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Normally-off AlN/$\beta$-Ga$_2$O$_3$ field-effect transistors using polarization-induced doping

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Abstract

III-nitrides and beta-phase gallium oxide ($\beta$-Ga$_2$O$_3$) are currently two intensively investigated wide bandgap semiconductor materials for power electronics. Due to the relatively low lattice mismatch between the two material systems and the availability of bulk AlN, GaN and $\beta$-Ga$_2$O$_3$ substrates, epitaxial growth of III-nitrides on $\beta$-Ga$_2$O$_3$ or vice versa has been realized. However, the design of power devices by integrating the two material systems is still lacking. Here we numerically investigate an AlN/$\beta$-Ga$_2$O$_3$ heterostructure by taking advantage of polarization-induced doping to realize high-performance enhancement-mode transistors. Induced by polarization effects at the AlN/$\beta$-Ga$_2$O$_3$ interface, a 2-dimensional electron gas concentration can reach up to $8.1 \times 10^{19}$ cm$^{-3}$ in the channel. On top of the channel, a p-GaN gate was introduced and eventually a normally-off AlN/$\beta$-Ga$_2$O$_3$ field-effect transistor with tunable positive threshold voltages was realized. Furthermore, we inserted an unintentionally doped GaN back barrier layer to suppress the drain leakage current. Eventually, the transfer and output characteristics of the proposed device with different structural parameters were further investigated and analyzed in the pursuit of high-performance III-nitrides/Ga$_2$O$_3$-based power devices.

Keywords: $\beta$-Ga$_2$O$_3$, p-GaN gate, field-effect transistors, normally-off, polarization-induced doping

(Some figures may appear in colour only in the online journal)

1. Introduction

Recently, beta-phase gallium oxide ($\beta$-Ga$_2$O$_3$) has attracted considerable attention due to its unique material properties such as wide bandgap (4.7 eV), high breakdown field (8 MV cm$^{-1}$) and high saturation velocity ($\sim 2 \times 10^7$ cm s$^{-1}$) for photodetector and power device applications [1–6]. Various $\beta$-Ga$_2$O$_3$ power electronic devices have been demonstrated, including Schottky barrier diodes (SBDs) [7–9] and field effect transistors (FETs) [10, 11].

Owing to the nonpolar nature of $\beta$-Ga$_2$O$_3$ crystals, modulation-doped heterostructure is one of the possible approaches to realize Ga$_2$O$_3$-based FETs. Recently, a modulation-doped two-dimensional electron gas (2DEG) at the $\beta$-(Al$_x$Ga$_{1-x}$)$_2$O$_3$/Ga$_2$O$_3$ heterojunction by silicon delta doping ($\delta$-doping) has been reported [12], followed by the demonstration of modulation-doped $\beta$-(Al$_x$Ga$_{1-x}$)$_2$O$_3$/Ga$_2$O$_3$ double heterostructure FETs [13]. However, the control of $\delta$-doping, such as the position and concentration of the $\delta$-doping, is rather challenging through the epitaxial growth
process. Fortunately, due to the presence of large spontaneous and piezoelectric polarization charges at nitride-based heterostructures (for example, the AlGaN/GaN heterostructure), an effective δ-doping can be created at the sharp heterointerface with atomic control and carrier concentration far beyond what is achievable by the impurity-based δ-doping technology [14]. Therefore, to further improve the performance of β-Ga2O3 based FETs, considering the advantage of the high breakdown field of Ga2O3 material and strong polarization fields of III-nitrides, a combination of the nonpolar β-Ga2O3 with polar III-nitrides to form a III-nitride/β-Ga2O3 heterostructure could be a promising device architecture to realize high-performance power electronics [15–18].

