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Analytical modeling of bare surface barrier height and charge density in AlGaN/GaN heterostructures

Nitin Goyal,[1,a)] Benjamin Iñiguez,[2] and Tor A. Fjeldly[1]
[1]*Department of Electronics and Telecommunication, Norwegian University of Science and Technology, Trondheim NO7034, Norway*
[2]*Department of Electronic Engineering, Universitat Rovira i Virgili, Tarragona, Spain*

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In this paper, a physics based analytical model for the bare surface barrier height and two dimensional electron gas density in AlGaN/GaN heterostructures is presented. The model is based on simple charge neutrality electrostatics across the AlGaN barrier layer and that a low density of surface donor states is the source of the two dimensional electron gas. The model shows good agreement with reported experimental results. © *2012 American Institute of Physics*. [http://dx.doi.org/10.1063/1.4751859]

GaN based high electron mobility transistors (HEMT) have shown great promise for the future high-power and high-frequency applications due to their wide band gap and high electron mobility. III–V based HEMTs also possess excellent thermal properties, which make them suitable candidates for high-temperature applications. The most interesting feature of these devices is the presence of a high mobility two-dimensional electron gas (2DEG) density of the order of $10^{13}\,cm^{-2}$ at the AlGaN/GaN interface even in the absence of both doping in the AlGaN barrier layer and gate metal (bare surface). This effect is attributed to the presence of strong piezoelectric as well as spontaneous polarization effects.[1] In the last few years, considerable research has been performed by different groups to explain the mechanism and source of electrons for the formation of this 2DEG. It has been shown, using experiments as well numerical simulations, that the presence of donor states at the AlGaN surface is the main source of the electrons in the 2DEG.[2–7] Till now, this is assumed to be the only valid theory to explain the behavior observed in the experiments. Even in the presence of a gate metal, the effect of surface states is only partially neutralized.[8] Understanding the formation of the 2DEG is very important to explain the mechanism of current collapse and various other effects in ac and dc characteristics[9,10] and is thus very crucial to the device design.

The surface donor model (SDM) by Ibbetson *et al.*[2] was proposed to explain the behavior of 2DEG charge concentration with variation in the barrier layer thickness. They assumed that a high density of surface donor states exists at a particular energy level E_{do} in the forbidden gap measured relative to the conduction band minimum of AlGaN surface (see Fig. 1). With increasing barrier thickness d, this level moves higher due to the constant electric field in the barrier. Once this level reaches the Fermi level, the surface donor states start donating electrons to form the 2DEG at the AlGaN/GaN interface. According to this model, the Fermi level at the surface will remain essentially constant (Fermi level pinning) once the barrier layer reaches the critical thickness d_{cr}, below which the 2DEG vanishes. Therefore, according to SDM, the surface barrier height $q\Phi_B$ remains almost constant (increases only in the range of kT/q) with increasing d once the donor level is reached. This model was justified by certain experimental data as well as by numerical simulations.[2,3]

However, this model could not be reconciled with experimental observations by Koley and Spencer[6] that the $q\Phi_B$ of the bare surface increases with increasing d. But these observations were explained by instead assuming low-density surface donor states distributed over a range of energies below a particular donor energy level E_d in the forbidden gap,[6] as indicated in Fig. 1. Hence, with increasing d, the conduction band can move up and, simultaneously, lift E_d with respect to Fermi level. Thus, when E_d crosses the Fermi level, the surface donor states start donating electrons to form the 2DEG at the hetero-interface. Therefore, in this model, $q\Phi_B$ will be able to increase with increasing d even in the active regime. Experiments and numerical simulations show that both the 2DEG charge concentration qn_s and $q\Phi_B$ first increase linearly and eventually saturate with increasing barrier thickness.[6,7]

Here, we present a physics based analytical model for the variation of the surface barrier height with the variation of the barrier layer thickness. This model is based on the charge neutrality condition across the barrier layer. We assume that the charge contribution due to the unintentional doping in GaN and AlGaN is negligible and that the polarization in combination with the distributed surface donor states is the responsible mechanism for the creation of the 2DEG.

Considering Fig. 1, we observe that to maintain charge neutrality, the electric field across the barrier layer is given by both left and right hand sides of the expression

$$(\sigma_{pz} - qn_s)/\varepsilon_{AlGaN} = (q\Phi_B + E_F - \Delta E_c)/dq, \qquad (1)$$

where ΔE_c is the conduction band offset, E_F is the difference between the Fermi level and the conduction band minimum (CBM) in the GaN at the hetero-interface, σ_{pz} is the positive polarization surface charge at the hetero-interface, and ε_{AlGaN} is the permittivity of the barrier layer. Here, we note that E_F does not change much, at most by a few kT/q, once we enter

a)Electronic mail: nitin@unik.no.

