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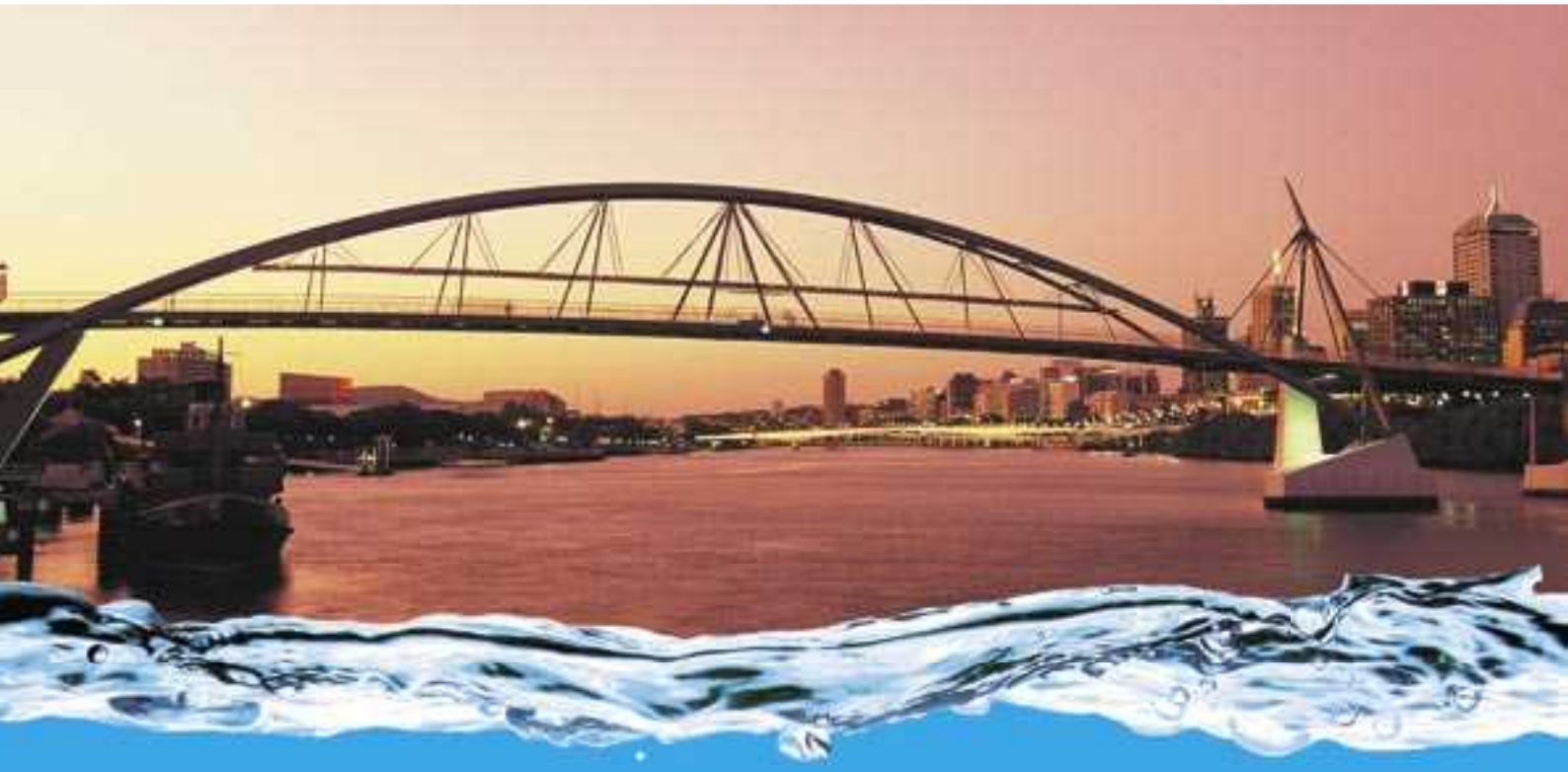

