Modeling of GaN-based heterostructure devices

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Self-consistent quantum models of GaN-based nanostructures are presented. We report on the calculation of electrical characteristics of AlGaN/GaN heterojunction field effect transistors through an optimized effective mass approach based on the self-consistent solution of the Schrödinger and Poisson equations coupled to a quasi-2D model for the current flow.

INTRODUCTION

The realization of green-blue LEDs and lasers on one side, and of power HEMTs on the other side, has focused a lot of attention to nitride-based heterostructures. While green-blue sources are sought for displays, light bulbs, DVD drivers, AlGaN/GaN modulation doped- field-effect transistors (MODFETs) are extremely attractive due to their potential use for high voltage and high power operation at microwave frequencies. High peak electron velocity, saturation velocity, thermal stability and breakdown fields are in fact very appealing properties of nitride materials for such applications. When grown in the wurtzite structure, actually the most interesting one, nitrides display a non-zero macroscopic polarization, comprising both a spontaneous and a piezoelectric component. Such polarization induces an internal electric field, which modifies quite profoundly the properties of nitride-based heterotructures with respect to more standard systems based for example on GaAs. Because of the polarization field, we can have a strong (width-dependent) Stark shift in the luminescence of nitride-based quantum wells, or growth-direction dependence of the channel properties of HEMTs. The complicate wurtzite structure and the presence of such internal field make the simulation of nitride-based devices a formidable task. Microscopic approaches are required in order to reduce the number of unknown parameters needed for device simulation.
In the following we consider the simulation of GaN-based nanostructured devices by means of self-consistent quantum mechanical approaches. For optical properties, where the detailed knowledge of both conduction and valence band is required, a tight-binding method should be considered [Di Carlo et al. (1), Della Sala et al. (2)]. However, for the calculation of the current in the quantized channel of a nitride HEMT, a self-consistent effective mass approach, tailored with tight-binding extract parameters, gives reliable results .

MODEL AND RESULTS

In order to study the mechanisms of channel formation and of current flow in GaN based MODFET, Schrödinger's equation can be used self-consistently coupled with Poisson equation .
Within the effective mass theory, Schrödinger's equation takes the form [Bastard (3), Lugli et al.(4)] :

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left(\frac{1}{m(z)}\frac{d}{dz}\right)\varphi + \left(eV(z)+\Delta E(z)\right)\varphi = E\varphi \qquad (1)$$

where *m(z)* is the position dependent effective mass, *V(x)* the electrostatic potential, *ΔE* the band discontinuity, φ the electron wavefunction and *E* the electron energy. Non-parabolicity may induce deviations from the simple parabolic band model, however this will not substantially change our results.
In the nitride semiconductors grown in the wurtzite structure, the presence of spontaneous and piezoelectric polarization effects implies that Poisson equation has to be solved for the displacement field, *D(z)*

$$\frac{d}{dz}D(z) = \frac{d}{dz}\left(-\varepsilon(z)\frac{d}{dz}V(z)+P(z)\right) = e\left(p(z)-n(z)+N_D^+-N_A^-\right) \qquad (2)$$

where *ε(z)* is the position-dependent dielectric constant, *P* the total polarization, *n(p)* the electron(holes) charge concentration and N_D^+(N_A^-) the ionized donor(acceptor) density. The total polarization charge can be written as P_{tot}= P_{piezo}+P_{spont} , where P_{piezo} is the piezoelectric charge caused by the lattice mismatch (mis) and by the thermal strain (ts) [P_{piezo} = P_{mis} + P_{ts}], whereas P_{spont} represents the spontaneous polarizability of the GaN/AlGaN interface, as clearly demonstrated by the recent works of Bernardini et al. [5]. The piezoelectric charge induced by the lattice in-plane

mismatch ($\sigma_{\parallel}$) can be calculated as given in [5]. Since the layers are grown on thick GaN buffer layers, we expect that the GaN layers are relaxed and take the bulk GaN lattice constant of the buffer (3.189 A). Moreover, we assume that the AlGaN layers grow pseudomorphically in our structures and undergo a tensile in-plane strain $\sigma_{\parallel}$. We neglect the thermal strain in our calculations. As far as the spontaneous polarization charge is concerned, we take the recent data of [5], leading to P_{sp}= -0.029 C/m^2 for the GaN and P^b_{sp}= -0.08 C/m^2, for the AlN. The spontaneous polarization for the AlGaN alloy has been obtained by linear interpolation of the binary compound values.

A self-consistent procedure has been set up, where the potential V is obtained using Eq. (2) from an initial guess of the mobile charge concentration, and then inserted into the Schrödinger's equation, (Eq. (1)) which is solved to obtain the energy levels and wavefunctions of the system. The new electron charge density is then calculated by applying Fermi statistics. The calculated density is than plugged into Poisson equation (Eq. (2)) and the iteration repeated until convergence is achieved. Convergence of the self-consistent algorithm can be improved by adopting special relaxation techniques.Here we have used a first order expansion of the model reported in Trellakis et al. [6].

