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ABSTRACT

In this computational study, the influence of GaN/Al$_x$Ga$_{1-x}$N layer stack parameters, such as surface potential, aluminum mole fraction, and background donor concentration, on the two-dimensional electron gas (2DEG) density in a heterostructure is verified. At a fixed Al mole fraction, the surface potential was identified to have the largest impact on the 2DEG density. The combination of a small aluminum mole fraction ($x < 0.12$) and large surface potential results in the absence of a 2DEG in the investigated heterostructures, while for a small surface potential value, a 2DEG will be present. For a large aluminum mole fraction ($x \geq 0.25$), a 2DEG is always present, independent of the surface potential value. In the case of an intermediate aluminum mole fraction, the background donor level is one key parameter strongly influencing the 2DEG density.

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I. INTRODUCTION

As technology of electronic devices develops, the systems become more complex, and hence, achieving lower power consumption without any loss of functionality becomes difficult. The trend of power amplifiers calls for higher channel conductivity and improved reliability. High electron mobility transistors (HEMTs) based on the wide bandgap semiconductor gallium nitride (GaN), exhibiting high electron saturation velocity, fulfill these demands and thus are perfect candidates for high-frequency, high-temperature, and high-voltage applications.1

Commonly, lateral GaN/AlGaN HEMTs, resembling field-effect transistor (FET) switching characteristics, operate in the depletion-mode (normally-on), i.e., at zero gate voltage, the source-drain channel is conductive. The normally-on switching behavior is not preferred for a fail-safe operation and attributed to the presence of a two-dimensional electron gas (2DEG) formed at a GaN/AlGaN interface due to polarization discontinuity, even without intentional doping.2 A few technological approaches have been explored to create enhancement-mode (normally-off) devices, such as etched gate recesses,3 p-doped GaN cap layers,4 fluorine ion implantation,5 or cascode circuits. All of this results in increased processing complexity and costs. Recently, it was reported that the presence of a 2DEG in GaN/AlGaN layer stacks depends on residual donor background impurity concentration.7,8 Consequently, HEMTs fabricated from ultrapure GaN/AlGaN heterostructures operate inherently in normally-off.

In this report, the influence of material parameters on the presence of a 2DEG in GaN/AlGaN layer stacks is investigated by means of technological computer aided design (TCAD) simulations. It is found that the GaN/AlGaN stack surface potential has the most significant influence on the 2DEG channel density, which is consistent with former experimental reports.9,10 A combination of a large surface potential and moderate aluminum mole fraction in the AlGaN layer results computationally in the inherent absence of a 2DEG. The comparison with experimental data indicates that in ultrapure GaN/AlGaN stacks, the Fermi level at the surface is pinned deep inside the GaN bandgap.

II. MODELING OF THE GaN/AlGaN HETEROSTRUCTURES AND CALCULATION OF 2DEG DENSITIES

The GaN/AlGaN heterostructures were modeled with the simulation tool Sentaurus Device (by Synopsis Inc.) using a finite
elements method. All heterostructures are composed of a 1 μm thick GaN layer with a fixed potential of 1.7 eV (assuming midgap Fermi level pinning) at the substrate side followed by an Al$_x$Ga$_{1-x}$N barrier with 16 nm thickness and capped with a 3 nm thick GaN layer. The surface potential $\Phi_S$ of the GaN cap, which is defined as the energy difference between the conduction band edge and the Fermi level at the surface, is a variable parameter in the simulations performed for a temperature of $T = 300$ K and for various Al mole fractions $x$. The hexagonal (wurtzite) lattice configuration and gallium polarity at the surface are assumed. For every finite element, material parameters (e.g., lattice or electrostatic parameters) are defined, resulting in a meshgrid of fundamental parameters and creating a model of the investigated structure. The quantitative modeling of the polarization discontinuities at the GaN/AlGaN and AlGaN/GaN interfaces is adopted from the descriptions by Ambacher et al. Apart from the bulk and surface potential values, the barrier and cap thicknesses, background donor concentration, and aluminum mole fraction can be varied, which represents a full set of layer stack parameters influencing the 2DEG density. In the model used, all donor impurities are ionized at all temperatures. The band diagrams and 2DEG wave functions are calculated by self-consistently solving the Schrödinger and Poisson equations. The sheet carrier concentration at the GaN/AlGaN interface is obtained by the integral over the wave function.

III. RESULTS AND DISCUSSION

In the following paragraphs, the influence of material parameters of the GaN/Al$_x$Ga$_{1-x}$N heterostructure, such as the surface potential $\Phi_S$, the aluminum mole fraction $x$ in the AlGaN barrier, and the background donor concentration in the whole layer stack, on the 2DEG sheet density will be discussed. For all layer stacks, the 2DEG density is largely influenced by the value of the surface potential. For relevant values of $\Phi_S$ between 0 and 3.4 eV, a 2DEG can be entirely absent at a small Al mole fraction, while at larger values ($x \geq 0.25$), it is always present. In the two regimes of small and large $x$, the variation of background donor impurity concentration is negligible, while at $x = 0.14$, the 2DEG density strongly depends on the impurity level.

The band diagrams shown in Fig. 1 represent the position of the conduction band energy relative to the Fermi level (set to 0 eV), while the surface potential was modified between 0 and 3.0 eV. The substrate potential is fixed at 1.7 eV for all cases, which assumes mid-gap Fermi level pinning at the substrate side. The background impurity concentration is set to zero for this GaN/Al$_{0.06}$Ga$_{0.94}$N heterostructure. For small surface potential values, the confinement potential at the GaN/AlGaN interface will be energetically located below the Fermi level, and thus, a 2DEG will be present. At larger values above 1.0 eV, however, a 2DEG will be absent.