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COUPLED MODELING OF STRAINED AlN/GaN HETEROJUNCTIONS

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Abstract
In this contribution, we report a model allowing to analyze simultaneously the effects of piezoelectricity, spontaneous polarization and the charge density on the electronic states and the quasi-Fermi level energy in wurtzite type semiconductor heterojunctions. We develop a self-consistent iterative scheme for the solution of the coupled Poisson-Schrödinger type integro-differential model and implement it in a finite element code. Results, demonstrated on an example of AlN/GaN heterojunctions, show a pronounced influence of charge density and piezoelectricity on the quasi-Fermi energy level.

Introduction
Wide bandgap wurtzite heterostructures, such as AlN/GaN and ZnO/MgO, are promising candidates for various optoelectronic device applications and some recent models have already emphasized the importance of piezoelectric effects in the development of their applications (e.g., Jogai et al 2003; Fonoberov and Balandin 2003). Our earlier results (Willatzen et al, 2006) highlighted the importance of coupled effects in the context of the influence of lattice misfit induced strain and the influence of the piezoelectric effect on the resonant frequency. For photonic device applications, an additional (integral) effect of the charge density becomes also important. This effect influences quantum-mechanical states of the system in a sense that the amount of net charges in the heterojunction determines the Fermi level energy of the device. Hence, it is important to determine how strongly the strain and the piezoelectric effect influence the Fermi level, in particular when the device size becomes smaller. In this case, it is essential to develop an efficient self-consistent scheme for the solution of the coupled Poisson-Schrödinger model, accounting for the effects discusssed above. We exemplify our theory with the analysis of a three-layer system.

Coupled Poisson-Schrödinger and Material Models
In what follows, we describe a coupling procedure for the Poisson and Schrödinger models in a consistent manner. The resulting nonlinear system of equations is solved numerically and our discussion is focused on a representative example of a three-layer system (a finite size AlN/GaN heterojunction), as depicted in Fig. 1. Let E_{FL} be the quasi-Fermi level energy and k_B be the Boltzmann constant. Then, the Fermi-Dirac distribution function is given by

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

where$(E^{(j,m,n)}, \Psi^{(j,m,n)})$ are the eigenpairs determined by the Schrödinger equation:

$$H\Psi = E\Psi \, . \tag{2}$$

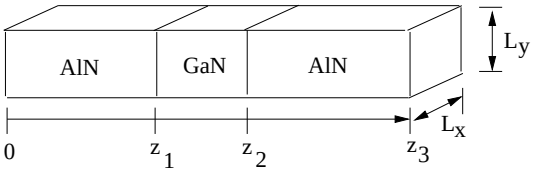


Figure 1: Three layer system with the GaN well in the AlN barriers.

For the one-band model, applicable to the depicted AlN/GaN heterojunction, we have

$$\Psi = \frac{1}{\sqrt{L_x L_y}} e^{ik_x^{(m)}x + ik_y^{(n)}y} \chi(z) \ , \quad k_x^{(m)} = m\frac{2\pi}{L_x} \ , \quad k_y^{(n)} = n\frac{2\pi}{L_y} \ , \tag{3}$$

where $m \in [0, m_{\max}]$, $n \in [0, n_{\max}]$ are chosen in such a way that approximately 5% of the Brillouin zone is included in the double integral connecting $n(z)$ and f. This integral, used in determining the electron density, acts as a coupling term which is changing through iterations until the system equilibrium is reached. As usual, the envelope function parts are normalized. Note that for the one-band model for electrons the Hamiltonian H in Eq. (2) can be represented in the following form

$$H = \frac{\hbar^2}{2m_0}\left[-\frac{\partial}{\partial z}\left(\frac{1}{m_e^{||}}\frac{\partial}{\partial z}\right)\right] + \frac{\hbar^2}{2m_0}\left[\frac{k_x^{(m)^2} + k_y^{(n)^2}}{m_e^{\perp}}\right] + H_c + H_c^{\varepsilon} + e\phi \ , \tag{4}$$

