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Analysis of Low-Dimensional Semiconductor Nanostructures with a Self-Consistent Iterative Scheme

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ABSTRACT

In this contribution we propose an iterative scheme for the solution of the coupled Poisson-Schrödinger system in a self-consistent manner. The developed methodology allows us to analyze the combined effects of piezoelectricity, spontaneous polarization, and the charge density in low-dimensional semiconductor nanostructures. These effects are analyzed here on an example of a wurtzite type semiconductor heterojunction. It is shown that such effects may influence substantially the electronic states and quasi-Fermi level energies of the nanostructures, in particular when compared to one-step calculations based on the conventional schemes. A major emphasis is given to two different types of mechanical boundary conditions.

1. INTRODUCTION

Finite element techniques provide a natural tool to apply in the analysis of low-dimensional semiconductor nanostructures. Optoelectronic properties of such structures can be analyzed mathematically with a coupled Poisson-Schrödinger model. However, a number of effects, that may influence the electronic states, are often omitted from such analyses. With new devices based on strained semiconductor heterojunctions, exploration of new technologies based on AlN/GaN, ZnO/MgO materials and other wide bandgap wurtzite heterostructures (e.g.[1–3]), there is an increasing need to incorporate such effects at the level of modelling. Recently, in ref.[4] we discussed the influence of lattice misfit induced strain and piezoelectric effect on the resonant frequency. New applications in photonics and optoelectronics and continuing technological miniaturizations require further attention to additional effects such as the charge density effect along with the quantification of its influence on the quantum-mechanical states of the nanostructures. Practical implementations of these effects into the existing codes require the development of self-consistent schemes for the Poisson-Schrödinger model.

2. MODEL FORMULATION

We start from the coupled equations of piezoelectricity:

$$\nabla \cdot \boldsymbol{\sigma} = 0 \,, \tag{1}$$

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

where e is the (positive) electronic charge, N_d is the donor density, and $n(\mathbf{x})$ is the carrier electron density. In what follows, the influence of acceptors and holes in the structure are neglected. The above equations are coupled by the following constitutive relationships, valid for the material model of the crystalline Bravais lattice of the wurtzite type:

$$\boldsymbol{\sigma} = \boldsymbol{c\varepsilon} - \boldsymbol{eE} \,, \tag{3}$$

$$\boldsymbol{D} = \boldsymbol{\epsilon E} + \boldsymbol{e\varepsilon} + \boldsymbol{P}_{\rm sp} \,, \tag{4}$$

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

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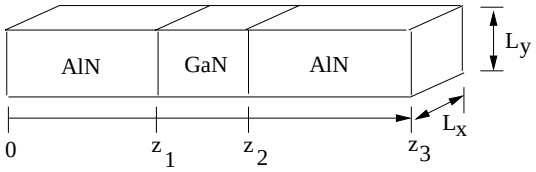

Figure 1. Three layer system with the GaN well in the AlN barriers.

of piezoelectric constants. The strain tensor is defined in a standard manner, accounting for thermal effects as follows:

$$\boldsymbol{\varepsilon} = \frac{1}{2}[(\nabla \boldsymbol{u}(\mathbf{x})) + (\nabla \boldsymbol{u}(\boldsymbol{x}))^T] - \boldsymbol{\varepsilon}^0(\mathbf{x}) + \boldsymbol{\alpha}\Delta T \ , \tag{5}$$

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). The last part on the right hand side of Eq. (5) is the thermal strain, where $\boldsymbol{\alpha}$ 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 its quasi-static approximation

$$\boldsymbol{E} = -\nabla\phi, \tag{6}$$

where ϕ is the electric potential. For simplicity, all discussions that follow will center around a three-layer nanostructure of the well type. In Fig. 1 such a structure is presented for the GaN well and the AlN barriers. In situations like this, the original problem can be reduced to a one-dimensional model where we consider the case: $n(\mathbf{x}) = n(z)$. According to the Fermi-Dirac distribution, we have

$$n(z) = 2\sum_{j=0}^{N} \int_{k_x^{(m)}=0}^{k_x^{(m_{\max})}} \int_{k_y^{(m)}=0}^{k_y^{(n_{\max})}} \frac{L_x L_y}{(2\pi)^2} |\Psi^{(j,m,n)}(z)|^2 f(E^{(j,m,n)}, E_{FL}) dk_x dk_y \ , \tag{7}$$

where N is the number of conduction subbands and the wavenumber $|\boldsymbol{k}|$ lies within approximately 5% of the Brillouin zone (sufficient to evaluate the integral accurately for typical carrier densities). The function f in Eq. (7) is the Fermi-Dirac distribution function given by

