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Poisson-Schrödinger Model in the Analysis of Coupled Effects in Quantum Well Nanostructures

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***Abstract*— In this contribution, we implement a self-consistent procedure for the solution of the Poisson-Schrödinger model applied here for the analysis of coupled effects in wide bandgap wurtzite heterostructures. Such effects are demonstrated on examples for three-layer systems, in particular AlN/GaN quantum well heterojunctions, which are promising components in a number of optoelectronic device applications. A major emphasis is given to the effects of boundary conditions, piezoelectricity and spontaneous polarization.**

I. Introduction

Electronic properties of wide bandgap wurtzite heterostructures can pronouncedly be influenced by a range of additional effects such as strain, piezoelectric effect, and spontaneous polarization. In designing new optoelectronic devices these effects should be taken into account. In [1], we have recently reported an illustrative study of lattice misfit induced strain and piezoelectric effect on the resonant frequency in AlN/GaN nanostructures. In such three-layer structures, a GaN well confined by AlN barriers. In the present contribution we continue the study of coupled effects in such nanostructures. First, we analyze the effect of boundary conditions in these structures, focusing on their influence on the strain and the electric potential distribution. The analysis is based on the Poisson-Schrödinger model. Then, in the same modeling framework we discuss the effect of piezoelectricity and spontaneous polarization, as well as the coupling between the Poisson and Schrödinger equations via the electron density.

II. Governing Equations

The geometry of the nanostructure is given in Fig. 1 and we are interested in the behavior of the carrier electron density in the z-direction, so that the following averaging, based on the Fermi-Dirac distribution, is carried out:

$$n(z) = 2\sum_{j=0}^{N} \int_{k_x^{(m)}=0}^{k_x^{(m_{\max})}} \int_{k_y^{(m)}=0}^{k_y^{(n_{\max})}} \frac{L_x L_y}{(2\pi)^2} |\Psi^{(j,m,n)}(z)|^2 f(E^{(j,m,n)}, E_{FL}) dk_x dk_y \ . \quad (1)$$

In Eq. (1) N is the number of conduction subbands. The wavenumber $|\mathbf{k}|$ lies within 5% of the Brillouin zone which allows us the evaluation of the integral accurately for typical carrier densities.

The function f in Eq. (1) is given by the Fermi-Dirac distribution with two arguments: E_{FL} being the quasi-Fermi level energy and $(E^{(j,m,n)}, \Psi^{(j,m,n)})$ being the eigenpairs of the Schrödinger equation:

$$H\Psi = E\Psi \ . \quad (2)$$

The one-band Hamiltonian models for electrons and holes are standard. We only note here that the Poisson equation should be solved prior to determining the electric potential entering these Hamiltonian models. Hence, the coupling between the Schrödinger and Poisson equations is effectively incorporated via the electron density in the system of coupled piezoelectricity, which in the general case can be written as follows:

$$\nabla \cdot \mathbf{D} = e(N_d - n(\mathbf{x})) \ , \quad (3a)$$

$$\nabla \cdot \boldsymbol{\sigma} = 0 \ . \quad (3b)$$

These two equations, in their turn, are coupled between themselves electro-mechanically via the constitutive equations given for the wurtzite type materials by:

$$\boldsymbol{\sigma} = \mathbf{c}\boldsymbol{\varepsilon} - \mathbf{e}\mathbf{E} \ , \quad (4a)$$

$$\mathbf{D} = \boldsymbol{\epsilon}\mathbf{E} + \mathbf{e}\boldsymbol{\varepsilon} + \mathbf{P}_{\rm sp} \ . \quad (4b)$$

In the above equations (3)–(4), we use the following notations: $\boldsymbol{\sigma}$, $\boldsymbol{\varepsilon}$, $\mathbf{D}$, $\mathbf{E}$ and $\mathbf{P}_{\rm sp}$ are the stress tensor, the strain tensor, the electric displacement, the electric field and the spontaneous polarization, respectively. $\mathbf{c}$ is the stiffness tensor, $\boldsymbol{\epsilon}$ is the dielectric tensor and $\mathbf{e}$ is the tensor of piezoelectric constants. e is the (positive) electronic charge, N_d is the donor density, and $n(\mathbf{x})$ is the carrier electron density (reduced in the one-dimensional case to $n(\mathbf{x}) = n(z)$).

