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A surface trap model and its application to analysis of III-nitride HEMT performance

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A polarity-dependent model of electron/hole traps on a free GaN:Si surface is suggested, accounting for both intrinsic and impurity-induced surface states. The model parameters are fitted to provide the best agreement with available observations. The suggested approach is invoked to explain a recently observed non-monotonic dependence of the surface barrier due to band bending upon the donor concentration in the GaN bulk. The model is used for analysis of DC performance of high-electron mobility transistors (HEMTs) with different cap layer design.

1 Introduction Electronic traps on III-nitride semiconductor surfaces are commonly believed to be responsible, at least partly, for the frequency-dependent current collapse and the so-called DC-to-RF current dispersion in AlGaN/GaN HEMTs. It has been shown that surface trap filling with electrons is the mechanisms that controls the charge on a free semiconductor surface and, hence, the band bending in bulk GaN and AlGaN/GaN heterostructures [1]. The band bending is known to depend remarkably on the technique used for GaN growth, while surface passivation with dielectrics is found to affect the surface trap density and, thus, the device performance (see [1] and references therein). Recently, an anomalous behavior of the band bending upon free electron concentration has been observed in GaN:Si grown by molecular beam epitaxy [2]. The bending is found to increase non-monotonically with the electron concentration despite the natural expectation of the opposite trend due to the surface charge screening by ionized donors in the material bulk.

In this paper we suggest a polarity-dependent model of surface traps on GaN:Si reproducing the trends reported in [2]. The model is used to analyze theoretically the DC performance of undoped and doped HEMTs with different cap layer design.

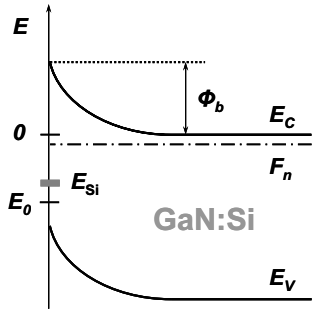

Fig. 1 Schematic band diagram of GaN: Si near the surface and energy level alignment.

2 Surface trap model We will assume surface traps on n-GaN to consist of two groups, intrinsic and donor-induced ones. Following [3], we assume the intrinsic traps to be uniformly distributed over the GaN bandgap with a density D_t dependent on the growth procedure and surface treatment. A neutrality

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level E_0 (see Fig.1) separates donor-like and acceptor-like traps. If the Fermi level F_n lies above the neutrality level, the traps are filled with electrons and form a negative surface charge. At $F_n < E_0$ the traps are filled with holes, and the surface becomes positively charged.

We will also assume that every Si atom creates on the GaN surface a number of surface states at an energy E_{Si} which can capture up to G_{Si} electrons and, thus, become negatively charged. The surface density of such atoms can be estimated as $N_{Si}^{2/3}$, where N_{Si} is the Si-donor concentration in the semiconductor bulk. If the levels E_0 and E_{Si} are deep enough, i.e. $F_n - E_0 - \Phi_b >> kT$ and $F_n - E_{Si} - \Phi_b >> kT$ (k is the Boltzmann's constant, T is temperature, and Φ_b is the height of the barrier due to the upward band bending at the semiconductor surface), the density of the negatively charged surface traps σ can be approximated by the expression

$$\sigma = D_t \cdot (F_n - E_0 - \Phi_b) + G_{Si} N_{Si}^{2/3} \quad . \tag{1}$$

The trap charge induces near the surface a space-charge region depleted with electrons. The height of the barrier due to the upward band bending in this region is $\Phi_b = q^2 \sigma^2 / 2\varepsilon_0 \varepsilon N_{Si}$, where q is the electron charge, ε_0 is the dielectric permittivity of vacuum, and ε is the dielectric constant of the semiconductor. Combining the latter expression with Eq. (1) and determining the Fermi level position from the electroneutrality condition in the material bulk, one can compute the barrier height Φ_b as a function of the donor concentration N_{Si} . For non-degenerate semiconductor the resulting equation is

$$\Phi_b = \frac{q^2}{2\varepsilon_0 \varepsilon N_{Si}} \left[D_t \cdot \left(E_C - E_0 + k\ T \cdot \ln \frac{N_{Si}}{N_C} - \Phi_b \right) + G_{Si} N_{Si}^{2/3} \right]^2 \quad , \tag{2}$$

where E_C is the conduction band edge and N_C is the electron density of states in the conduction band.

