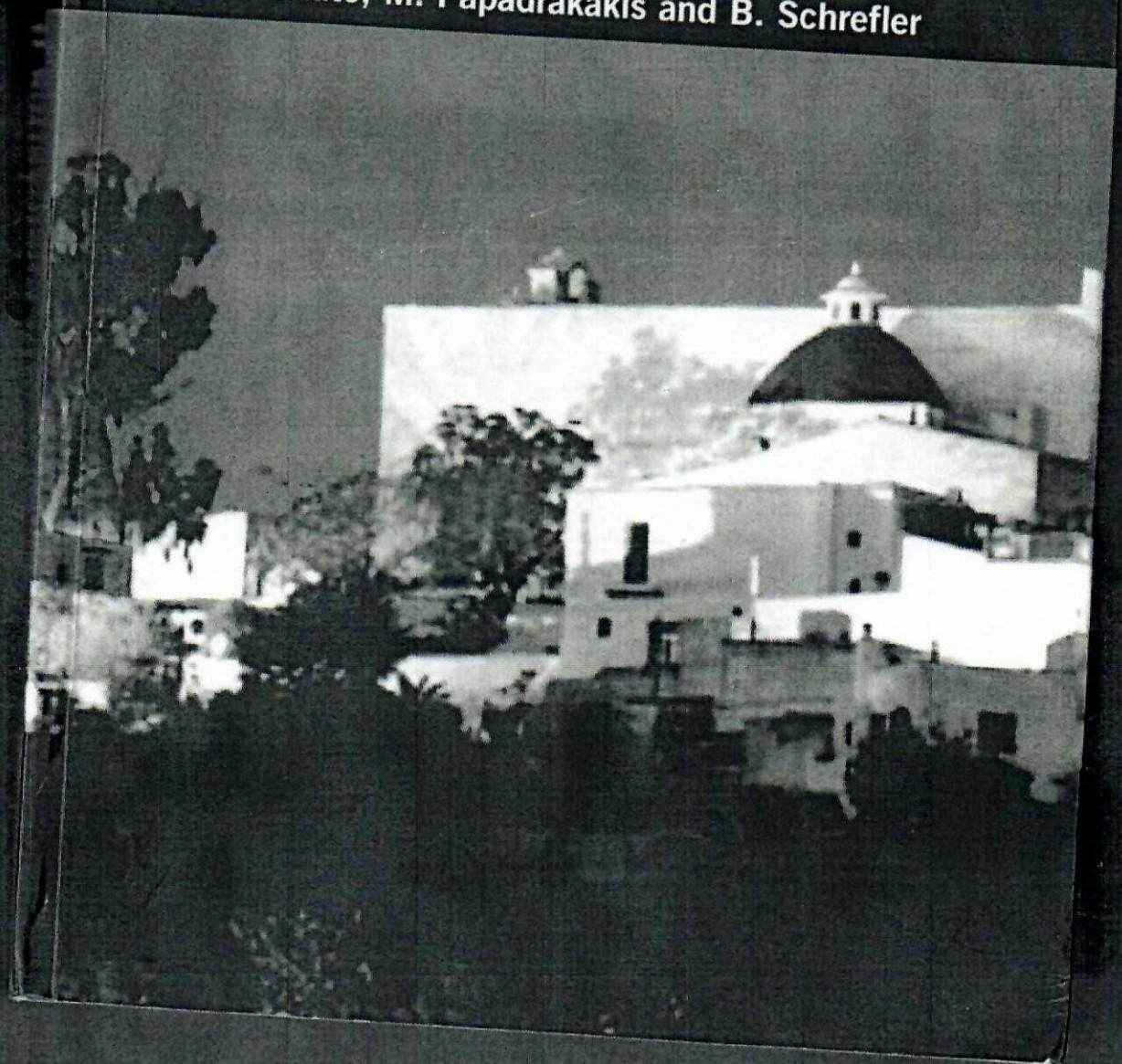
Computational Methods for Coupled Problems in Science and Engineering II

Edited by:
E. Oñate, M. Papadrakakis and B. Schrefler



Computational Methods for Coupled Problems in Science and Engineering II
Coupled Problems 2007

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MULTI-PHYSICS SELF-CONSISTENT MODELING IN NANOTECHNOLOGICAL APPLICATIONS: QUANTUM DOTS AND QUANTUM-WELL LASERS

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Key words: Quantum dot, quantum well, strain, piezoelectricity, Fermi energy.

Abstract. This paper reports a self-consistent Poisson-Schrödinger scheme including the effects of the piezoelectricity, the spontaneous polarization and the charge density on the electronic states and the quasi-Fermi level energy in wurtzite type semiconductor heterojunction and quantum-laser.

