Iron-Induced Acceptor Centers in the Gallium Nitride High Electron Mobility Transistor: Thermal Simulation and Analysis

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Abstract—The effect of the presence of iron-induced acceptor centers in the gallium nitride high electron mobility transistor is studied using device physics simulations at elevated temperatures (up to 600 K), as a lattice heat flow equation is solved self-consistently with the Poisson and the continuity equations to account for self-heating effects. It is shown that the acceptor centers intentionally introduced in the buffer layer of the device cause a shift of the input characteristics in the positive direction.

I. INTRODUCTION

Gallium nitride (GaN) is a binary III/V semiconductor with a wide band gap of 3.4 eV, which affords it outstanding properties for applications in high power, high frequency and optoelectronic devices. The excellent breakdown and reasonable transport characteristics of GaN are made full use of in heterojunction field-effect transistors or high electron mobility transistors (HEMTs), which are currently the most widespread electronic nitride devices. The HEMT is a field-effect transistor with a junction between two materials with different band gaps, i.e. heterojunction, used to confine electrons to a triangular-like quantum well.

Unlike the case of some other popular III/V materials such as gallium arsenide and indium phosphide, GaN substrates have only recently been commercially available in semi-insulating and n-conducting forms with dimensions required for electronic device fabrication [1]. The high-pressure growth, processing and dc characterization of HEMTs over semi-insulating bulk GaN substrates were first reported by Khan et al. in 2000 [2]. A continuous-wave power density of 9.4 W/mm at 10 GHz with an associated power-added efficiency of 40 % was obtained by Chu et al. in 2004 for HEMTs on low-dislocation semi-insulting GaN substrates [3]. However, the size and quality limitations and the high production cost of free-standing GaN wafers have yet to be overcome for the commercial success of the GaN-on-GaN technology.

For modern power electronics and microwave applications, GaN films are generally grown at a high temperature by metal organic chemical vapor deposition (MOCVD) or molecular beam epitaxy techniques on silicon, sapphire or silicon carbide substrates. Nowadays, the fabrication of GaN HEMTs is conducted mainly by MOCVD due to its high efficiency and adequate precision. A major problem for nonoptimized growth conditions is unintentional doping responsible for an extremely high background donor concentration and thus persistent electron conductivity. The n-type conductivity of GaN films had earlier been ascribed to the generation of nitrogen vacancies in the GaN crystal [4]. According to a more detailed research, though, the main source of residual electrons is oxygen, an omnipresent shallow-level donor impurity in the MOCVD reactor [5]. Since the buffer layer in the HEMT structure must be designed to insulate the device and confine electrons in the channel, the residual donors should be compensated by deep-level acceptor centers to obtain high resistivity. In [6], the use of iron (Fe) doping to suppress the premature off-state breakdown in GaN HEMTs is described. In this paper, we investigate the effect of the presence of Fe-induced deep-level acceptor centers treated as trap states on the dc characteristics of the GaN HEMT using device physics simulations at elevated temperatures (up to 600 K).

II. STRUCTURE

A two-dimensional schematic representation of the GaN HEMT device structure is shown in Fig. 1. The heterostructure consists of a 1.5 μm GaN buffer layer and a 20 nm aluminum gallium nitride ($Al_{0.21}Ga_{0.79}N$) barrier layer. The thickness and the length of the gate are equal to 3 μm and 0.5 μm, respectively.

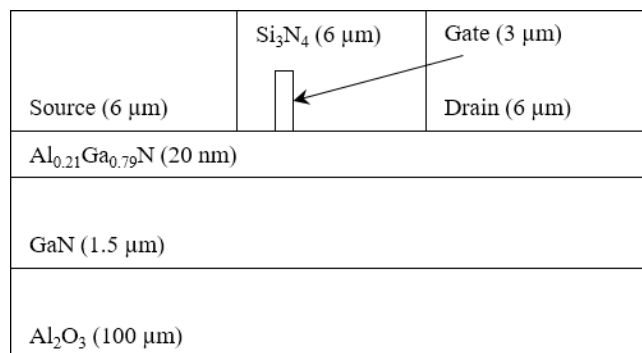The source-to-gate and the gate-to-drain distances are 1 μm and 3.5 μm, respectively.

Fig. 1. GaN HEMT structure (in brackets, the thickness values are indicated)

The surface of the structure is passivated by a 6 μm silicon nitride (Si₃N₄) layer. The thickness of the sapphire (Al₂O₃) substrate is 100 μm. The length of the whole structure equals to 17 μm. The scale factor that represents the third dimension (unsimulated) in two-dimensional simulations is 150 μm.

