Strain and Piezoelectric Effects in Quantum-Dot Structures

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Abstract—A discussion of computational methods for calculating strain and piezoelectric fields in nanostructures is presented. Emphasis is on a comparison of continuum and valence force field atomistic models and the validity of the former in predicting, accurately, strain fields for nanostructures with dimensions down to a few nm. This is done on the experimentally relevant InAs/InGaAs quantum-dot wetting layer structures and on spherical quantum dot structures. We next address the influence of boundary conditions imposed at the computational domain for strain fields near and inside the quantum dot; a point largely missing in literature. Boundary conditions discussed include fixed, free, fixed-free, and periodic, and it is shown that the particular choice of boundary conditions is unimportant for the strain results; a conclusion that allows to choose the computationally most effective one being the fixed-free boundary conditions as it requires the smallest computational domain for obtaining convergent results. While this result is fortunate, it is not obvious from a mathematical point of view. A further important, and *a priori* not obvious conclusion, is that a continuum model captures well atomistic strain results; a fact that allows us to use a continuum formulation even in cases where structure dimensions are down to only a few lattice constants.

In realistically grown structures, inhomogeneous concentration profiling exists. We present investigations for strain and piezoelectric results in the case where a spherical quantum dot region is gradually profiled from GaAs to InAs assuming the concentration is a function of the distance to the quantum dot sphere center. It is shown that quantum dot concentration profiling affects strain fields and biaxial strains in particular, electronic states and hence optical properties.

We finally present some effective quasi-analytical studies of electronic states and strain fields in curved quantum dots based on applications of differential geometry and perturbation theory.

I. INTRODUCTION

Strain and piezoelectric fields play a major role in determining electronic eigenstates and optical properties of quantum dot structures. In this work we examine the influence of size and shape of structures, different material constituents, and concentration profiles that occur inevitably under experimental growth conditions. At the same time, the many structural parameters allow to tailor and optimize nanostructure properties toward certain applications [1]. In this work we put emphasis to effective computational methods and their advantages and limitations. In particular, we address the influence of boundary conditions imposed at the computational domain boundaries [2]. Further, we compare continuum and atomistic models, the latter based on Keating's valence force field model and the former's applicability to capture strain fields in nanostructures with dimensions down to a few lattice constants. It is demonstrated that the precise choice of boundary conditions is not important for the strain fields near and inside the quantum dot. Moreover, it is confirmed that a continuum model captures well strain fields even for small nanostructures by comparing with atomistic results. These important and non-trivial conclusions allow us to use a computationally fast continuum model where multiphysics effects such as piezoelectricity (and possibly electrostriction) [3], [4] are easily accounted for even for complicated structures such as quantum dot wetting layer structures where some dimensions including the wetting layer contain few monolayers. It is further demonstrated that concentration gradings in the quantum dot region lead to modifications in the biaxial strain component that significantly affect electronic states and, eventually, optical properties.

In the second part of the paper, a perturbative differential-geometry based model is used to examine strain effects quasi-analytically in curved structures. As a corollary, a very effective method for obtaining quasi-analytical results for electron eigenstates and energies is outlined. The model applicability includes problems where simple Dirichlet (hard-wall) boundary conditions are replaced by Neumann conditions (relevant for some electromagnetics or acoustics problems) and mixed boundary conditions.

A. Strain fields in inhomogeneous InGaAs quantum dot structures

Realistically grown quantum dot structures are subject to concentration gradients. We discuss the influence of a radially-varying concentration gradient c in $In_cGa_{1-c}As$ spherical quantum dots embedded in a GaAs matrix. Continuum strain field results are computed for a quantum dot with radius $R = 1.5$ nm and subject to a constant concentration $c = 1$ inside the quantum dot, a linear profile $c = 1 - r/R$, and a quadratic profile $c = 1 - r^2/R^2$, respectively, where r denotes the distance from the quantum dot center. Results for the biaxial strain component are shown in Figure 1. Firstly,
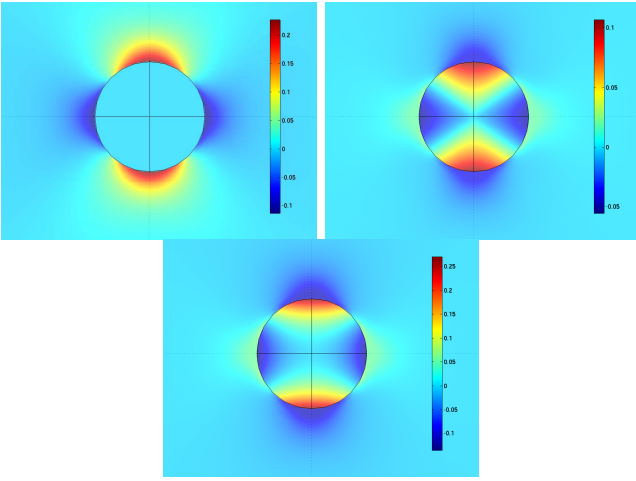
167