Moreover, due to the presence of 2DEG in the channel at zero gate bias, the β-(Al0.2Ga0.8)2O3/Ga2O3 modulation-doped FET showed a normally-on operation [12]. However, normally-off enhancement mode devices with positive threshold voltages (Vth) are highly desirable in power electronics applications, especially in designing fail-safe power switches, RF power amplifiers, and simpliﬁed driving circuits [19, 20]. To pursue the normally-off devices, there are several device structures being proposed: metal-insulator-semiconductor FET (MISFET) [21, 22], ﬂuorine implantation under the gate [23, 24], p-GaN gate [25–27] and Cascade conﬁguration [28]. Among those structures, it is generally accepted that the p-GaN-based gate is a relatively stable and reliable approach. The Vth is not affected by the interface states at the channel as in the MISFETs, and it is stable over time as opposed to the devices based on ﬂuorine implantation [29, 30].

In this work, we propose a p-GaN gated FET structure based on Al-polar AlN/β-Ga2O3 heterojunction. The proposed device structure can be possibly realized via those mature growth techniques such as MOCVD, MBE, or PLD since many studies have been carried out in the investigation of the growth process of nitrides/Ga2O3 heterostructures in the past [15, 31–34]. The band diagram and 2DEG concentration at the interface of the heterostructure were investigated. It was found that a channel is formed at the interface with a high 2DEG concentration due to the band offset and polarization effects. A p-GaN gate was employed to obtain a normally-off operation with a positive Vth. In order to suppress the drain leakage current, a Ga-polar UID GaN back barrier layer was inserted so that positive polarization charges can be formed at the interface. Those positive charges can draw the electrons away from the bulk Ga2O3 (the region below the channel) and thus form a high-resistive region to suppress the leakage current. Herein, we demonstrated a polarization-induced-doped field effect transistor (PIDFET), where its electrical characteristics were comprehensively investigated and computed by a 2D device drift-diﬀusion-based simulation (Silvaco Atlas).

2. Simulation

2.1. Device structures

Simulations for the normally-off III-nitride/β-Ga2O3 PIDFET were carried out using a 2D device simulator Silvaco Atlas. As shown in figure 1, the designed PIDFET consisted of a 70 nm p-type doped GaN cap layer with varying gate length (0.1, 0.2, 0.3, 0.4 μm) and hole concentration (1 × 1017, 1 × 1018, 2 × 1018, 4 × 1018, 6 × 1018 cm−3), a UID Al-polar AlN polarization layer with different thickness (from 4 to 14 nm), 100 nm of UID β-Ga2O3 channel layer, and a 100 nm of UID Ga-polar GaN back barrier layer. For comparison, we also designed a structure without this GaN back barrier layer to show its effect on the leakage current suppression. Two 20 nm thick heavily n-doped β-Ga2O3 contact layers were adopted under the source/drain to reduce the serial resistance and enhance the device working current. The source-drain and the gate-source spacing were set as 1.3 μm and 0.2 μm, respectively. Aluminum (work function: 4.6 eV) was used for the gate Schottky contact. As for the source and drain, the ideal ohmic contacts were implemented in carrying out the simulation. It is suggested to have ohmic contacts to measure the device performance in device fabrication and demonstration. In the real device implementation, we need to carefully control the surface donor since it signiﬁcantly impacts the device performance [35, 36], thus, in our simulation setup, we included a thick layer of silicon oxide to passivate the AlN layer. We normally use silicon oxide or silicon nitride as the passivation layer [37].

2.2. Physical models

The material structure, spontaneous polarization (Psp), and piezoelectric polarization (Ppz) parameters were calibrated in the simulation to produce correct polarization charges at the heterointerface according to the following equations [38]

\[
P_{\text{tot}} = P_{\text{sp}} + P_{\text{pz}}
\]

\[
P_{\text{pz}} = 
\epsilon_{33} \epsilon_{zz} + \epsilon_{31} (\epsilon_{xx} + \epsilon_{yy})
\]

\[
\epsilon_{zz} = (c - c_0) / c_0, \quad \epsilon_{xx} = \epsilon_{yy} = (a - a_0) / a_0
\]
Figure 2. Polarization charge distribution schematic of PIDFET (AlN/β-Ga$_2$O$_3$/GaN).

Table 1. Parameters used for polarization calculation of AlN/β-Ga$_2$O$_3$/GaN heterostructure.