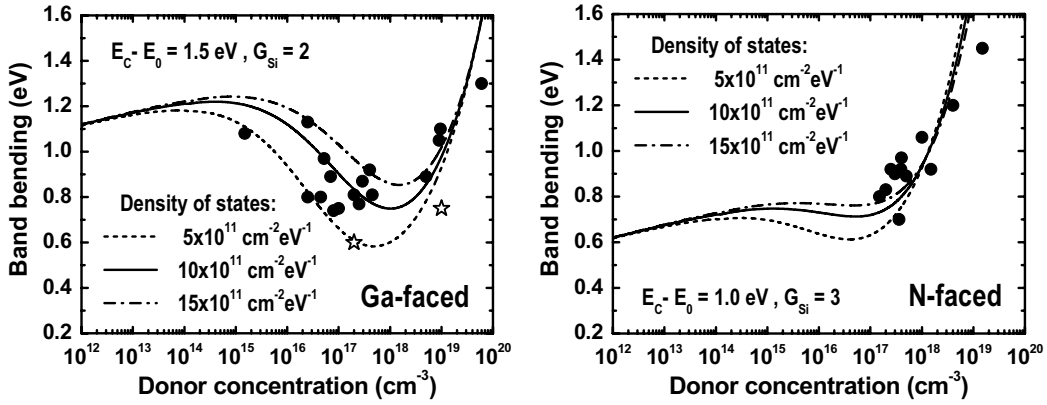

Fig. 2 Surface barrier height as a function of donor concentration for Ga-faced and N-faced GaN:Si. Lines are computations made for different intrinsic densities of states, symbols are the data borrowed from [2] (circles) and [1, 4] (stars).

The above model has been applied to experimental data reported in [1, 2, 4] for Ga-faced and N-faced GaN:Si. To fit better observations, we varied the position of the neutrality level E_0 and the number of electrons that could be captured by a donor-induced surface trap G_{Si} . The comparison of the adjusted theoretical predictions with experiment is shown in Fig. 2. Here, we have neglected the difference between the free-electron and donor concentrations at high doping level due to reduction in the impurity ionization energy. It is seen from Fig. 2 that the model predictions reproduce well the non-monotonous dependence of the band-bending barrier height upon the donor concentration reported for the Ga-faced GaN in [2]. The gradual increase in the barrier height at a low doping level, is related to the rise in the surface charge caused by the Fermi level ascent with the impurity concentration. Then the barrier height falls down due to the electric field screening by ionized donors. The further rise in the barrier height at a high doping level is explained by an additional contribution of the donor-induced surface traps to the

negative surface charge. As the simulations show, the scatter in the measurements, especially pronounced in the range of donor concentration from 5×10^{16} cm^{-3} to 5×10^{18} cm^{-3}, may be attributed to a variation of the intrinsic surface state density from sample to sample.

Within the suggested model, a steeper rise in the surface barrier height with donor concentration observed on N-faced GaN may be associated with the increase of the number of electrons G_{Si} which can be captured by a donor-induced surface trap. Our model predicts a smaller band banding in a low-doped material and a weaker scatter in the surface barrier height caused by the intrinsic surface state density variation. Unfortunately, there is lack of data enabled validation of these predictions.

On a Ga-faced p-GaN ([Mg] = 5×10^{17} cm^{-3}), a downward band bending of 0.75 eV has been observed in [4]. It is interesting that our model is capable of reproducing this result. Without donor-induced traps the model predicts such a downward barrier height at the same neutrality level position and the density of intrinsic states $D_t = 1.8\times10^{12}$ cm^{-3}eV^{-1}.

3 Surface traps and HEMT DC performance In DC operation, the principal impact of surface traps on the transistor characteristics is related to the band bending and its influence on the sheet electron concentration in the channel regions located between the source, gate, and drain electrodes. Actually, this effect controls the channel conductivity in the inter-electrode regions, which should be made as high as possible in order to improve the device performance.

Here, we consider three different HEMT heterostructures. Structure A consists of a thick unintentionally doped (UID) GaN capped by an UID-$Al_{0.2}Ga_{0.8}N$ 30 nm thick. Structure B differs from structure A by an additional 3 nm UID-GaN cap layer grown on the AlGaN top. Structure C contains in series: a thick UID-GaN, 10 nm UID-$Al_{0.2}Ga_{0.8}N$, 15 nm n-$Al_{0.2}Ga_{0.8}N$ ([Si] = 4×10^{18} cm^{-3}), 5 nm UID-$Al_{0.2}Ga_{0.8}N$, and 3 nm UID-GaN cap. The structure is different from structure B only in doping of the AlGaN layer. Two latter HEMT heterostructures are generally similar to those reported in [5, 6].