III. SIMULATION DETAILS

The electrical behavior of a semiconductor device is operated by a mathematical model, which consists of a coupled set of basic partial differential equations linking together the electrostatic potential and the carrier concentration. The general framework of the model is provided by the Poisson and carrier continuity equations. To incorporate the self-heating effects into the simulation, a heat flow equation is solved self-consistently with the primary equations.

A. Poisson and Carrier Continuity Equations

The Poisson equation governs the interaction of the electrostatic potential with the space charge density:

$$\nabla^2\varphi = \frac{q(N_d - N_a - n + p)}{\varepsilon\varepsilon_0}, \tag{1}$$

where φ is the electrostatic potential, q is the elementary charge, N_d and N_a are the donor and acceptor densities, n and p are the electron and hole concentrations, ε is the relative permittivity and ε_0 is the electric constant.

The continuity equations describe how the electron and hole concentrations change during the transport, generation and recombination processes. In a steady state, the generation and recombination rates are equal, the electron and hole concentrations are constant and the continuity equations are given as follows:

$$q\frac{\partial n}{\partial t} = \nabla J_n = 0, \tag{2}$$

$$q\frac{\partial p}{\partial t} = \nabla J_p = 0, \tag{3}$$

where J_n and J_p are the electron and hole current densities (for simplicity, referred to hereafter as the currents).

In accordance with the drift-diffusion transport theory, the driving force for the carriers is the quasi-Fermi level gradients:

$$J_n = q\mu_n n\nabla\varphi_n, \tag{4}$$

$$J_p = q\mu_p p\nabla\varphi_p, \tag{5}$$

where μ_n and μ_p are the electron and hole mobilities, φ_n and φ_p are the quasi-Fermi levels for electrons and holes.

By neglecting the gradient of the intrinsic carrier concentration, the currents can be decomposed into the drift and diffusion ingredients:

$$J_n = q\mu_n nE + qD_n\nabla n, \tag{6}$$

$$J_p = q\mu_p pE + qD_p\nabla p, \tag{7}$$

where D_n and D_p are the diffusivities and E denotes the electric field related to the potential through the Gauss law:

$$E = -\nabla\varphi. \tag{8}$$

It should be noted that the Einstein relationship is tacitly assumed to hold:

$$D_n = V_T\mu_n, \tag{9}$$

$$D_p = V_T\mu_p, \tag{10}$$

where V_T is the thermal voltage:

$$V_T = \frac{\kappa T}{q}, \tag{11}$$

where κ is the Boltzmann constant and T is the temperature.

In case of a single AlGaN/GaN heterostructure, GaN is specified as a reference material, since it has a lower band gap. The electron and hole concentrations are linked to the potential in AlGaN through the following expressions:

$$n = \frac{n_i^{GaN} N_c^{AlGaN}}{N_c^{GaN}}\exp\left(\frac{\varphi + \varphi_n - \chi^{GaN} + \chi^{AlGaN}}{V_T}\right), \tag{12}$$

$$p = \frac{(n_i^{AlGaN})^2 N_c^{GaN}}{n_i^{GaN} N_c^{AlGaN}}\exp\left(\frac{\chi^{GaN} - \chi^{AlGaN} - \varphi - \varphi_p}{V_T}\right), \tag{13}$$

where n_i is the carrier intrinsic concentration, N_c is the effective density of states for electrons and χ is the electron affinity.

The corresponding expressions for GaN are given as follows:

$$n = n_i^{GaN}\exp\left(\frac{\varphi + \varphi_n}{V_T}\right), \tag{14}$$

$$p = n_i^{GaN}\exp\left(\frac{-\varphi - \varphi_p}{V_T}\right). \tag{15}$$

The carrier intrinsic concentration is defined by

$$n_i = \sqrt{N_c N_v}\exp\left(-\frac{E_g}{2V_T}\right), \tag{16}$$

where N_v is the effective density of states for holes and E_g is the band gap.

For calculating the electron mobility in the channel of the GaN HEMT, we employ a user-specified model, which describes the mobility of a two-dimensional electron gas formed at the AlGaN/GaN heterostructure as a function of the carrier concentration and the temperature [7].

Polarization modeling is critical for GaN devices. When polarization effects are simulated, the space charge density in the Poisson equation, which is solved at the nodes located at a heterointerface, is augmented by a polarization-induced charge.