where the first term in the right hand side denotes the z-part kinetic energy term with $m_0 m_e^{||}$ ($m_0 m_e^{\perp}$) being the effective mass of the electron for motion parallel (perpendicular) to [0001]. The second term in Eq. (4) is the x, y-part kinetic energy assuming parabolic bands for the lateral directions. H_c is the conduction-band offset for the unstrained material, and $H_c^{\varepsilon} = a_c \mathrm{Tr}(\boldsymbol{\varepsilon})$ is the conduction band energy offset due to strain and piezoelectricity (see ref. [**?**]). The last two terms in the right hand side of Eq. (4) are obtained by solving the Poisson equation within an iterative loop.

The coupled equations of piezoelectricity for this system can be presented in the following general form:

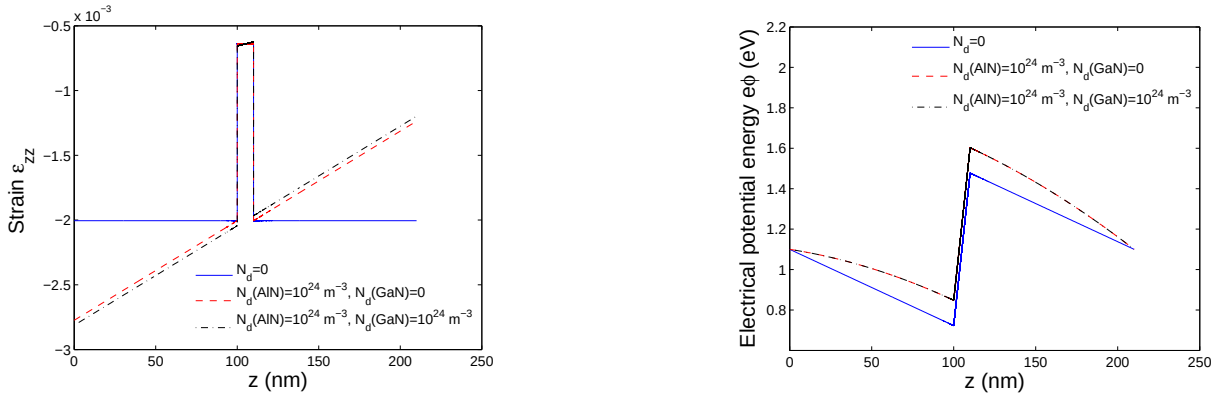
$$\nabla \cdot \boldsymbol{\sigma} = 0 \ , \tag{5a}$$

$$\nabla \cdot \boldsymbol{D} = e(N_d - n(\mathbf{x})) \ , \tag{5b}$$

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 acceptors and holes in the structure. Equations (5a) and (5b) are converted into the 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.

Results and Discussion

First, we analyzed the effect of piezoelectricity and spontaneous polarization based on comparison of four cases: (1) without lattice misfit, piezoelectricity, and spontaneous polarization, (2) without spontaneous polarization, with lattice misfit and piezoelectricity, (3) without lattice misfit and piezoelectricity, with spontaneous polarization, and (4) with lattice misfit, piezoelectricity, and spontaneous polarization. By applying the developed iterative scheme, we obtained the Fermi level energy, the magnitude of $n(z)$ at the well center and the band energies. For all the above four cases, we have observed confinement shapes very similar to those obtained without iteration. However, the results obtained with the developed iterative scheme, clearly indicate that the Fermi



(a) (b)

Figure 2: (a) Strain ε_{zz} and (b) electrical potential energy $e\phi$ due to various values of the net donor density N_d.

level shifts significantly due to piezoelectricity, spontaneous polarization, and coupling effects. Our implementation procedure was based on the finite element methodology, so that the strain field and the electric field were equilibriated due to the minimization of total energies in a variational sense.