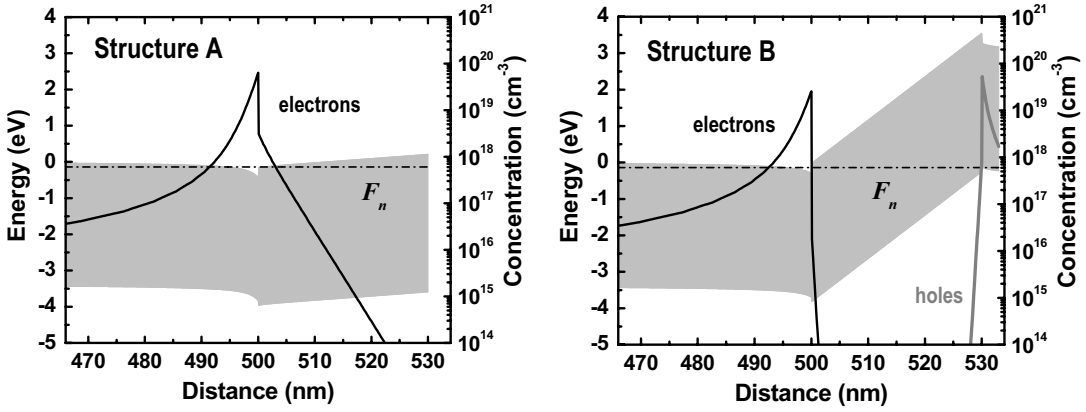

Fig. 3 Equilibrium band diagrams of the HEMT structures A and B in the inter-electrode region computed for the intrinsic density of surface states $D_t = 5\times10^{11}$ cm^{-3}eV^{-1}. The bandgap of the structures is shadowed, and F_n denotes the Fermi level.

Figure 3 shows the equilibrium band diagrams of structures A and B computed for the inter-electrode region, a low density of surface states, and E_C–E_0 = 1.5 V, which corresponds to a Ga-faced free surface. The computations are carried out with the FETIS package based on a self-consistent solution of the Poisson and Schrödinger equations for both electrons and holes and accounting for the surface-trap charge via boundary conditions [7]. No difference between the GaN and AlGaN surface properties is enabled in the computations.

It is seen from Fig. 3 that in conventional structure A, the Fermi level is located near the bottom of the conduction band, producing negatively charged surface and upward band bending in the AlGaN cap. A thin UID-GaN cap grown on the top of the AlGaN layer (structure B) favours parasitic hole formation at

the inverted GaN/AlGaN interface due to a negative polarization charge induced. This results in a drammatic band diagram transformation with the Fermi level lying near the valence band edge (Fig. 3). In this case, the surface becomes positively charged, and a built-in electric field of ~1.2 MV/cm is formed in AlGaN pushing electrons out of the cap. Additional doping of the AlGaN layer with Si (structure C) is found to increase the electron and to decrease the hole concentration. In the gate region, where a Schottky barrier of 1.2 V is assumed to be formed, the hole generation is avoided in all the structures.

Table 1 Sheet electron and parasitic hole concentrations in the gate and inter-electrode regions of different HEMT heterostructures.

Structure	**Inter-electrode region**		**Parasitic holes**		**Gate region**
Density of states ($cm^{-2}eV^{-1}$)	5×10^{11}	5×10^{12}	5×10^{11}	5×10^{12}	Φ_{SB} = 1.2 V
(A) $Al_{0.2}Ga_{0.8}N$/GaN	9.55×10^{12}	8.29×10^{12}	—	—	8.18×10^{12}
(B) GaN/$Al_{0.2}Ga_{0.8}N$/GaN	4.32×10^{12}	5.20×10^{12}	3.41×10^{12}	5.55×10^{12}	7.09×10^{12}
(C) GaN/n-$Al_{0.2}Ga_{0.8}N$/GaN	6.92×10^{12}	8.63×10^{12}	4.21×10^{10}	—	9.81×10^{12}

Table 1 presents the sheet electron and hole concentrations in the HEMT heterostructures as a function of surface density of states D_t . A decrease of D_t results in a higher inter-electrode electron concentration in structure A. Thus, surface passivation commonly associated with a reduction in the trap density of states improves the channel conductivity in such a structure. For structures B and C, however, an opposite tendency is predicted by our model – reduction in D_t leads to a lowering of the inter-electrode electron concentration. In these structures, an unpassivated surface seems to be more beneficial for the device performance.

It should be also mentioned that structure A provides the highest gate/inter-electrode ratio of electron concentrations among all the structures considered (see Table 1), which is important for better transfer characteristics of a HEMT. This conclusion, however, does not allow for additional traps that may be induced by chemically reactive Al surface atoms. More experimental efforts are required to clarify the difference in the properties of GaN and AlGaN surfaces.

4 Summary We have suggested the polarity-dependent model of surface traps on GaN:Si, which is capable of reproducing a non-trivial dependence of the surface band bending upon the bulk donor concentration observed in [2]. The model is found to be applicable to both n- and p-GaN. Using the model, we have performed a theoretical analysis of the surface trap effect on the channel electron concentration in the gate and inter-electrode regions of HEMTs with different cap layer design. HEMTs with AlGaN and GaN/AlGaN caps are predicted to provide qualitatively different behaviour of the inter-electrode sheet electron concentration, which may be attributed to an additional negative polarization charge accumulated in the cap at the GaN/AlGaN interface. The polarization charge is also responsible for parasitic hole generation in the cap layer under certain conditions. Surface passivation is found to be beneficial for HEMTs with AlGaN cap layer, while the passivation effect is questionable for the transistors with combined GaN/AlGaN caps. The latter conclusion seems to be valid, if the surface properties of UID GaN and AlGaN differ insignificantly.

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