In the following, we show the results for a single heterojunction AlGaN/GaN MODFET, consisting of a 150 Å n-doped (n=10^{18}cm^{-3}) AlGaN layer, a 50 Å unintentionally doped AlGaN region and a thick GaN buffer, and for an inverted double heterojunction DHMODFET consisting of 300 Å unintentionally doped GaN, 50 Å unintentionally doped AlGaN, 150 Å n-doped (n=10^{18}cm^{-3}) AlGaN, 300 Å unintentionally doped AlGaN layers on a thick GaN buffer. We consider a residual doping of 10^{17} cm^{-3} for both GaN and AlGaN layers. Calculations have been performed for $Al_xGa_{1-x}N$ regions with Al concentration of x=0.1, 0.2, 0.3, 0.4. As discussed above, polarization effects are quite important in nitride-based MODFET's. The conduction band edge profile for the MODFET grown along the [0001] direction is depicted in Fig. 1 for the cases i) with both spontaneous and piezoelectric polarization fields, ii) without considering any polarization field, iii) with only the piezoelectric polarization fields. The difference in piezoelectric and spontaneous polarization between AlGaN and GaN layer determines a fixed 2D charge density at the interface between the two materials. For the [0001] growth direction the polarization difference between the two materials induces a positive charge (σ = +1.12x10^{13} cm^{-2}) at the AlGaN/GaN interface. Electrons are attracted by this positive charge, and tend to accumulate at the interface, thus forming a conductive channel. Moreover, the high electric field induced by the interface charge, favors the build up of a large channel density and of a strong channel confinement. The distribution of the free electron charge in the channel is shown in Fig. 2 for several values of the Al concentration of the AlGaN layer. Increasing the Al content induces a larger polarization charge at the GaN/AlGaN interface and consequently a higher channel electron concentration.

The conduction band edge profile and electron and hole densities for the DHMODFET grown in the [000-1] direction are shown in Fig. 3. As for the MODFET, the presence of the fixed and positive polarization charge at the GaN/AlGaN interface induces the formation of an electron channel, which is not present in the absence of the polarization charge. For the DHMODFET, a $-\sigma$ polarization charge is also present at the end of AlGaN region (i.e. at the AlGaN/GaN interface), and an accumulation region for holes can be present, if holes are available. Similarly to the [0001] grown MODFET, a larger Al content of the AlGaN layer induces a larger polarization charge at the GaN/AlGaN interface and consequently an increase of electron concentration in the channel.

The channel charge density is therefore controlled by two factors: i) the gate bias as in traditional MODFET device, ii) the Al content of the AlGaN layer, which tailors the polarization field. Charge control in nitride-based devices can be achieved by adjusting two independent parameters and thus with a larger degree of flexibility with respect to traditional devices.

We have also calculated the I-V characteristics of nitride based HEMT by using a quasi two-dimensional transport model. In such model, we solve for the quantized states and electron density in a series of 1D sections perpendicular to the gate. For each section, Schrödinger-Poisson equations are solved taking as a boundary condition the proper potential (determined from the source-to-drain bias). When a drain bias (V_D) is applied, the potential along the channel may be considered to vary gradually from the source to the drain. In this situation it is possible to calculate the sheet charge density in different sections of the channel, provided that one considers the proper potential V(x) (on the top surface). Since generally V_D is positive, while V_S is zero, V(x) contributes to the channel depletion. The numerical solution is based on a discretization of the gate region on N sections, each one with amplitude *h*. Given the (*i*-1)-th section potential, the *i*-th potential is $V_i = V_i - 1 + F_i\, h$ where F_i is the *i*-th section electric field. We have then N relations:

$$I_{DS} = qW \frac{\mu_0 F_i}{1+\frac{F_i}{F_C}} n\left(V_G - V_{i-1} - F_i h\right) \qquad (3)$$

Since the (*i*-1)-th section potential is known from the previous step, this is a non-linear equation in the unknown F_i. Solving iteratively for all the N sections, one obtains the value of drain voltage V_D consistent with the assumed current. Repeating this procedure for a suitable range of values of I_{DS}, one obtains the set of corresponding V_{DS} values and builds the device I-V characteristics. We show in fig. 4 the simulated I_{DS} vs. V_{DS} characteristics for a $Al_{0.2}Ga_{0.8}N$/GaN HEMT, grown in the [0001] direction, with gate length L = 0.3 μm. We have chosen a drain and source contact resistivity of about 1 Ωmm. We use a saturation velocity of 2.5 x 10^7 cm/s [Morkoc (7)], while for the low field mobility

we choose a value of μ_0 = 1100 cm^2/Vs, slightly higher than the GaN bulk value, according to the experimental and theoretical results for similar devices [Oberhuber et al.(8), Bhapkar et al.(9), Murphy et al (10), Wu et al. (11)]. By comparing the results of fig. 4 with those obtained with a larger Al concentration in the barrier we find that the current flowing in the devices depends strongly on the Al content of the top layer. This is essentially due to the increasing of the channel electron density induced by the enhanced polarization charge when increasing the Al contents. This peculiarity of the MODFET should be considered in the design of these devices since fluctuation of the alloy composition of the top layer may induce large variation with respect to nominal electrical values of the device.