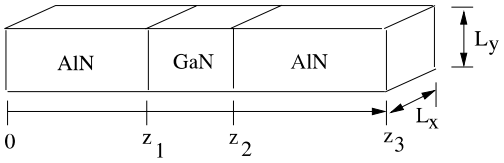

Fig. 1. Geometry of the nanostructure.

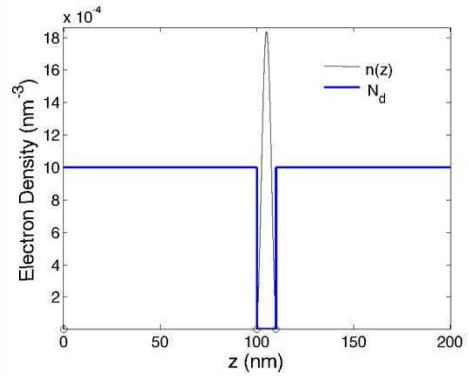

Fig. 2. Electron density distribution in the nanostructure (under fixed-fixed mechanical boundary condition).

III. Self-Consistent Scheme of the Solution

Recall that in the usually uncoupled solution of the Schrödinger-Poisson model, a typical conventional numerical procedure requires to solve the Poisson equation first under the assumption of a known distribution of charge, followed by the computation of the band structure for an assumed value of the quasi-Fermi level energy. The latter value may not be determined accurately in such one-step procedures which results in inaccuracies in determining the shape of quantum confinement.

In the self-consistent implementation of the Schrödinger-Poisson model applied in this paper, we first initialize the quasi-Fermi level energy E_{FL} and set $n(z)$ to zero. We solve the Poisson equation based on the coupled system of piezoelectricity with respect to the displacement (u) and the electric potential (φ). This is followed by the solution of the Schrödinger equation with the Hamiltonian based on the determined values of u and φ. Then, we determine the electron density $n(z)$ and verify the convergence condition for the finite element implementation of the problem. If it is satisfied, we store the final values of the band edge potential, energy states, and the charge distribution. Otherwise, we update the quasi-Fermi level energy E_{FL} and proceed to the solution of the Poisson equation, repeating the multi-step coupled procedure described above.

IV. Results

Based on the self-consistent scheme described above, a number of computational experiments have been carried out, some of which are reported below.

TABLE I

Conduction band energies (eV) under different types of mechanical boundary conditions.

State	Fixed-free $E_{\mathrm{FL}} = -0.0965$ eV $\max(n(z)) = 1.846 \times 10^{-3}$ nm^{-3}	Fixed-fixed $E_{\mathrm{FL}} = -0.1265$ eV $\max(n(z)) = 1.836 \times 10^{-3}$ nm^{-3}
1	1.0395	1.0671
2	1.2913	1.2474
3	1.3666	1.3951
4	1.5006	1.5294
5	1.6434	1.6724
6	1.8156	1.8446

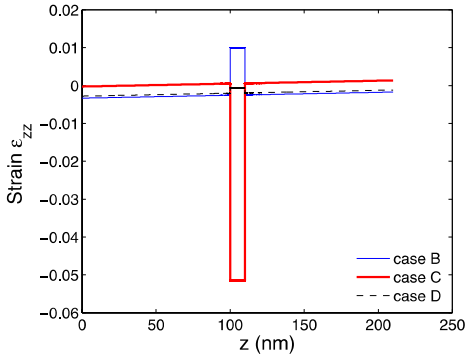

Fig. 3. Strain ε_{zz} in the nanostructure.