$$f(E^{(j,m,n)}) = \left[1 + \exp\left(\frac{E^{(j,m,n)} - E_{FL}}{k_B T}\right)\right]^{-1} \ , \tag{8}$$

where E_{FL} is the quasi-Fermi level energy, k_B is the Boltzmann constant, and $(E^{(j,m,n)}, \Psi^{(j,m,n)})$ are the eigen-pairs in the Schrödinger equation:

$$H\Psi = E\Psi \ . \tag{9}$$

3. SOLVING POISSON-SCHRÖDINGER EQUATIONS VIA AN ITERATIVE SCHEME

Conventional methodologies typically lead to one-step calculations where, assuming some known distribution of charge, the Poisson equation is solved first. Then, the band structure is computed for an assumed value of the Fermi level energy. Although simple, this approach has a number of serious disadvantages. Indeed, to get a better approximation to the problem solution, we have to determine the quasi-Fermi level energy accurately. This is the main idea of the proposed scheme where both, the Fermi level energy and the quantum-mechanical states, are determined through iterations. Piezoelectricity and spontaneous polarization are also accounted for while solving the Poisson equation. The iterative procedures is summarized in Fig. 2.

4. COMPUTATIONAL EXPERIMENTS

We analyze two types of mechanical boundary conditions:

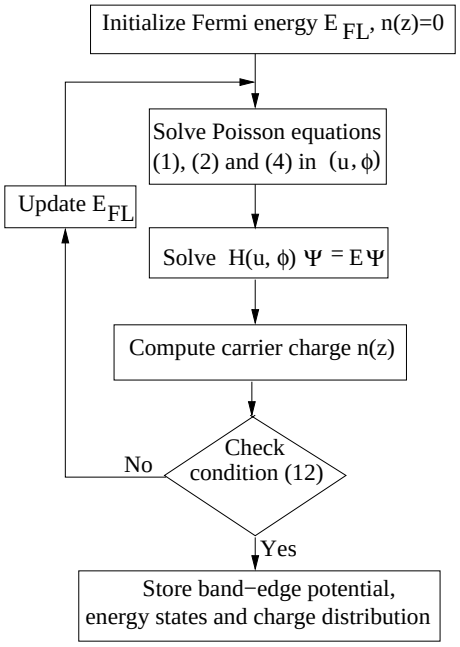

Figure 2. Block diagram showing the self-consistent Poisson-Schrodinger scheme.

Table 1. Conduction band energies (eV) under the fixed-fixed boundary condition ($u(0)_z = 0$, $u(z_3) = 0$) and the fixed-free boundary condition ($u(0)_z = 0$, $\sigma(z_3)_{zz} = 0$) without the self-consistent Poisson-Schrodinger scheme. Conduction-band offset: $H_c = 0$ in GaN and $H_c = 1.955$ eV in AlN.

State	Fixed-free	Fixed-fixed
1	1.0522	1.0798
2	1.2320	1.2601
3	1.3793	1.4078
4	1.5132	1.5421
5	1.6561	1.6851
6	1.8282	1.8572
7	2.0345	2.0636
8	2.2736	2.3028

- perfectly restrained boundary condition: $u(0) = 0$, $u(L_z) = 0$, and
- stress-free boundary condition: $u(0)_z = 0$, $\sigma(L_z)_{zz} = 0$.

Figures 3(a), (b), (c) and (d) show the displacement, electric potential, strain and electric field, respectively, for these two cases. Note that the stress-free boundary condition represents a free-surface condition at $z = L_z$. We apply the electrical boundary conditions at $z = 0, L_z$: $e\phi(0) = e\phi(L_z) = 1.1$ eV, that is approximately 60% of the conduction-band energy offset. All the effects, such as lattice misfit, piezoelectricity and spontaneous polarization have been included in the calculations.

Observe by comparing Figs. 3(a) and (c) that the magnitude of strain changes drastically due to change in the mechanical boundary condition without any significant change in the electric potential. Such a change in the strain affects the conduction band energies, which is clear from Table 1. Figs. 3(b) indicates that although constant electrical potential ($\phi = 1.1/e$ V) is applied at the boundaries, there is a significant change in the