1 INTRODUCTION

In recent years, several detailed computational methods for analyzing the electronic properties of strained semiconductor heterojunction have been reported (See refs. [1, 2]). AlN/GaN, ZnO/MgO and several other wide bandgap wurtzite heterostructures are promising candidates for various optoelectronic device applications. An illustrative study has been reported in ref. [3] within the context of lattice misfit induced strain and piezoelectric effect on the resonant frequency. Some of the contradictions reported earlier regarding the order of magnitude of piezoelectricity in wurtzite AlN/GaN heterojunction (see refs. [1, 4]) have been addressed in the recent analytical development in ref. [3]. In the context of lasing applications, an additional integral effect, namely the charge density effect on the quantum-mechanical states [5]) is not well estimated. Also, it is not well known how strongly the strain and piezoelectricity influence the Fermi level and the evolved quantum-mechanical states.

1.1 Coupled Problems in the Engineering of Quantum Dot Heterostructures

Coupled effects, similar to those discussed above for GaN/AlN and other wide-bandgap wurtzite quantum wells, become much more complicated when one considers 3D quantum dot growth and their lasing applications. The main objective behind employing a quantum dot, as in a lasing device, is to first confine the electron motion spatially and then produce stimulated emission by applying electric field. Although in the physics literature, a quantum dot is called 0-dimensional structure, actually the 3D effects due to the crystalline arrangement of the constituent atoms and the nearfield effects due to the interfaces become important. For lasing, which is a process of charge pumping, followed by optical emission, it becomes a competition between the strain energy and the excitonic energy. In addition, in many wide bandgap heterostructures, wurtzite type crystals are grown and they exhibit strong piezoelectric polarization (including spontaneous polarization during lasing). In literature, the strain effects in quantum dots have been included in an uncoupled manner [2, 6] and the semi-coupled Green's function based approach were employed by Jogai *et al.* [1]. We consider extension of such idea (but using finite element approach) beyond 1D type assumption and give a rigorous treatment to the coupled problem, first for a problem with finite 1D for growth axis ($\|$ direction) and finite 2D normal plane ($\perp$ plane) for a multilayer GaN/AlN quantum well structure, and next, a full 3D treatment to a GaAs/InAs pyramidal quantum dot. Due to intersecting interfaces and corners in many types of quantum dots (e.g., pyramidal or hexagonal types, depending on their constituent crystallographic properties), the growth process leaves several characteristic signatures, e.g., lattice misfit, diffused phases near interfaces and nonlinear strain as a source of defect formation. Hence, it is understood that, the effect of interface conditions and phase inhomogeneity need to be considered in deriving the energy density. Such an energy density description must also account for the spatial distribution of the density of states in the structure via Maxwell's equations.

2 Material model, lattice misfit and polarization induced strain

We define the material model for the crystalline Bravais lattice as

$$\boldsymbol{\sigma} = \boldsymbol{c}\boldsymbol{\varepsilon} - \boldsymbol{e}\boldsymbol{E}\,, \quad \boldsymbol{D} = \boldsymbol{\epsilon}\boldsymbol{E} + \boldsymbol{e}\boldsymbol{\varepsilon} + \boldsymbol{P}_{\rm sp}\,. \tag{1a}$$

where $\boldsymbol{\sigma}$, $\boldsymbol{\varepsilon}$, $\boldsymbol{D}$, $\boldsymbol{E}$ and $\boldsymbol{P}_{\rm sp}$ are the stress tensor, the strain tensor, the electric displacement, the electric field and the spontaneous polarization, respectively. $\boldsymbol{c}$ is the stiffness tensor, $\boldsymbol{\epsilon}$ is the dielectric tensor and $\boldsymbol{e}$ is the tensor of piezoelectric constants. The strain tensor is expressed as $\boldsymbol{\varepsilon} = \frac{1}{2}[(\nabla \boldsymbol{u}(\mathbf{x})) + (\nabla \boldsymbol{u}(\mathbf{x}))^{\mathbf{T}}] - \boldsymbol{\varepsilon}^0(\mathbf{x}) + \boldsymbol{\alpha}\Delta\mathbf{T}$, where $\boldsymbol{u}(\mathbf{x}) = (u_x, u_y, u_z)$ denotes displacement of a material point $\mathbf{x}$ and $\boldsymbol{\varepsilon}^0(\mathbf{x})$ denotes the compressive residual strain due to lattice misfit (see ref. [2] for details). $\boldsymbol{\alpha}$ is the tensor of thermal expansion coefficients and ΔT denotes the difference between the device temperature and the equilibrium temperature. The electric field is given by $\boldsymbol{E} = -\nabla\phi$, where ϕ is the electric potential.

For an assumed distribution of donors and electrons, it is possible to find an analytical solution of the full piezoelectric problem only for simple geometries and thus estimate the band edge potential, and subsequently the energy states, accurately. Such analytical results can be found in refs. [1, 3, 7]. Taking note of these developments, optimization the effect of size (e.g., length of the well relative to the barrier) as a mechanism of relaxing the strain due to lattice misfit, electrical polarization etc., which are important factors to influence the band structure, require detailed analysis. However, in lasing applications, where the charge density also affects the electric field [5] and the equilibrium strain, the overall effect due to the size of the well region, as well as the shape of electron/hole confinements for various subbands are not well understood, and it requires a self-consistent model as discussed next.

