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Simulation of characteristics of microwave transistors with AlGaN heterostructures

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Abstract. In work results of researches in the area of simulation of electrical characteristics of the AlGaN/GaN field-effect transistor are provided. The considerable difference of transport processes in case of the strong and feeble electrical polarization is shown. The role of capture of centers in volume of a buffer layer GaN is analyzed and it is shown that deep interruptions can influence considerably on distribution of electrostatic potential and density of electrons in a buffer layer. In case of high concentration of interruptions there is a sharp lowering of density of the free electrons with increase of distance from the channel, the current density in the depth of a buffer layer decreases.

1. Introduction

GaN field-effect heterojunction transistors became the main type of high-power semiconductor microwave devices. Large band-gap width of gallium nitride (3.4 eV) and low collisional ionization coefficient enable operation of devices with high bias voltages. AlGaN/GaN heterojunction transistors provide quite high electron density in the channel (about 10^{13} cm^{-2}), which taking into account large value of saturated electron velocity ($2.7 \cdot 10^7$ cm/s) may provide drain current of several amperes per millimeter of channel width.

At present, a number of publications are dedicated to aspects of instrumental-technological modeling of GaN-based transistor structures (see, for example, [1-5]), but the results obtained in these publications are not sufficiently complete. Within the framework of this paper, we propose methods for modeling effects associated with existence of deep centers and polarization and their influence on performance of microwave transistors and present corresponding numerical calculations.

2. Formulation of the problem

Mechanisms of high electron density appearance in the channel were considered in [6 and 7]. These mechanisms are associated with the effects of spontaneous and piezoelectric polarization in nitride semiconductor materials with wurtzite type crystal lattice. Hexagonal wurtzite lattice has no center of symmetry, and interatomic bond contains a considerable proportion of ionic component. Therefore, spontaneous polarization P_{SP} occurs in such crystals. P_{SP} vector is parallel to axis c of the lattice and is directed opposite to the direction of normal to crystal face, on the surface of which cations (Ga$^+$, Al$^+$) are located. Polarization value depends on chemical composition of the material. In Al$_x$Ga$_{1-x}$N P_{SP} value is approximately linearly dependent on Al content, and at x=1 it is three times higher than in

GaN. Piezoelectric polarization P$_{PE}$ depends on deformation of crystal lattice under mechanical stresses. Relationship between P$_{PE}$ value and direction with tensor of mechanical stresses is determined by tensor of piezoelectric coefficients.

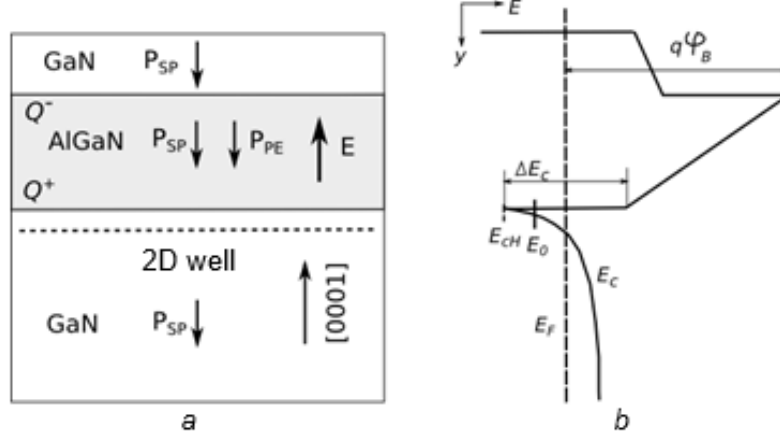Polarization pattern in heterostructure typical of gallium nitride transistors is shown in Fig. 1.

Figure 1. Location of layers (*a*) and dependence of energy of *Ec* conductivity band bottom on distance from the surface (*b*) in the structure of field-effect transistor. Energy diagram corresponds with thermodynamic equilibrium condition and presence of metal electrode on the surface.

Structure oriented along the crystal axis [0001] consists of thick lower GaN layer, AlGaN layer and thin upper GaN layer. Spontaneous polarization P$_{SP}$ occurs in each of these layers. Due to difference in lattice parameter *a* in AlGaN and GaN, middle layer is exposed to extension, so piezoelectric polarization P$_{PE}$ coincident in direction with spontaneous polarization occurs in it. In upper rather thin GaN layer piezopolarization is insignificant due to relaxation. Condition for continuity of electrical induction in the presence of difference in polarization values in different sides of heterojunction is taken into account by introducing Q^+ and Q^- charges on corresponding heterointerfaces. Surface density of Q^+ charges may exceed surface density of qN$_D$d donors in Al$_x$Ga$_{1-x}$N layer with thickness d. As calculated in [4], $Q^+/q=1.4 \times 10^{13}$cm^{-2} at x=0.25; where q – value of elementary charge.