The total spontaneous polarization is defined by the difference between the values for two adjacent materials:

$$P_{sp} = P_{sp}^{GaN} - P_{sp}^{AlGaN}. \tag{17}$$

The relatively thick GaN layer is assumed unstrained, and so the piezoelectric component of polarization is calculated only for the thin AlGaN layer:

$$P_{pe} = 2\frac{a^{GaN} - a^{AlGaN}}{a^{AlGaN}}\left(e_{31} - \frac{e_{33}c_{13}}{c_{33}}\right), \tag{18}$$

where a is the lattice constant, e_{31} and e_{33} are the piezoelectric constants for AlGaN and c_{13} and c_{33} are the elastic constants for AlGaN.

Finally, the total polarization is determined as follows:

$$P = P_{sp} - P_{pe}. \tag{19}$$

Table I compiles the parameters for the AlN/GaN material system used for the polarization simulation.

The temperature dependence of the band gaps for AlN and GaN is commonly fitted to the empirical Varshni form

$$E_g(T) = E_g(0\,\text{K}) - \frac{\alpha T^2}{T + \beta}, \tag{20}$$

where α and β are adjustable parameters.

For AlGaN, the dependence of the band gap on composition is fitted to a simple quadratic form

$$E_g^{AlGaN} = E_g^{AlN}x + E_g^{GaN}(1-x) - \gamma x(1-x), \tag{21}$$

where x is the composition and γ is the so-called bowing parameter equal to 1 [8].

The behavior of a heterojunction depends crucially on the alignment of the energy bands at the interface. According to Anderson's rule, the conduction band discontinuity (offset) is defined by the difference between the two materials electron affinities [9]:

$$\chi^{GaN} - \chi^{AlGaN} = \rho\left(E_g^{AlGaN} - E_g^{GaN}\right), \tag{22}$$

where ρ determines the portion of the band gap difference assigned to the conduction band offset. We take ρ equal to 0.7 and independent of the temperature.

The effective mass in wurtzite crystals is anisotropic. In case of a single band minimum characterized by a longitudinal mass and two transverse masses, the effective mass for the density of states is calculated as the geometric mean of the three masses:

$$m = \left(m_l m_t^2\right)^{1/3}, \tag{23}$$

where m_l and m_t are the longitudinal and transverse effective masses for the density of states.

Equation (23) is valid for both electrons and holes.

The effective density of states for electrons is defined through the electron effective mass as follows:

$$N_c = 2\left(\frac{2\pi m\kappa T}{h^2}\right)^{3/2}, \tag{24}$$

where h is the Planck constant.

The effective density of states for holes is analogous.

Table II shows the band parameters used in the simulations. With the exception of (21), the parameter values for AlGaN are linearly interpolated against composition.

B. Lattice Heat Flow Equation

Simulation of the self-heating effect implies the addition of a lattice heat flow equation to the set of the primary semiconductor device equations. According to Wachutka's thermodynamically accurate model of lattice heating [14], in a steady-state, the lattice heat flow equation is given by

$$H = -\lambda\nabla^2 T, \tag{25}$$

where H is the heat generation rate and λ is the thermal conductivity.

The heat generation rate in the simplest form can be regarded as Joule heat:

$$H = \left(J_n + J_p\right)E. \tag{26}$$

Since the thermal conductivity depends on temperature, the following models are employed for AlN/GaN [15] and Al_2O_3 [16], respectively:

$$\lambda(T) = \lambda(300\,\text{K})\left(\frac{T}{300}\right)^{\delta_1}, \tag{27}$$

$$\lambda(T) = 0.01\left(\frac{\delta_2}{T^{\delta_3}} + \delta_4 T\right), \tag{28}$$

TABLE II.   BAND PARAMETERS

Parameter	Material		Units	References
	AlN	GaN		
E_g (0 K)	6.23	3.507	eV	[8]
α	0.001719	0.000909	eV/K	[8]
β	1462	830	K	[8]
m_l (for electrons)	$0.2938m_e$[a]	$0.1846m_e$	kg	[10]
m_t (for electrons)	$0.3433m_e$	$0.2283m_e$	kg	[10]
m_l (for holes)	$3.53m_e$	$2m_e$	kg	[11]
m_t (for holes)	$11.14m_e$	$2.04m_e$	kg	[11]
ε	8.5	9.5	–	[12][13]

[a.] m_e denotes the electron rest mass

TABLE I.   PARAMETERS FOR THE POLARIZATION SIMULATION [8]

Parameter (300 K)	Material		Units
	AlN	GaN	
a	3.112	3.189	Å
c_{13}	108	106	GPa
c_{33}	373	398	GPa
e_{31}	–0.5	–0.35	C/m²
e_{33}	1.79	1.27	C/m²
P_{sp}	-0.081	-0.029	C/m²

where δ_1, δ_2, δ_3 and δ_4 are the temperature dependence coefficients.