<table>
<thead>
<tr>
<th>Lattice mismatch with β-Ga$_2$O$_3$</th>
<th>$\varepsilon_{33}$ (C m$^{-2}$)</th>
<th>$\varepsilon_{31}$ (C m$^{-2}$)</th>
<th>$P_{sp}$ (C m$^{-2}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>AlN</td>
<td>2.4% [15]</td>
<td>1.46 [38]</td>
<td>−0.60 [38]</td>
</tr>
<tr>
<td>GaN</td>
<td>4.7% [32]</td>
<td>0.73 [38]</td>
<td>−0.49 [38]</td>
</tr>
</tbody>
</table>

where $P_{tot}$ is the total polarization, $P_{sp}$ and $P_{pz}$ are the spontaneous polarization and piezoelectric polarization, respectively; $\varepsilon_{33}$ and $\varepsilon_{31}$ are piezoelectric coefficients parallel and perpendicular to the c axis, respectively, $\varepsilon_{xx}$ and $\varepsilon_{yy}$ are the biaxial stresses in c plane, and $\varepsilon_{zz}$ is the stress along the c axis.

Table 1 lists polarization related parameters that used for AlN/β-Ga$_2$O$_3$/GaN heterostructure. It is worth noting that the proposed III-nitride/β-Ga$_2$O$_3$ heterojunctions are all based on the (−201) plane of β-Ga$_2$O$_3$ and (001) of III-nitride. A very small lattice mismatch (~2.4%) between the AlN and β-Ga$_2$O$_3$ was adopted [15]. At the interface between Al-polar AlN and β-Ga$_2$O$_3$, $P_{SP}$ is dominant and induces an electric field along the growth direction and thus provides a driving force for the electron flowing into the channel. At the β-Ga$_2$O$_3$/Ga-polar GaN interface, $P_{PZ}$ dominates polarization charges and a reverse electric direction is formed, drawing the electrons from bulk Ga$_2$O$_3$ (the region beneath the 2DEG channel). The interface charge distributions of those two interfaces are schematically shown in figure 2.

The calculated energy band diagram (red line) and electron distribution (blue line) at the AlN/β-Ga$_2$O$_3$ and the β-Ga$_2$O$_3$/GaN heterointerface are shown in figure 3(a). According to the diagram, there are obvious conduction band offsets at both interfaces and high concentration of 2DEGs can be formed. The electron concentration as high as $8.1 \times 10^{19}$ cm$^{-3}$ was obtained at the upper interface, providing a conductive channel for the PIDFET. The electron density of the bulk Ga$_2$O$_3$ was controlled down to $1.36 \times 10^{16}$ cm$^{-3}$ due to the existence of the GaN back barrier layer which can be further confirmed in figures 3(b) and (c). This much reduced electron density can suppress the drain leakage current and decrease the subthreshold swing.

The models used in the simulations include parallel electric field model for velocity saturation (FLDMOB), Shockley–Read–Hall model (SRH), Fermi–Dirac model (FERMI), incomplete ionization model (INCOMPLETE) and polarization model (POLARIZATION). The Caughey–Thomas expression for β-Ga$_2$O$_3$ was also applied with a saturation velocity of $2 \times 10^7$ cm s$^{-1}$ and a channel hall mobility.
Figure 4. Simulated transfer characteristics with varying AlN thickness of 4, 6, 8, 10 and 12 nm in (a) linear and (b) semi-logarithmic scale; (c) linearly dependent \( V_{th} \) vs AlN thickness curve extracted from (b); (d) electron density in the channel with varying AlN thickness at 10 V and 0 V gate biases, respectively; and (e) \( g_m - V_{gs} \) curves with varying AlN thickness of 4, 6, 8, 10 and 12 nm.