Positive charge on heteroboundary pulls free electrons and, as illustrated in Fig. 1b, potential well with surface electron density n_S is formed on the surface of lower buffer layer. Value of this electron density may be determined using formula given in [3], which defines the change of *Ec* on the thickness of middle barrier layer assumed that there are no charges in it,

$$\frac{dq^2}{\varepsilon_0}\left(\frac{Q^+}{q} - n_s\right) = q\varphi_B - \Delta E_c + \left(E_F - E_{cH}\right) \quad , \qquad (1)$$

where ε_0 – electrical permittivity of vacuum, ε – material relative permeability, $q\varphi_B$ – potential barrier height, ΔE_c – discontinuity of E_c on the boundary, E_F–E_{cH} – distance between Fermi level and conduction band bottom of buffer layer on the boundary. The latter value may be represented in the following form E_F-E_{cH}=(E_F-E_0)+(E_0-E_{cH}), where E_0 – absolute value of energy of the bottom of lower subband in two-dimensional quantum well of triangular profile. Energy intervals included in the latter equation may be expressed in terms of n_S:

$$\left(E_F - E_0\right) = \frac{\pi\hbar}{m}n_S \text{ and } \left(E_0 - E_{cH}\right) = \left(\frac{9\pi\hbar q^2}{g\varepsilon_0\sqrt{gm}}n_S\right)^{2/3} , \qquad (2)$$

where *m* – effective mass of electrons. It should be noted that in the above formulas variables and material parameters depend on composition of Al$_x$Ga$_{1-x}$N. According to numerical calculation performed in [3] n_S=1·10^{13} cm^{-2} at *d*=20 nm and *x*=0.25.

3. Modeling of GaN field-effect transistor

Modeling of characteristics of AlGaN/GaN field-effect transistors was performed in Sentaurus TCAD modeling system. Structural components of the considered transistor are shown in Fig.2. Source/drain contacts are buried, so that they overlap the thickness of channel area of buffer layer. Distance between source and drain is 5 μm, gate length is 0.8 μm, drain is 3 μm away from the gate.
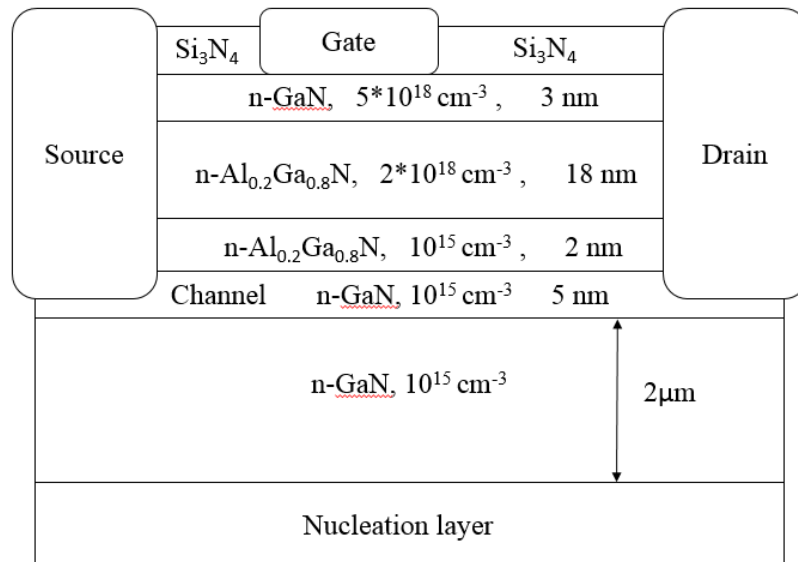

Figure 2. Field-effect transistor structure.