Fig. 1.   The upper-left, upper-right, and lower plots show biaxial strain fields in constant, linear, and quadratic concentration profiled InGaAs quantum dots embedded in a GaAs matrix, respectively.

we observe that results are anisotropic despite the quantum dot is spherical. This stems from the zincblende nature of the underlying crystal lattice. It is interesting to observe that the biaxial strain component vanishes inside the quantum dot in the homogeneous concentration case while biaxial strains are nonzero in the cases with a linear and a quadratic concentration gradient. Albeit calculations are done in the linear strain regime, biaxial strain values inside the quantum dot are locally above 20 % in the quadratic profiling case and up to 10 % in the linear profiling case. This shows that concentration gradients significantly change the strain state and thus optoelectronic properties of the quantum dot structure since deformation potentials are $5 - 10$ eV's in InGaAs!

B. Strain distributions in curved nanostructures

In the second part of the paper, we present a powerful quasi-analytical technique to obtain electronic eigenstates in curved finite nanowire structures where the presence of strain is solely due to bending. Hence, the structure is in equilibrium in the absence of strain, i.e, when it takes the form of a straight nanowire. The study of static and dynamic deformations in nanostructures is important when examining, e.g., energy harvesting generators based on bending of piezoactive nanorods [5]. Further relevant examples are nanomechanical piezoelectric actuation using GaAs and the nonlinear resonance of piezoelectric nanowires.

The strain tensor ϵ_{ij} becomes diagonal in the case of a nanowire structure with cross-sectional dimensions considerably smaller than its length. In this case, one finds for zincblende grown nanowires

$$\epsilon_{22} = \epsilon_{33} = -\frac{c_{12}}{c_{11} + c_{12}}\epsilon_{11}, \qquad (1)$$

where c_{ij} is the stiffness tensor components, and

$$\epsilon_{11} = \frac{u^2}{R} + \frac{1}{2}\left(\frac{u^2}{R}\right)^2, \qquad (2)$$

where R is the local radius-of-curvature. Note that we keep second-order terms in the strain tensor not because strain values are big rather as energy changes from bending strains are of order $\frac{1}{R^2}$.

The Schrödinger equation for electrons of effective mass m_e, written in general curved coordinates u^1, u^2, u^3, is a separable problem even in the presence of strain since the strain tensor depends on u^2 only:

$$-\frac{\hbar^2}{2}\nabla \cdot \left(\frac{1}{m_{eff}(\mathbf{r})}\nabla\right)\psi(\mathbf{r}) +$$
$$[V_{BE}(\mathbf{r}) + D_e (\epsilon_{11} + \epsilon_{22} + \epsilon_{33})]\psi(\mathbf{r}) = E\psi(\mathbf{r}), \qquad (3)$$

where V_{BE} is the band-edge potential (zero inside and infinite outside the nanowire in the infinite-barrier case), D_e is the hydrostatic deformation potential, and E is the electron energy. Separability of the Schrödinger problem allows a quasi-analytical solution. Equation (3) is solved for various bent structures and it is shown that that moderate bendings lead to significant changes in electronic eigenstates and their energies.

II. CONCLUSION

A discussion of strain fields in quantum dot structures is presented using continuum and atomistic models and it is shown that even for smaller quantum dots (a few nanometers in diameter) continuum model results agree well with atomistic results. It is shown that strain results in and near the quantum dot are insensitive to the precise choice of boundary conditions. This important result allows to choose the computationally most effective boundary conditions. Our calculations are carried out for InGaAs structures embedded in a GaAs matrix and particular emphasis is given to changes in strain fields in cases with a homogeneous concentration of In in the quantum dot as compared to cases where the In content changes linearly or quadratically from 0 at the quantum dot radius to 1 at the quantum dot center. It is demonstrated that the biaxial strain field is very sensitive to concentration gradients, a result that severely affects hole bandstructures and optical properties. We also provide a discussion of effective ways to solve the one-band effective mass equation for electronic eigenstates and energies quasi-analytically using differential geometry and perturbation theory.

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