Effects of gate work function on E-mode AlGaN/GaN HEMTs with stack gate \(\beta\)-Ga\(_2\)O\(_3\)/p-GaN structure

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Abstract
This research investigates electrical properties of E-mode AlGaN/GaN HEMTs with n-type \(\beta\)-Ga\(_2\)O\(_3\)/p-GaN gate stack under different gate work functions of 4.6, 5.1 and 5.7 eV, respectively. The simulated results show that the device with gate work function of 5.7 eV exhibits the largest threshold voltage of 2.8 V while having the lowest saturation drain current of 0.15 A mm\(^{-1}\), which can be ascribed to the device having the highest Schottky barrier, leading to the least electrons collected at the AlGaN/GaN interface. Moreover, the device with gate work function of 5.7 eV shows the largest gate breakdown voltage as well as the lowest off-state gate leakage, which can be attributed to the least strength of electric field in the Ga\(_2\)O\(_3\) layer. Additionally, the Fowler–Nordheim equation was used to study the mechanisms of off-state leakage.

Keywords: AlGaN/GaN, HEMT, Ga\(_2\)O\(_3\), gate work function

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

1. Introduction

Gallium nitride (GaN) based high electron mobility transistors (HEMTs) have drawn considerable attention in high power electronics due to their superior properties, such as low specific on-resistance, high operation switching frequency, high breakdown voltage, and good-thermal stability [1, 2]. Conventional AlGaN/GaN HEMTs show a normally-on behavior, which is caused by the fact that two-dimensional electron gas (2DEG) inherently exists at the interface due to the strong built-in polarization electric field in the AlGaN/GaN hetero-structure [3]. Nevertheless, to meet the needs of most power electronic applications, normally-off devices are more desirable [4]. Several technologies have been developed to achieve normally-off operation, including recessed gate, fluorine-base plasma treatment, floating charges, the piezo neutralization layer, and the p-type GaN cap layer [5–9]. Among these different methods, the p-GaN gate structure is considered to be the most promising structure for commercialization due to its well-balanced features between device performance, reliability and manufacturing capability [10, 11].

More recently, a GaN-based p-n junction gate HEMT featuring an n-GaN/p-GaN/AlGaN/GaN gate stack has been demonstrated to improve the performance of the device with a larger gate breakdown and a lower gate leakage thanks to the wider depletion region in the p–n junction at forward gate voltages [12]. Moreover, \(\beta\)-Ga\(_2\)O\(_3\) is an attractive ultrawide band gap semiconductor, and shows tremendous

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potential to outperform current high-power semiconductors such as GaN and SiC [13–15]. More inspringly, the construction of p–n heterojunctions between mechanically exfoliated n-type β-Ga2O3 and p-type GaN have been fabricated [16, 17]. Thus, a GaN-based p–n junction gate HEMT featuring an n-type β-Ga2O3/p-GaN/AlGaN/GaN gate stack could be an appealing consideration which needs further studies.

For conventional p-GaN gate HEMTs, 2DEG carriers in the channel are modulated by the Schottky gate. Schottky barrier heights were observed to vary with different gate work functions, which determine the electric characteristics including threshold voltage, gate breakdown, gate leakage etc [18–22]. Thus, the choice of gate work function is important to obtain a proper barrier height to maintain device operations. In this work, we investigate the effects of work functions for Schottky gate contacts on the performance of the n–β-Ga2O3/p-GaN/AlGaN/GaN HEMT. The gate work functions are selected as 4.6, 5.1 and 5.7 eV [19], with corresponding metals of Cu, Ni and Pt [23, 24]. The electrical characteristics including threshold voltage ($V_{TH}$), saturation drain current ($I_{D,S}$), gate breakdown and off-state gate leakage of the proposed device are studied. Notably, a trade-off behavior between threshold voltage and output current with different gate work functions is observed. Also, gate work functions can control gate breakdown and off-state gate leakage of the device. Moreover, band diagrams, electron concentrations, and distribution of electric field are simulated to analyze the mechanisms.