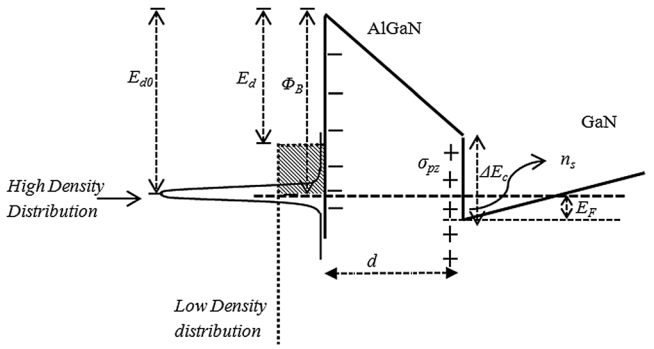

FIG. 1. Band diagrams of a AlGaN/GaN HEMT showing various charges at the different interfaces and illustrating the formation of a 2DEG with electrons supplied by surface donor states. Two cases with different distributions of the surface donor states in the energy gap are shown: (a) single surface donor level with high density; (b) distributed surface donor states with low density.The shaded box shows the number of electrons per unit area donated by low density surface donor states.

the active regime. As a reasonable approximation, we therefore assume $E_F \approx 0$ (see further comments below). Next, we assume a constant surface donor density below the donor level E_d with the population n_o states per unit area and energy, as proposed by Gordon *et al.*[7] The number of empty surface donor states above the Fermi level can then be written as $n_o(q\Phi_B - E_d)$ per unit area, which corresponds to the 2DEG electron density n_s at the hetero-interface. Applying this to Eq. (1) and solving for the surface barrier, we find

$$q\Phi_B \approx \frac{K_1 d + K_2}{n_0(d + K_3)}, \tag{2}$$

where $K_1 = \sigma_{pz}/q + n_o E_d$, $K_2 = \varepsilon_{AlGaN}\Delta E_c/q^2$, and $K_3 = \varepsilon_{AlGaN}/q^2 n_o$. From Eq. (2), we see that for sufficiently thick barriers, the barrier height saturates at the value $q\Phi_B \approx E_d + \sigma_{pz}/qn_o$. Moreover, when the surface state density is high, $q\Phi_B$ approaches the value E_d.

Figure 2 shows a comparison of the modeled barrier height versus barrier thickness against experimental data from Gordon *et al.*[7] for two different Al compositions in the barrier layer. The experimentally determined values for n_o and E_d were used in the model. The model is found to reproduce quite well the experimental results, especially for small barrier thicknesses. At higher thicknesses, there is a slight deviation between model and experimental data, which can be attributed to the strain relaxation in the barrier layer[7] as well as the finite value of the difference between Fermi level and the CBM in GaN at the AlGaN/GaN interface[10] that we have neglected in order to simplify the mathematical analysis. As can be seen from Fig. 2 and from additional experimental results in Ref. 7, the model is fairly accurate up to a barrier layer thickness of close 25 nm at the Al composition of 19%. For higher Al compositions, the range of accuracy decreases to about 15 nm at 24% Al. For this practical range of barrier compositions, the present model explains the effect of barrier thickness in a simple manner, which can be used to understand and develop new concepts of GaN HEMTs. Figure 3 illustrates graphically how E_F and $q\Phi_B$ behave with increasing d, and why the approximation for E_F is justified for thin barriers.

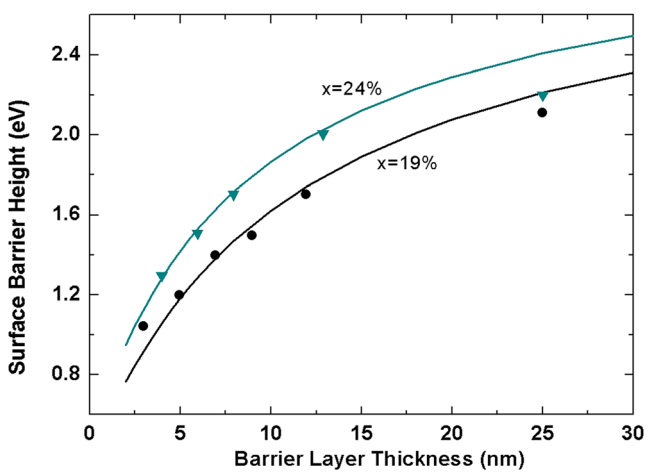

FIG. 2. Comparison between the model (curves) and experimental data (symbols) obtained from Ref. 7, for two different Al compositions in the barrier. The density of surface donor states used were $n_o(x = 0.19) = 4.6 \times 10^{12}\,\mathrm{cm}^{-2}\mathrm{V}^{-1}$ and $n_o(x = 0.24) = 6.1 \times 10^{12}\,\mathrm{cm}^{-2}\mathrm{V}^{-1}$.[7]

