermore, an important point which, unfortunately, is largely neglected in the literature, is the discussion of appropriate boundary conditions when computing electromechanical fields.

The goal of the present work is to compare electromechanical field distributions of quantum-dot nanostructures used in novel optoelectronic applications obtained from a continuum electromechanical model and a VFF atomistic method while emphasizing the importance of the chosen boundary conditions.

In the continuum-model case, a total free energy density change $d\mathcal{U}$ of a piezoelectric medium reads

$$d\mathcal{U} = d\mathcal{U}^{mech} + d\mathcal{U}^{elec} = TdS + \sigma_{ik}d\varepsilon_{ik} + E_i dD_i, \tag{1.1}$$

where the mechanical and electrical energy contributions are

$$d\mathcal{U}^{mech} = TdS + \sigma_{ik}d\varepsilon_{ik}, \tag{1.2a}$$

$$d\mathcal{U}^{elec} = E_i dD_i, \tag{1.2b}$$

respectively. Here, T, S, σ_{ik}, ε_{ik}, E_i, and D_i denote the temperature, entropy, stress tensor, strain tensor, electric field, and electric displacement, respectively. For a zincblende