3 COUPLED POISSON-SCHRÖDINGER MODEL

The coupled equations of piezoelectricity has the general form:

$$\nabla \cdot \boldsymbol{\sigma} = 0\,, \quad \nabla \cdot \boldsymbol{D} = e(N_d - n(\mathbf{x}))\,. \tag{2a}$$

where e is the (positive) electronic charge, N_d is the donor density, and $n(\mathbf{x})$ is the carrier electron density. In this paper, we neglected the influence of donors and holes in the structure. Equations (2a) and (2b) are converted into Poisson equation with the stress $\boldsymbol{\sigma}$ expressed in terms of the displacement gradient $\nabla \boldsymbol{u}$ and the electric potential ϕ. Similarly, the electric displacement $\boldsymbol{D}$ is also expressed in terms of the displacement gradient and the electric potential.

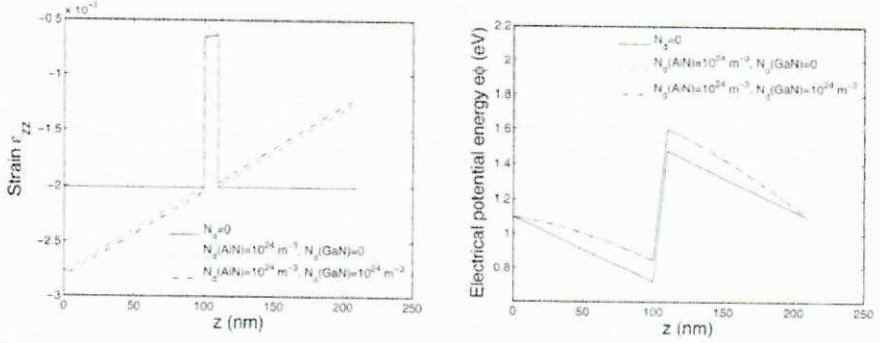
The electron density $n(\mathbf{x})$ is found by solving the Schrödinger equation. We choose to use the effective-mass approximation, so that the conduction-band envelope functions and corresponding energies are found by solving the equation:

$$H(\nabla(\hbar^2/(2m))\nabla, \boldsymbol{\varepsilon}, \phi)\Psi^{(j)} = E^{(j)}\Psi^{(j)}\,. \tag{3}$$

where H is the Hamiltonian. The $(\boldsymbol{\varepsilon}, \phi)$ dependent terms in H are obtained by solving the Poisson equation (Eq. (2a)-(2)) within a loop of iteration. According to the Fermi-Dirac distribution,

$$n(\mathbf{x}) = 2\sum_j |\Psi^{(j)}(\mathbf{x})|^2 f(E^{(j)}, E_{FL}, T)\,. \tag{4}$$

In order to obtain the converged values of the Fermi level energy, we start with $E_{FL}^{(i)} = E_{FL}^{(0)} = H_b$, such that $H_b \ll H_c$ for the well, that is, the initial value H_b (in the order of few meV) lies at the bottom of the relative conduction band edge. With this initial value assigned to E_{FL} and $n(z) = n(z)^{(i)} = 0$, we first solve the Poisson equation (combined form of Eqs. (2a) and (2a) along with Eqs. (1)). Next, we solve the eigenvalue problem based on Eq. (3) and then evaluate $n(z) = n(z)^{(i+1)}$. Next, the Fermi level energy is updated as



(a) (b)

Figure 1: (a) Strain ε_{zz} and (b) electrical potential energy $e\phi$ due to various values of the net donor density N_d.

$E_{FL}^{(i+1)} = E_{FL}^{(i)} + \Delta E_{FL}$. This process is repeated until an equilibrium is reached, that is, until

$$N_d L_z - \int_0^{L_z} n(z)dz \to 0\,. \tag{5}$$

3.1 Effect of Electron Carrier Distributions in GaN/AlN Quantum Well

Figures 1(a) and (b) show the strain and the electric potential. The strain does not change whereas the electric potential increases by approximately 0.4 eV when nonzero N_d is assumed. The calculated ground state conduction band energy is found to drop by 12.7 meV and the Fermi energy deviates by ≈ 100 meV when compared to decoupled band structure-piezoelectric calculation (i.e., one-step calculation).

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CONTENTS

PLENARY LECTURES

C.S. - ELECTRO-MAGNETIC COUPLING

This book contains the Abstracts of the papers presented at the Second International Conference on Computational Methods for Coupled Problems in Science and Engineering (COUPLED PROBLEMS 2007) held in Santa Eulalia, Ibiza, Spain from May 21-23, 2007.

The objective of the conference was to present and discuss state of the art mathematical models, numerical methods and computational techniques for solving accurately and with affordable computing times coupled problems of multidisciplinary character in science and engineering. Emphasis was given to showing the potential of new computational methods for solving practical problems of industrial interest.

The papers included in the book provide an overview of the formulation and computational solutions of real life problems with a multidisciplinary vision, accounting for all the complex couplings involved in their physical description.

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