The thermal conductivity for Si_3N_4 is taken constant and equal to 0.027 W/(cm·K) [17].

Table III shows the thermal conductivity model parameters used throughout the simulations:

The parameter values for AlGaN are linearly interpolated against composition.

To solve the lattice heat flow equation, thermal boundary conditions must be imposed. In case of a field-effect transistor, the thermal boundary condition is commonly set at the lowest points of the substrate and has the following form:

$$-\lambda \nabla T = \sigma (T - T_0), \qquad (29)$$

where σ is the heat-transfer coefficient between a material and ambient medium, T_0 is the room temperature.

C. Trapped Charge in the Poisson Equation

Trap centers with an associated energy lying in a band gap exchange charges with the conduction and valence bands through the emission and the capture of carriers. Trap centers influence the charge distribution in semiconductor bulk. In case of acceptor traps, the space charge density in the Poisson equation is reduced by the density of states for ionized acceptor traps, which is determined as follows:

$$N_{ta}^- = P N_{ta}, \qquad (30)$$

where N_{ta} is the density of states for acceptor traps and P is the ionization probability defined by

$$P = \frac{n}{n + \tau N_c \exp\left(\dfrac{E_{ta} - E_c}{V_T}\right)}, \qquad (31)$$

where τ is the degeneracy factor, E_{ta} is the trap energy level and E_c is the conduction band edge.

IV. RESULTS

To investigate the effect of the presence of Fe-induced deep-level acceptor centers treated as trap states on the dc characteristics of the GaN HEMT at elevated temperatures, intentional doping of Fe is implemented for the GaN buffer layer with three different residual channel concentrations, denoted as low- (10^{16} cm^{-3}), medium- (10^{17} cm^{-3}) and high-Fe (10^{18} cm^{-3}). Fig. 2 illustrates the distributions of the Fe-induced acceptor traps with the associated energy of 0.7 eV [18] from the channel to the substrate described by a Gaussian profile with a peak

concentration of $5 \cdot 10^{18}$ cm^{-3} close to the bottom of the buffer layer to mimic the fact that the material quality deteriorates towards the substrate.

In Fig. 3, the distributions of the ionization probability for the acceptor traps are presented. As can be seen, when the acceptor trap concentration at the device channel is increased from the value of 10^{16} cm^{-3} to 10^{18} cm^{-3}, the thickness of the buffer layer where the traps are almost completely ionized ($P \geq 0.99$) decreases from the value of 0.013 μm to 0.006 μm. For low-Fe, the trap centers are not ionized ($P \leq 0.01$) at the distances of 0.16 μm and higher, while for high-Fe the limit is located at 0.061 μm.

The drain current vs gate voltage characteristics of the GaN HEMT at the drain voltage of 1 V are shown in Fig. 4. When the acceptor trap concentration at the channel is raised, the input characteristics are shifted in the positive direction. For low-Fe, the threshold voltage equals to –3.47 V, while for high-Fe, the threshold voltage is –2.5 V.

The drain current vs drain voltage characteristics of the GaN HEMT at the gate voltage of 0 V are presented in Fig. 5. The shift of the input curves caused by the acceptor traps leads to a decrease in the drain current at the same bias conditions.
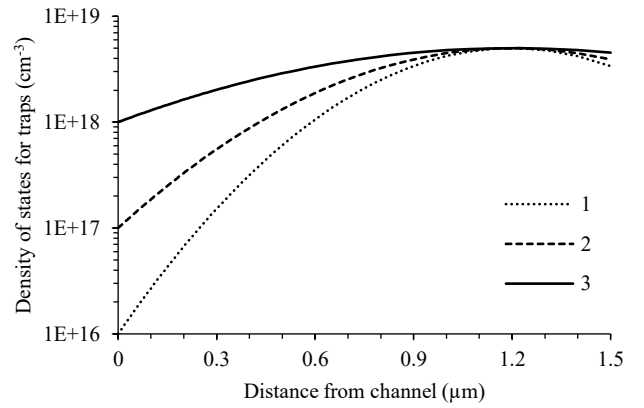