of 200 cm\(^2\) V\(^{-1}\) s\(^{-1}\). These two are typical values for \(\beta\)-Ga\(_2\)O\(_3\) based field-effect transistors [39]. We have validated our polarization model by performing calculation on the 2DEG in the AlN/GaN [40] and AlGaN/GaN heterostructures [41, 42], and similar results were obtained. Additionally, it has to be noted that those polarization parameters can be significant different in the calculation of polarization field in those heterostructures if different reference models are adopted (zincblende or hexagonal references) [43]. Moreover, the electron transport model was also calibrated by doing the simulation on an \((\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3/\text{Ga}_2\text{O}_3\) MODFET experimentally reported before [12]. In addition, the channel mobility in this AlN/\(\beta\)-Ga\(_2\)O\(_3\) PIDFET may be higher than that in \((\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3/\text{Ga}_2\text{O}_3\) MODFET due to the elimination of the alloy scattering which is one of the significant scattering mechanisms for the electron transportation [43]. The p-type doped buffer was simulated with incomplete ionization model due to the nature of the dopant material (usually Mg in the case of III-nitrides) [44]. All UID layers in the simulator were doped with a low donor background concentration of \(10^{15}\) cm\(^{-3}\). In the following section, the influences of some key structural and device parameters on the device performance are investigated in detail, including AlN polarization layer, p-GaN gate layer and GaN back barrier layer.

3. Results and discussions

3.1. AlN polarization layer

Figures 4(a) and (b) show the simulated transfer characteristics with varying AlN thickness in linear and semi-logarithmic scale, respectively. The \(V_{th}\) and the saturation current
increased with decreasing AlN thickness. The $V_{th}$ values extracted from the semi-logarithmic $I_{ds}$–$V_{gs}$ curves are 0.3, 0.9, 1.4, 2.0 and 2.6 V for AlN thicknesses of 12, 10, 8, 6 and 4 nm, respectively, as shown in figure 4(b). Further analysis reveals that $V_{th}$ is linearly dependent on the AlN thickness, as plotted in figure 4(c). This means the $V_{th}$ is tunable by varying AlN thickness, and it provides a straightforward approach to achieving the desired $V_{th}$.

Another obvious trend can be found in figure 4(a) is that the saturation current increases with a decreasing AlN thickness. It is well known that the current density is formulated as equation: $J = \frac{-nq\bar{v}_d}{E} = nq\mu E$, where $n$ is the electron density, $q$ is the charge of an electron, $\bar{v}_d$ is the average electron drift velocity, $\mu$ is the electron mobility, and $E$ is the lateral electric field intensity. The increment of the saturation current can be explained by an enhanced electron density in the channel with a thinner AlN thickness, as shown in figure 4(d). At the gate bias of 0 V, the electron density in the channel, which is only influenced by the polarization charges at the interface, remains almost a constant with varying AlN thickness. At the gate bias of 10 V, however, the electric potential in the channel gets higher and assists the polarization electric field in forming...
Figure 7. (a) Output characteristics of AlN/β-Ga$_2$O$_3$ PIDFET without back barrier layer; (b) output characteristics of AlN/β-Ga$_2$O$_3$ PIDFET with GaN back barrier layer; (c) transfer characteristics of AlN/β-Ga$_2$O$_3$ PIDFET without back barrier layer under $V_{ds} = 10$ V; and (d) transfer characteristics of AlN/β-Ga$_2$O$_3$ PIDFET with GaN back barrier layer under $V_{ds} = 10$ V.

a higher electron density. In addition, a higher transconductance is also obtained in figure 4(e) with a thinner AlN layer, indicating a better gate control.

Figure 6 exhibits the effect of hole concentration of p-GaN gate to the transfer characteristic. The $V_{th}$ extracted from the semi-logarithmic $I_{ds}$–$V_{gs}$ curves are $-0.5$, $-0.3$, $0$, $1.2$, and $2.6$ V for acceptor concentration of $1 \times 10^{17}$, $1 \times 10^{18}$, $2 \times 10^{18}$, $4 \times 10^{18}$ and $6 \times 10^{18}$ cm$^{-3}$ respectively. It is obvious that with the increased hole concentration, the $V_{th}$ becomes higher. This trend can be explained by the broadened depletion area in n-type Ga$_2$O$_3$ with an increased hole concentration of the p-GaN. Therefore, a higher turn-on voltage, which is desirable in the normally-off operation devices, is needed to form the channel.