Modeling of structures with heterojunctions and corresponding calculations in particular are based on generalization of Shockley diode theory (Anderson model) and special models of charge transfer process in heterojunctions, which take into account recombination of carriers through surface states, tunneling and both effects simultaneously. At initial stage we investigated dependence of states of spontaneous and piezoelectric polarization of $Al_XGa_{1-X}N$ barrier layer on aluminum content in its composition and the way it affects characteristics of such devices. According to model proposed in [4] at pseudomorphic growth of AlGaN on GaN with AlGaN barrier layer thickness of more than 15 nm, carriers concentration is in quadratic dependence on Al molar content in AlGaN. However, spontaneous polarization is determined not by the absolute value of dipole moment averaged by volume, but by difference of polarization in two different system states, at that the value of macroscopic polarization is also determined by piezoelectric polarization arising due to mismatch of the lattice parameters on heterointerfaces. Polarization effects considered in the program – batch file of characteristics modeling, may be seen in band diagrams and space-charge density distributions shown in Fig. 3.
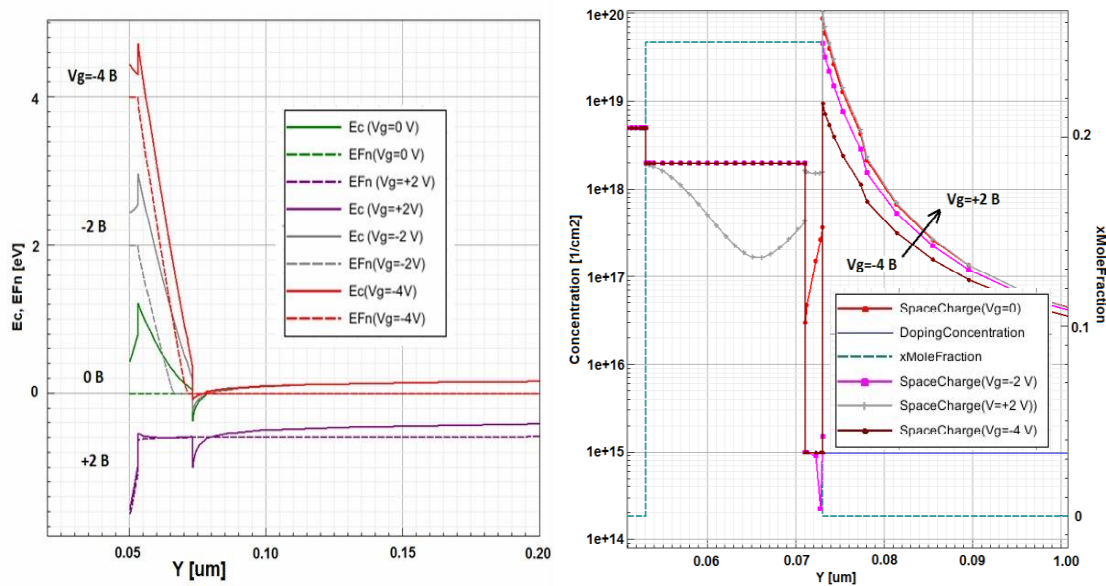
Figure 3. Band diagrams (on the left) and space-charge density distributions (on the right) in section passing through the middle of the gate length at different voltages V_{gs} on it and at voltage on drain V_{ds}=0.

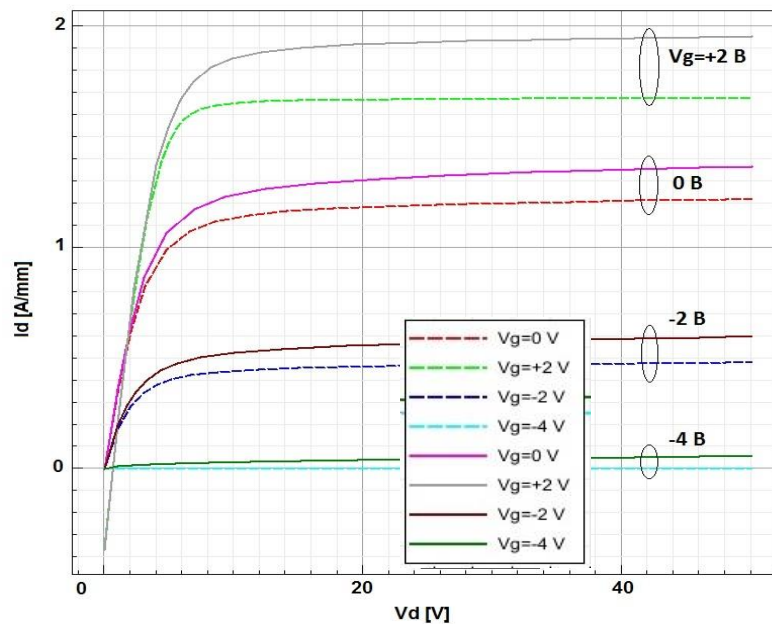$I_d(V_{gs})$ output current-voltage characteristics are shown in Fig. 4.

Figure 4. Families of output current-voltage characteristics of the model without (solid lines) and with (dashed lines) traps in GaN layer.