## 2. TCAD modeling

### 2.1 Models

To access the performance of the proposed E-mode AlGaN/GaN HEMTs with n-type β-Ga2O3/p-GaN gate stack, we used the Silvaco Atlas 2D drift-diffusion simulator. A low field mobility model was used to consider various types of scattering mechanisms [25]. Shockley–Read–Hall recombination was used to model trapping effects [26]. Polarization models were taken into account due to the strong spontaneous and piezoelectric polarization effects of nitride semiconductors [27]. The Fowler–Nordheim tunneling model was used to treat the tunnel effect [28]. Parallel electric field model was adopted to model velocity saturation effect and all calculations are based on the Fermi–Dirac statistics [29].

### 2.2 Device structure

The proposed E-mode AlGaN/GaN HEMT with stack gate β-Ga2O3/p-GaN structure consists of a 5 nm β-Ga2O3 layer with a carrier concentration of $1 \times 10^{17}$ cm$^{-3}$, a 50 nm p-GaN layer, a 15 nm Al0.23Ga0.77N barrier layer, and a 2 μm GaN buffer layer as shown in figure 1(a). The hole density in the p-GaN layer is $3 \times 10^{17}$ cm$^{-3}$ and the electron density in AlGaN layer is $1 \times 10^{13}$ cm$^{-3}$. The unintentional doping carrier concentration in the GaN buffer is $1 \times 10^{16}$ cm$^{-3}$. The gate-source distance, gate length, and gate-drain distance of the proposed device are 1, 1, and 6 μm, respectively. The gate electrode was defined as the Schottky contact, and the source and drain electrodes were defined as ohmic contacts. The work functions of the gate metal were selected as 4.6, 5.1, and 5.7 eV to investigate the effects of gate work function on the performance of the proposed device. The contact of gate metal and semiconductor is shown in figure 1(b), and the Schottky barrier height is determined by the energy differences between gate metal work function and semiconductor conduction band.

## 3. Results and discussion

### 3.1 Effect of gate work functions on the $V_{TH}$ and $I_{D,S}$

Figures 2(a) and (b) show the transfer and output characteristics of the E-mode HEMT. As shown in figure 2(a), the threshold voltages of the device are 1.7, 2.3 and 2.8 V at drain voltage of 5 V with a work function of the gate metal as 4.6, 5.1 and 5.7 eV, respectively. Thus, the threshold voltage obtained from the slope of the linear region in the $I_D$–$V_G$ curve increases with the increase of gate work functions. Figure 2(b) shows $I_D$–$V_D$ curves of the device at gate voltage of 4 V, and in this work the saturation drain current is defined as the output drain current at drain voltage of 20 V in $I_D$–$V_D$ curves. As acquired from figure 2(b), the saturation drain currents are 0.34, 0.23, and 0.15 A mm$^{-1}$ with gate work functions of 4.6, 5.1 and 5.7 eV, respectively. Hence, the saturation drain current decreases with the increase of the gate work functions. Therefore, there is a trade-off between $V_{TH}$ and saturation drain current with different gate work functions, as shown in figure 2(c). This can be attributed to the difference of band diagrams resulting from different Schottky barrier heights caused by different gate work functions.

Band diagrams were simulated to investigate the impacts of work functions on threshold voltage of the device, as shown in figures 3(a) and (b). The gate voltage and drain voltage are both set as 0 V, and the fermi level is at 0 eV. Figure 3(a) shows the conduction band diagrams of the device with the three work functions. The theoretical Schottky barrier height can be obtained from figure 3(a) as 0.6, 1.1 and 1.7 eV with gate work function of 4.6, 5.1, and 5.7 eV, respectively. Conduction band diagrams are above the fermi level at gate voltage of 0 V, hence few electrons are collected in the potential well of the AlGaN/GaN heterojunction. Forward gate bias...
Figure 2. (a) Transfer characteristics of the device at drain voltage of 5 V and (b) output characteristics of the device at gate voltage of 4 V. (c) A trade-off between threshold voltage and saturation drain current with different gate work functions. The work functions of the gate metal are 4.6, 5.1 and 5.7 eV.