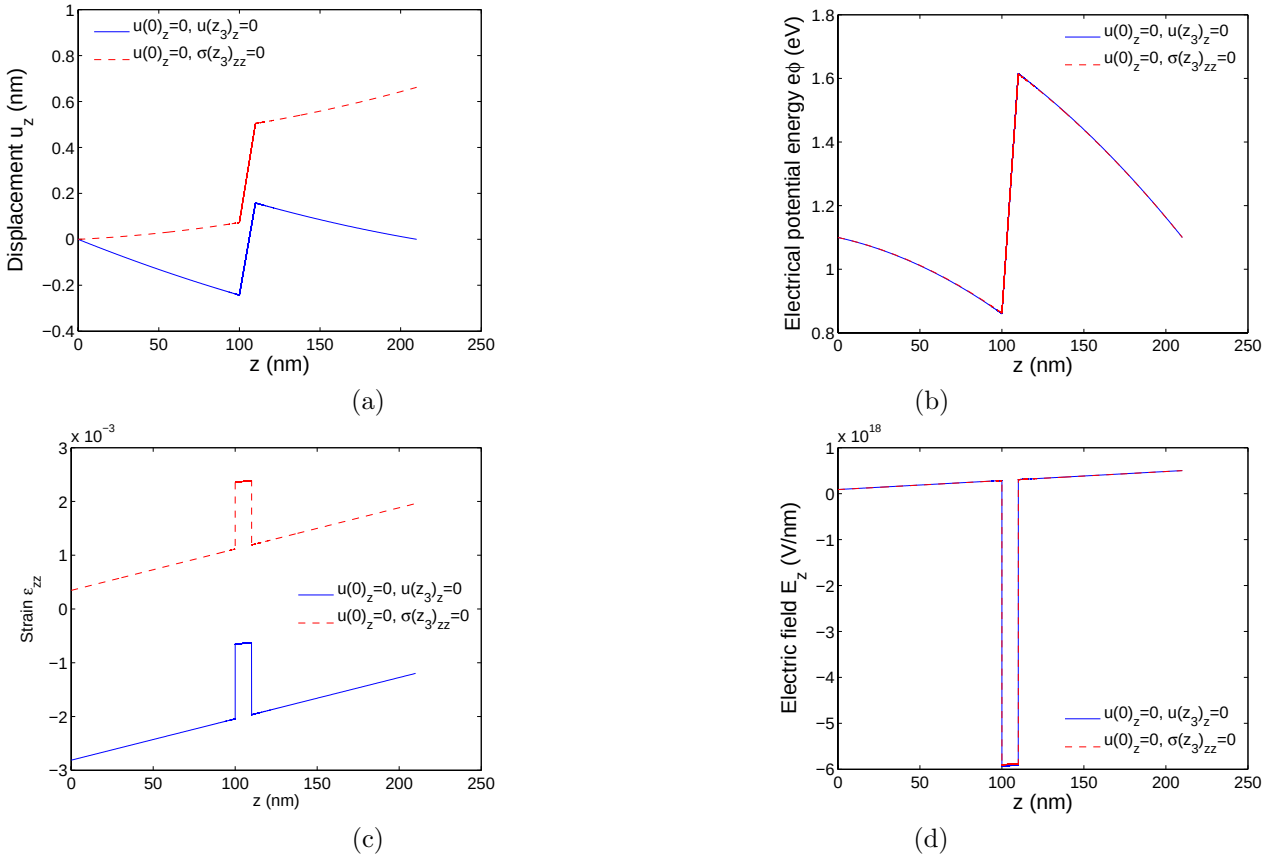

Figure 3. (a) Displacement u_z (b) electrical potential energy $e\phi$ (c) strain ε_{zz} and (d) electric field E_z under fixed-fixed and fixed-free boundary conditions applied at the two outer edges of the AlN barrier. Electric potential applied at the boundaries: $\phi(z=0) = \phi(z_3 = L_z) = 1.1/e$ V.

electric potential (≈ 0.8 V) across the interfaces and accordingly in the electric field as shown in Fig. 3(d). This effect is due due to the coupled nature of piezoelectricity in the heterojunction.

5. CONCLUSIONS

A self-consistent iterative scheme for solving the coupled Poisson-Schrödinger system has been developed and applied to the analysis of optoelectronic properties of low-dimensional semiconductor nanostructures, with examplifications given for AlN/GaN heterojunctions.

REFERENCES

1. B. Jogai, J.D. Albrecht and E. Pan, J. Appl. Phy., **94**(10), 6566-6572 (2003).
2. V.A. Fonoberov and A.A. Balandin, J. Appl. Phys., **94**(11), 7178-7186 (2003).
3. V.A. Fonoberov and A.A. Balandin, J. Vac. Sci. Technol. B, **22**(4), 2190-2194 (2004).
4. M. Willatzen, B. Lassen, L.C. Lew Yan Voon and R.V.N. Melnik, J. Appl. Phys. **100**, 024302 (2006).