The quantitative dependence of 2DEG density on surface potential for various Al mole fractions $x$ is shown in Fig. 2. Surface potential values from 0 to 0.5 eV for a GaN/Al$_{0.06}$Ga$_{0.94}$N heterostructure result in a 2DEG sheet density between $1 \times 10^{12}$ cm$^{-2}$ and $2 \times 10^{12}$ cm$^{-2}$, which is consistent with experimental data. The trends presented in Fig. 2 also indicate that for even larger values of $x = 0.18$, a 2DEG can be absent at a large surface potential above 3.0 eV. Experimentally, this would correspond to pinning of the Fermi level close to the valence band, which can be achieved, for example, by magnesium doping of the cap layer.

In contrast to the absence of a 2DEG at a small Al mole fraction $x$ and large surface potential $\Phi_S$, a 2DEG will always exist at $x \geq 0.25$, even for $\Phi_S$ values $> 3.4$ eV, which are unphysical (Fig. 3). This is attributed to the emergence of a two-dimensional hole gas (2DHG) at the AlGaN/GaN (barrier/cap) interface.

![Fig. 1. Conduction band diagrams of a GaN/Al$_{0.06}$Ga$_{0.94}$N heterostructure (see the main text and the inset of Fig. 2) with varying values of the surface potential between 0 and 3.0 eV. The Fermi level is set to 0, and the potential at the substrate side is fixed at 1.7 eV for all plots. At large surface potential values, the confinement potential at the GaN/AlGaN interface lies energetically above the Fermi level, and, as a consequence, a 2DEG is not present. At small values, however, the confinement potential is pushed toward the Fermi level, and the calculated quantum mechanical states can be occupied with electrons, resulting in the presence of a 2DEG. The quantitative trend is shown in Fig. 2.](image-url)

![Fig. 2. 2DEG sheet carrier concentration vs surface potential at different Al mole fractions for other identical layer stacks (lines are guides to the eye). While a 2DEG is already absent at a surface potential of 1.0 eV for an Al mole fraction of $x = 0.06$, for higher Al mole fractions, larger surface potentials are required to suppress its formation. At $x = 0.25$, a 2DEG will always be present for any surface potential within the range of the bandgap. However, within this range, between 0 and 3.4 eV, the 2DEG density can vary between $2 \times 10^{12}$ cm$^{-2}$ and $1 \times 10^{13}$ cm$^{-2}$. The inset shows the layer stack of the discussed GaN/AlGaN heterostructure (not to scale).](image-url)
Undoped GaN/AlGaN heterostructures were considered in the calculations presented so far, and it was shown that the surface potential \( \Phi \) massively impacts the 2DEG density at the GaN/AlGaN interface. Recently, it was speculated that the presence or absence of a 2DEG is related to residual background donors in the range between \( 10^{16} \) cm\(^{-3} \) and \( 10^{17} \) cm\(^{-3} \) in GaN/Al\(_{0.16}\)Ga\(_{0.84}\)N heterostructures. In this computational study, this behavior could not be verified. Although insignificant for small and large Al mole fractions, an intermediate regime \( x \approx 0.14 \) is identified where background impurities at the aforementioned levels strongly influence the 2DEG sheet density. This intermediate regime is characterized by a combination of the surface potential and Al mole fraction, which results in an energetic position of the confinement potential at the GaN/AlGaN interface close to the Fermi level. Depending on the surface potential assumed, the formation of a 2DEG can be impeded by reducing the background donor concentration significantly below \( 10^{17} \) cm\(^{-3} \). For example, at \( x = 0.12 \) and an assumed surface potential of 1.7 eV, the 2DEG density increases from \( 4 \times 10^{11} \) cm\(^{-2} \) to \( 7 \times 10^{12} \) cm\(^{-2} \) once an active donor impurity level of \( 8 \times 10^{16} \) cm\(^{-3} \) is introduced (Fig. 4). These low doping levels between \( 10^{16} \) cm\(^{-3} \) and \( 10^{17} \) cm\(^{-3} \) are technologically relevant since the growth of such pure GaN material with oxygen as the only donor impurity has been independently demonstrated recently.\(^{11}\)

Following the presented data, the absence of a 2DEG in ultrapure GaN/Al\(_{0.16}\)Ga\(_{0.84}\)N heterostructures experimentally realized recently\(^ {12}\) is consistent with pinning of the Fermi level deep inside the bandgap of the GaN surface at a background donor level significantly below \( 10^{17} \) cm\(^{-3} \). Technologically, the observed behavior results in the desired normally-off operation of lateral field-effect transistors. In these devices, a positive voltage applied to a surface gate electrode will shift the confinement potential at the GaN/AlGaN interface below the Fermi level and thus create a conductive 2DEG channel. The microscopic nature of the large surface potential is still under discussion; a suitable candidate for a deep level inside the bandgap pinning the Fermi level could be residual carbon\(^ {17}\) at an unverifiable level.

IV. CONCLUSIONS

The 2DEG density in GaN/AlGaN heterostructures is significantly influenced by material parameters such as surface potential, aluminum mole fraction, and background donor concentration. In contrast to aluminum mole fraction and background donor concentration, the surface potential is a crucial parameter which decides the presence or absence of a 2DEG in GaN/Al\(_{1-x}\)Ga\(_{x}\)N layer stacks with a low Al mole fraction \( x \).

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