The critical thickness $d = d_{cr}$ is the barrier layer thickness below which n_s can be approximated to be very small. It can easily be calculated from Eq. (1) by setting $n_s = 0$, $q\Phi_B = E_d$, and $E_F = 0$, resulting in

$$d_{cr} = \left(\frac{\varepsilon_{AlGaN}}{\sigma_{pz} q}\right)(E_D - \Delta E_c). \tag{3}$$

Finally, we may also develop an explicit expression for n_s versus d for a given d_{cr} by combining Eq. (1) to (3). This results in the following expression:

$$n_s = \frac{\sigma_{pz}}{K_4 q}\left(1 - \frac{d_{cr}}{d}\right), \tag{4}$$

where $K_4 = 1 + \varepsilon_{AlGaN}/dqn_o$ can be regarded as a correction factor relative to SDM by accounting for the variation in the surface barrier height with increasing barrier layer thickness. For large n_o, K_4 approaches unity, which corresponds to SDM. This correction is illustrated in Fig. 4, where we choose $E_d = E_{d0}$ to emphasize the magnitude of the correction.

The importance of this work lays in the fact that this model predicts the experimental observations in AlGaN/GaN HEMTs in a simple analytical manner. For any given HEMT structure, only the donor level of the surface states and the surface state density are required for this model to calculate barrier height as well as the 2DEG for any value of the barrier

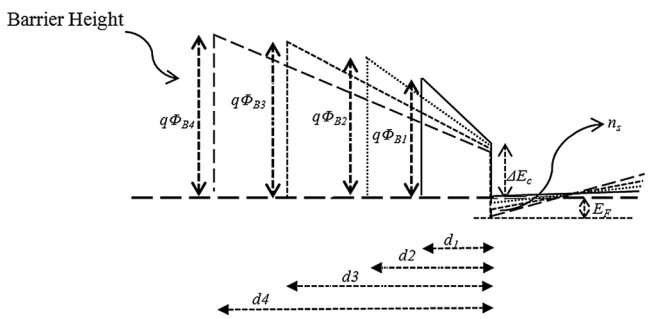

FIG. 3. Schematic view of band diagrams of a AlGaN/GaN HEMT showing surface barrier heights versus barrier layer thicknesses (not to the scale). Here, E_F is indicated for a relatively thick barrier.

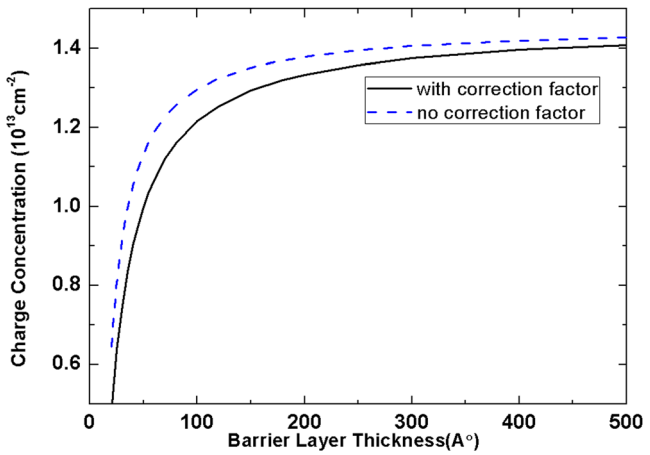

FIG. 4. Comparison between the proposed model according to Eq. (4) (low density surface states) and the model given by Ibbetson *et al.*[2] (high density of surface states where $K_4 = 1$) for dependence of n_s versus barrier layer thickness.

thickness. We have also verified that using the corresponding values in Ref. 6, the saturating value of barrier height has been observed as approximately 1.7 eV, which demonstrates the validity of the model for different sets of samples. From our analysis, we can observe that d_{crit} is dependent on σ_{pz} and ΔE_c. Therefore, to design HEMTs with better gate control, there is a need for new materials for barrier layers that can provide strong polarization as well as large conduction band off-set values. AlN/GaN and lattice matched InAlN/AlN/GaN are such material combinations and have been demonstrated to possess superior gate control as well as high n_s at small barrier layer thicknesses due to strong spontaneous polarization and large effective ΔE_c. These materials can be used for high aspect ratio designs.

In conclusion, we have presented a physics based model for the sheet carrier density (2DEG) at the AlGaN/GaN interface, including the effect of piezoelectric and spontaneous polarization charges. We have shown that the sheet carrier density as well as barrier layer height are functions of the density, location in the band gap, and distribution of surface donor states. By assuming a uniform distribution, a completely analytical model has been presented, which can be used to further understand the physics of AlGaN/GaN based HEMTs. The present model is in good agreement with the reported experimental data.

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