Fig. 2. Fe-induced acceptor traps distributions in the GaN buffer layer: 1 – low-Fe, 2 – medium-Fe, 3 – high-Fe
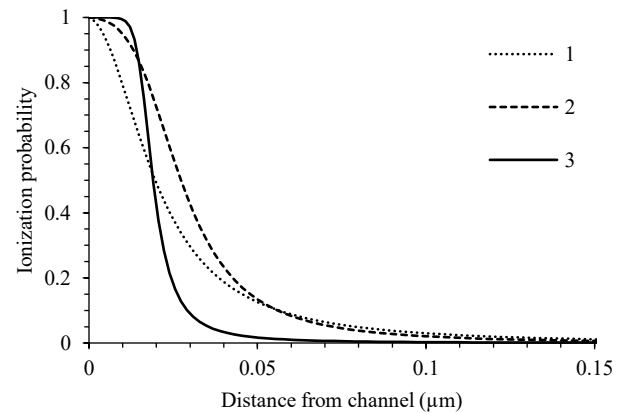

Fig. 3. Ionization probability distributions for the Fe-induced acceptor traps in the GaN buffer layer: 1 – low-Fe, 2 – medium-Fe, 3 – high-Fe

TABLE III. THERMAL CONDUCTIVITY MODEL PARAMETERS

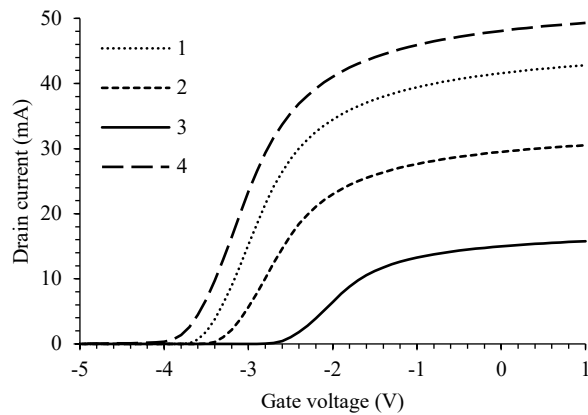| Parameter	Material		
	AlN	GaN	Al₂O₃
λ (300 K)	2.85	1.3	–
δ_1	–1.64	–0.28	–
δ_2	–	–	51292
δ_3	–	–	1.2868
δ_4	–	–	0.0001769

Fig. 4. Drain current vs gate voltage characteristics at the drain voltage of 1 V of the GaN HEMT: 1 – low-Fe, 2 – medium-Fe, 3 – high-Fe, 4 – traps not accounted for
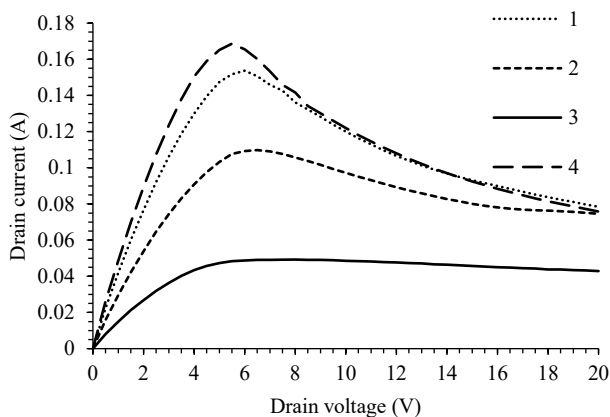

Fig. 5. Drain current vs drain voltage characteristics at the gate voltage of 0 V of the GaN HEMT: 1 – low-Fe, 2 – medium-Fe, 3 – high-Fe, 4 – traps not accounted for

For instance, at the gate voltage of 0 V and the drain voltage of 6 V, the drain current is 0.154 A for low-Fe and 0.049 A for high-Fe. In all cases, the drain current decreases, when the drain voltage is raised, due to the self-heating effect.

For the reason of comparison, the current-voltage characteristics simulated without the acceptor centers in the buffer layer are presented.

Conclusions

The effect of the presence of Fe-induced deep-level acceptor centers treated as trap states on the dc characteristics of the GaN HEMT at elevated temperatures (up to 600 K) was studied. The simulation results show that the acceptor centers intentionally introduced in the buffer layer of the device cause a shift of the input characteristics in the positive direction. The distribution of the traps in the buffer layer can be subject to optimization.

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