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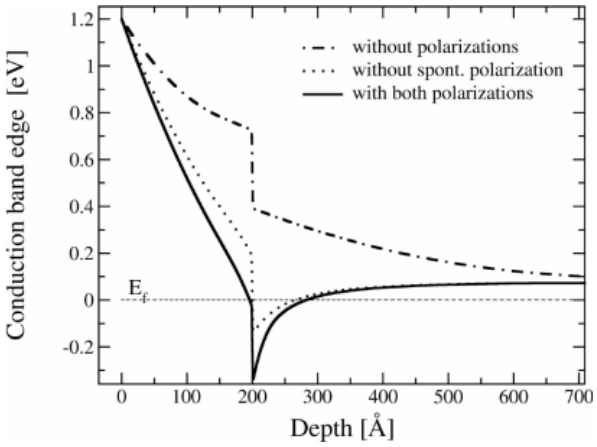

Fig. 1 Conduction band profiles for an AlGaN/GaN MODFET

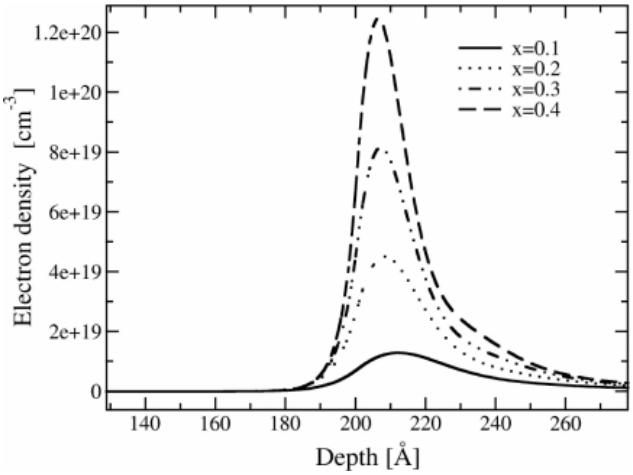

Fig. 2 Electron density distribution in the MODFET channel as a function of Al concentration x

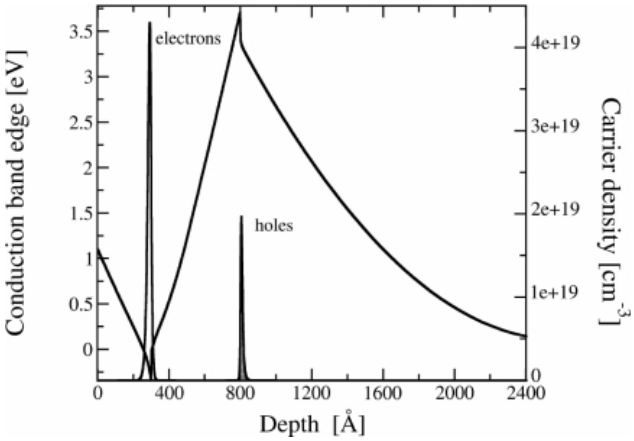

Fig. 3 Conduction band edge and electron and hole densities in an inverted DHMODFET

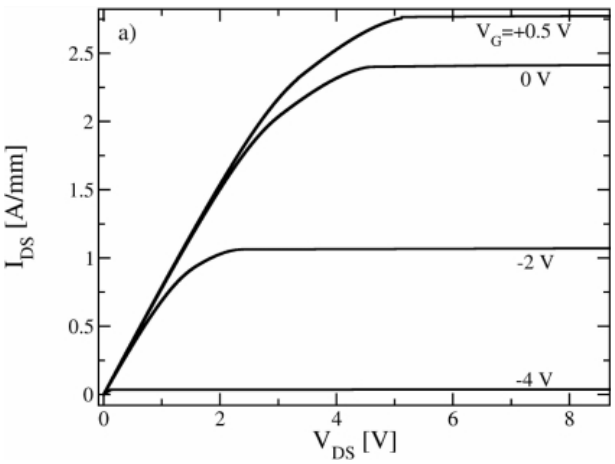

Fig. 4 I-V characteristics for $Al_{0.2}Ga_{0.8}N/GaN$ MODFET