We have observed differences in the values of the energies calculated with the standard uncoupled one-step scheme and the multi-step coupled procedure developed here. Such differences were observed for different types of mechanical boundary conditions, including perfectly restrained boundary conditions (displacements at both ends are zeros) as well as stress-free boundary conditions. The developed coupled iterative procedure has been applied to the analysis of confinement in the heterojunction (see Fig. 1). The confinement produces the electron density distribution $n(z)$ shown in Fig. 2. In Table I we provide details on the converged value of the quasi-Fermi level energy, the maximum value of $n(z)$ (located at the center of the well), and the converged band energies.

The analysis of these results reveals that the difference in the quasi-Fermi energy between the fixed-fixed and fixed-free boundary conditions can be as large as 30 meV. Further we note that the magnitude of strain may change drastically due to change in the mechanical boundary condition without any significant change in the electric potential. Further details of these observations will be reported elsewhere.

Next, we analyze the effect of piezoelectricity and spontaneous polarization by considering the following four cases: (a) the case without lattice misfit, piezoelectricity, and spontaneous polarization, (b) the case without spontaneous polarization, with lattice misfit and piezoelectricity, (c) the case without lattice misfit and piezoelectricity, with spontaneous

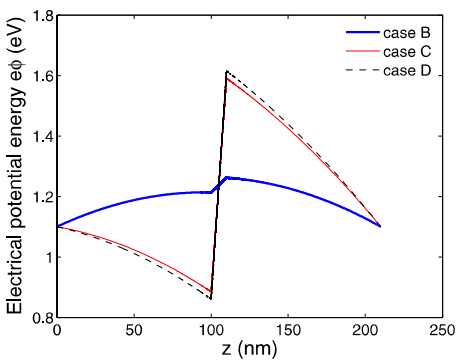

Fig. 4. Electrical potential energy $e\phi$ in the nanostructure.

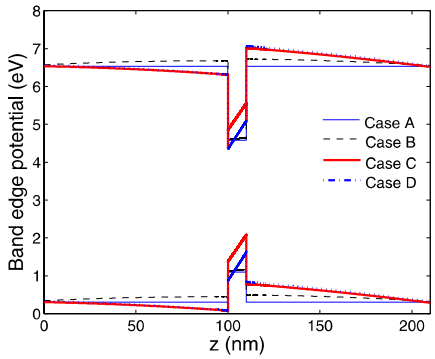

Fig. 5. Band edge potentials for the nanostructure (with conduction-band offset $H_c = 0$ in GaN and $H_c = 1.955$ eV in AlN).

polarization, and, finally, (d) the case with lattice misfit, piezoelectricity, and spontaneous polarization.

The standard uncoupled calculations with $N_d = 10^{14}$ m^{-3} in the barrier and $N_d = 0$ in the well lead to the result presented in Figure 3 and Figure 4 where we plot the strain and the electric potential, respectively. The change in sign is due to the absence of lattice misfit and the fact that in this case the spontaneous polarization effect dominates over the piezoelectric strain. We also observe significant changes in the band edge potential from the case (a) to the cases (b)–(d), as demonstrated by Fig. 5. Note that unstrained band gap for the analyzed case is $E_g = 3.475$ eV for GaN and $E_g = 6.23$ eV for AlN.

Other observations, that will be discussed in detail elsewhere, demonstrate also significant influence of charge density and piezoelectricity on the quasi-Fermi energy level with the deviation as large as 100 meV when compared to one-step uncoupled calculations.

V. Conclusions

Based on the self-consistent finite element implementation of the Poisson-Schrödinger model, we analyzed coupled effects in wide bandgap wurtzite heterostructures with examples given for three-layer AlN/GaN quantum heterojunctions. The results demonstrated that the effect of mechanical boundary conditions, piezoelectric effect and spontaneous polarization on the electronic states and the quasi-Fermi level energy can be substantial. These effects will become increasingly important for new photonic and optoelectronic device applications.