Next, the effect of electron carrier distributions is analyzed with the developed iterative scheme and compared for three profiles of the net donor density distribution: (1): $N_d = 0$, (2): $N_d = 1 \times 10^{24}$ m^{-3} throughout the AlN barrier layers and $N_d = 0$ in the well, (3): $N_d = 1 \times 10^{24}$ m^{-3} throughout the barrier and well. In this computational experiment fixed-fixed boundary conditions ($u(0) = 0$, $u(L_z) = 0$) have been employed. Figures 2(a) and (b) show the resulting strain and the electric potential, respectively. While the strain does not change in a pronounced manner, the electric potential increases by approximately 0.4 eV when nonzero N_d is applied.

Conclusions

A self-consistent iterative scheme was developed for the solution of the coupled Poisson-Schrödinger model. The implementation of the scheme was carried out in the finite element methodology framework and the results were presented for AlN/GaN heterojunctions. The results demonstrated a pronounced influence of charge density and piezoelectricity on the quasi-Fermi energy level. The developed scheme can be applied to the analysis of other nano-devices subjected to different optoelectronic excitations.

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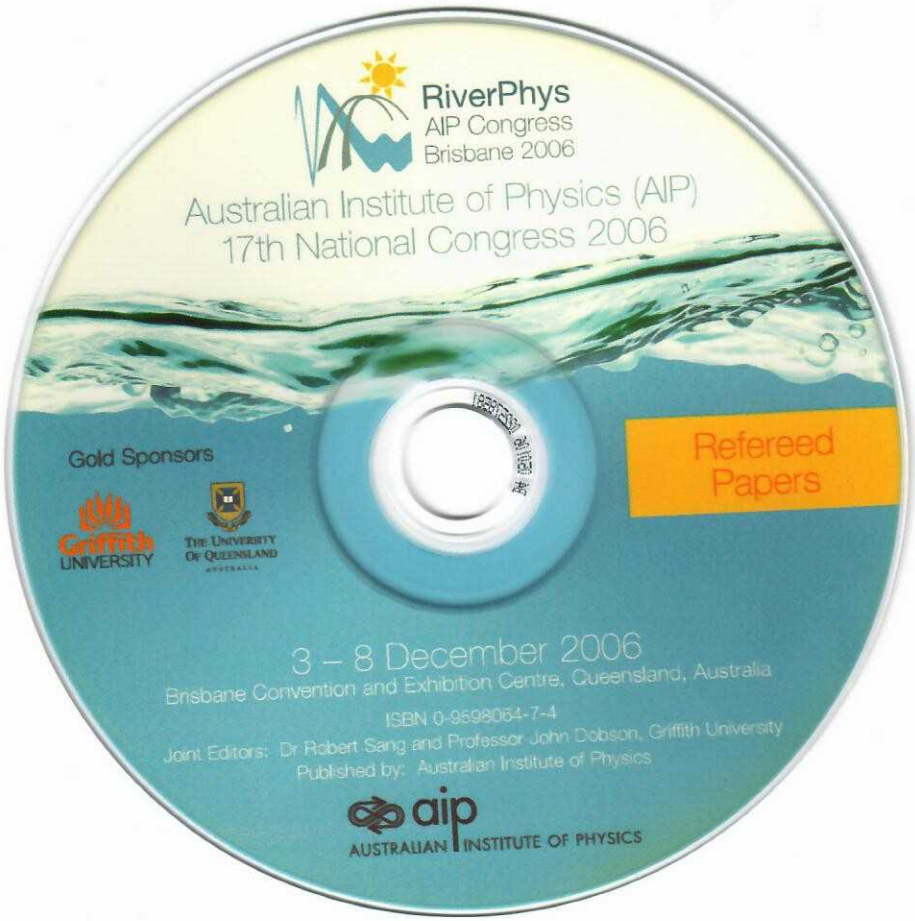
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