3.2. p-GaN gate

In order to further investigate the normally-off operation, we simulated the dependence of the transfer characteristics on different p-GaN gate parameters in terms of the gate length and the hole concentration. Figures 5(a) and (b) show the $I_{ds}$–$V_{gs}$ curves with different gate length in linear and semi-logarithmic scale, respectively. The threshold voltages extracted from the semi-logarithmic curves (figure 5(b)) are $2.6$, $3.3$, $3.4$ and $3.4$ V for the gate length of $0.1$, $0.2$, $0.3$, and $0.4$ µm, respectively. The curves of transconductance versus gate voltage with varying gate length are shown in figure 5(c). The maximum values of transconductance extracted from the $g_m$–$V_{gs}$ are $404.3$, $379.6$, $364.1$ and $348.8$ mS mm$^{-1}$ for the gate length of $0.1$, $0.2$, $0.3$, and $0.4$ µm, respectively, which suggests that there is a tradeoff between the threshold voltage and the transconductance.

3.3. GaN back barrier layer

The output characteristics of the PIDFET without and with back barrier layer are also compared, and the results are shown in figures 7(a) and (b). From figure 7(a), it is found that the drain current ($I_{ds}$) is not saturated and the off-state $I_{ds}$ (the purple line) arises significantly, indicating the existence of drain leakage current. In figure 7(b), the drain current is saturated, and a maximum $I_{ds}$ of $1698$ mA mm$^{-1}$ is obtained. The off-state drain leakage current can be fully suppressed by the GaN back barrier layer. The detailed principles of the suppression effect of the inserted GaN back barrier were elaborated in section 2.2 as schematically shown in figures 2 and 3. Figures 7(c) and (d) demonstrate the transfer characteristics of the PIDFET without and with the GaN back barrier layer. We can find that the current at the subthreshold region ($0 \sim 4$ V in figure 7(c)) is much suppressed by adding the GaN back barrier layer.

4. Conclusion

To unleash the full potential of Ga$_2$O$_3$ and III-nitride materials in power device applications and realize a normally-off field-effect transistor, herein, we proposed a normally-off AlN/β-Ga$_2$O$_3$ PIDFET via forming a polarization-induced 2DEG channel within the device.
Although early experimental demonstrations of the formation of the III-nitrides/gallium oxide heterostructures have shown the promise for their implementation in III-nitrides/Ga$_2$O$_3$-based power electronics, due to the obvious difference in their crystal structures, it is still challenging to grow AlN or Al-rich AlGaN thin films on β-Ga$_2$O$_3$ templates or vice versa to form high-quality interfaces \[15, 33, 34\]. Significant efforts have to be dedicated to the growth optimization. Many growth approaches, such as substrate temperatures, gas flow sequences and rates, film stress control, and initial stage nucleation, are the keys to achieve high-quality epitaxial layers and thus to realize high performance transistors based on III-nitrides/Ga$_2$O$_3$ heterostructures in the future \[33, 34\]. Additionally, due to the narrower bandgap of GaN in comparison with Ga$_2$O$_3$, the p-GaN itself has lower critical field which may compromise the breakdown performance in the proposed devices. Other wider bandgap p-type material, for example p-AlGaN layer, may serve better as the gate material, which can be an interesting topic for further investigation.

Nevertheless, in this work, the proposed PIDFET exhibits decent output characteristics, including high source-drain current and high transconductance, which can be attributed to the large 2DEG concentration. We comprehensively investigated the transfer characteristics of the PIDFET with different AlN thickness, p-GaN gate length and doping concentration of p-GaN gate. In order to suppress the off-state drain leakage current and decrease the subthreshold swing, we adopted an AlN/β-Ga$_2$O$_3$ PIFET with a Ga-polar GaN back barrier layer. Our approach could fully leverage the benefits of III-nitrides and Ga$_2$O$_3$ materials by taking advantage of the polarization effect at the III-N/Ga$_2$O$_3$ interface in the pursuit of future field-effect transistor.

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