Increase of negative voltage on the gate reduces electron density n_S in the channel; however, permanence of Q^+ polarization charge causes the intensity of electric field in the barrier to increase, and almost all V_{gs} voltage falls on the barrier layer. At positive V_{gs}, n_S increases and voltage on barrier layer decreases. With further growth of V_{gs}, accumulation of n_S is limited due to electrons pass to the gate through ΔE_c permanent barrier. Fermi quasi-level shift in buffer layer is shown in Fig. 4 and is probably related to the use of ohmic contacts to barrier type source/drain in initial program. This figure shows the

decrease of current increment and, consequently, the decrease of transmission steepness at positive gate bias, which is connected with the above-mentioned dependence of n_S on V_{gs}. Maximum value of steepness in transistor without traps is 3.7 S/mm. In order to clarify the role of traps in GaN they were included in batch file for modeling of instrument characteristics. Specified concentration is 10^{16} cm^{-2}, energy position is in the middle of band-gap, electrons and holes capture cross section is 10^{-18} cm^2. The results obtained are presented in Fig. 5.
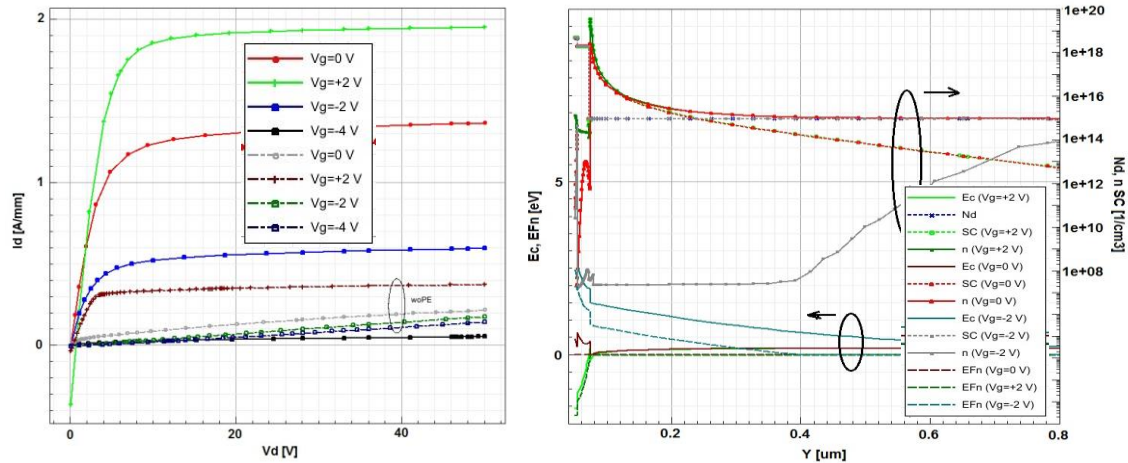

Figure 5. Left field shows output characteristics without (dashed lines) and with (solid lines) taking into account polarization. Right field shows energy diagrams (axis of ordinates is on the left), distribution of electron density and space charge density (axis of ordinates is on the right) in section passing through the middle of the gate length at various V_{gs} and at V_{ds}=0.

As can be seen from Fig. 5, such traps reduce drain current in saturation region by about 10%. Of particular interest is the comparison of modeling results with and without taking into account polarization effects, for which purpose polarization models call commands were excluded from the program. Design and material parameters remained the same. Absence of polarization results in sharp decrease of drain current and change of characteristics of charge carrier transfer in the channel. Insufficient concentration of donors in barrier layer cannot provide high surface electron density in the channel quantum well even at V_{gs}=0 (see the right-hand side of Fig. 5). At negative gate voltage the well is emptied and electric field penetrates into the depth of buffer layer. At V_{gs}=-2 V, thickness of depletion region takes significant part of this layer. Drain current is determined by transfer of electrons through non-depleted part of the buffer.

4. Conclusions
The authors believe that the following provisions and results are new in this paper. Modeling of electrical characteristics of AlGaN/GaN field-effect transistor was performed. Significant difference in transfer of charge carriers in case of strong and weak electric polarization in structural elements is shown. In the absence of polarization effects, localization of current in the region of quantum well is noticeably reduced. Consideration of the role of trapping centers in the volume of GaN buffer layer showed that deep traps may significantly affect distribution of electrostatic potential and electron density in the volume of buffer layer. In case of high concentration of traps, their capture of electrons results in sharper decrease of free electron density with increasing distance from the channel, current density in the depth of buffer layer becomes smaller.

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