References

[1] M. Willatzen, B. Lassen, L.C. Lew Yan Voon and R.V.N. Melnik, Dynamic coupling of piezoelectric effects, spontaneous polarization, and strain in lattice-mismatched semiconductor quantum-well heterostructures, *J. Appl. Phys.*, **100**, 024302, 2006.

PREFACE

This Proceedings provides a lasting record of the highly successful Conference on Optoelectronic and Microelectronic Materials and Devices (COMMAD) which was held in Perth, Australia, at The University of Western Australia, from 6th to 8th of December, 2006. COMMAD is usually organised every two years and provides a forum to bring together industrial collaborators, scientists, engineers and students to discuss new and exciting advances in the fields of optoelectronic, MEMS, and microelectronic materials and devices, as well as advanced materials and various aspects of nanotechnology as they relate to optoelectronics, MEMS, and nanoelectronics. The conference attracted more than 120 participants, from more than 20 different countries, and consisted of two and a half days of oral presentations and two days of evening poster sessions. In addition, there were 4 short courses presented as part of the one-day Workshop on Nanoelectronics, which took place prior to the conference on Tuesday 5th December.

COMMAD'06 provided a forum to present and discuss recent advances in:

- Materials: growth, processing, and characterisation.
- Devices: physics, design, fabrication, testing, and applications.

COMMAD'06 covered nano- and micro-electronic and optoelectronic materials and technologies such as Si, SiGe, SiC, ZnO, GaAs, InP, GaN, ZnSe, HgCdTe, $LiNbO_3$ etc, and nano- and micro-electronic, optoelectronic, and MEMS devices such as lasers, modulators, photovoltaic devices, photonic crystals, photodetectors, optical switches, waveguides, HBTs, HEMTs, MISFETs, sensors, etc.

The conference was opened by Professor Doug McEachern, Deputy Vice-Chancellor (Research and Innovation), The University of Western Australia. There were 44 oral and 57 poster presentations. We are particularly grateful to the plenary speakers, Hiroshi Iwai, Sajeev John and Hideki Hasegawa, (who set the overall scene and provided orientation for the conference on each day), and to the invited speakers Martin Stutzmann, Sanjay Krishna, Andrej Kusnetsov, Roberto Menozzi, Oskar Painter, Carl-Mikael Zetterling, Leonard Chen, Erhard Kohn, Angela Rizzi, Anant Agarwal, Joseph Talghader, Sebastian Lourdudoss, Charles Ironside, Hiroshi Mizuta, and Elisabetta Comini, for excellent up-to-date overviews of a wide range of topics.

The student prizes were awarded at the conference dinner to Jonathan Klamkin and Michael Fraser (joint winners of best oral presentation) and Ryan Westerhout (best poster presentation).

These proceedings contain both invited and contributed papers. All contributed papers published in these Proceedings were accepted for publication after anonymous peer review by at least two distinguished reviewers. We would like to express our appreciation for the excellent and timely work of the reviewers.

COMMAD 2006 Technical Co-Sponsors were The Institute of Electrical and Electronic Engineers (IEEE) Electron Device Society (EDS) and Lasers and Electro-Optics Society (LEOS). The conference was supported by The University of Western Australia, the School of Electrical, Electronic and Computer Engineering, The Australian Research Council Nano-technology Network, and The Australian Research Network for Advanced Materials.

Finally, on behalf of all attendees of COMMAD 2006, I would like to express sincere thanks to all members of the Scientific Advisory Committee, the Organising Committee, staff at the UWA Institute of Advanced Studies and, in particular, to Ms Sabine Betts and members of the Microelectronics Research Group for all their contributions in making COMMAD 2006 such a successful conference and a truly memorable event.

COMMAD 2008 will be held in Sydney from July 28 to August 1, 2008, in conjunction with the International Conference on Electronic Materials (ICEM 2008). See http://www.aumrs.com.au/ICEM-08/

Professor Lorenzo Faraone

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