Figure 3. (a) Conduction band diagrams, (b) valence band diagrams of the E-mode device and (c) electron concentrations at AlGaN/GaN interface. The gate voltage and drain voltage are both 0 V, and the gate work functions are set as 4.6, 5.1, and 5.7 eV.
should be applied on the gate to collect electrons in the potential well to form the channel current and open the device. Thus, a larger gate voltage should be applied on the gate to open the device with less electrons in the potential well. As can be found from figures 3(a) and (c), the conduction band with work function of 5.7 eV shows shallowest potential well, and the electron concentrations at AlGaN/GaN interface decreases with the increase of the gate work functions. Thus, the device with gate work function of 5.7 eV shows the largest threshold voltage, as shown in figure 2(a). Figure 3(b) plots the valance band diagrams of the device at gate voltage of 0 V, in which the valance band diagrams are under the fermi level, where few holes exist at p-GaN/AlGaN interface. With the increase of gate bias, holes will be collected at the p-GaN/AlGaN interface and drift further to the AlGaN/GaN interface.

In order to study the effects of gate work functions on the saturation drain current of the device, band diagrams and distribution of electron concentrations were simulated, as shown in figure 4. The device is at on-state with gate voltage of 4 V and the conduction band diagram is under the Fermi level at the AlGaN/GaN interface, hence, a large number of electrons exist at the AlGaN/GaN potential well, as shown in figure 4(a). These electrons then flow to the drain terminal which usually called a drain current. When all the electrons collected at the AlGaN/GaN interface are attracted to the drain terminal, the saturation current of the device is acquired. That is, the more electrons exist at the AlGaN/GaN interface, the larger saturation drain current will be. Figure 4(b) shows distribution of electron concentrations of the device, and electron concentrations at the AlGaN/GaN interface with the three gate work functions are exhibited in figure 4(c) accurately. As can be noted from the figure 4(c), electron concentrations decrease with the increase of gate work functions. Therefore, the device with gate work function of 4.6 eV exhibits the largest saturation drain current as shown in figure 2(b).

3.2. Effect of gate work functions on the gate breakdown and off-state gate leakage

$I_G$–$V_G$ characteristics of the proposed device were simulated to investigate the impacts of work functions on gate breakdown and off-state gate leakage. As shown in figure 5(a), the drain voltage is 5 V and the gate voltage is scanned from –1 V to 15 V at 0.3 V per step. The gate breakdown voltages are defined as the gate voltages at the gate current of 0.01 A mm$^{-1}$ in this work, whose values are 11.6, 12.1 and 12.7 V correspond to the work functions of 4.6, 5.1, and 5.7 eV, respectively. Thus, the gate breakdown voltage increases with increase of gate work functions, which can be ascribed to the different strength of electric field in the gate region due to the different Schottky barriers. Figure 5(b) shows $I_G$–$V_G$ characteristics with the three gate work functions at
Figure 5. $I_G$–$V_G$ curves of the device at drain voltage of (a) 5 V and (b) 0 V. The gate work functions are 4.6, 5.1, and 5.7 eV.

Figure 6. (a) Distributions of electric field at gate voltage of 8 V with gate work functions of 4.6, 5.1 and 5.7 eV. (b) Distributions of electric field at gate voltages of 3, 4 and 5 V with a gate work function of 5.7 eV.

drain voltage of 0 V with logarithmic coordinate. The off-state gate leakage currents at gate voltage of 0 V are $1 \times 10^{-24}$, $1 \times 10^{-34}$ and $1 \times 10^{-44}$ A mm$^{-1}$ with the work function of 4.6, 5.1 and 5.7 eV respectively. Hence, the off-state gate leakage decreases with increase of gate work functions. Moreover, the device with gate work function of 5.7 eV exhibits an off-state leakage magnitude 20 orders smaller than the device with gate work function of 4.6 eV. It should be pointed out that in this paper, high dislocation defects in GaN or Ga$_2$O$_3$ are not considered. In addition, the practical Schottky barrier will not be ideal, thus, the proposed device exhibits very low gate leakage current in our simulation, which can be ascribed to the tunnel current due to the thin Ga$_2$O$_3$ layer. The tunnel current is too small to measure, but is of great importance to study. Therefore, increasing gate work functions can increase the gate breakdown voltage and reduce the off-state leakage current of the device. In this work the device with gate work function of 5.7 eV exhibits the best performance with the largest gate breakdown as well as the lowest off-state gate leakage.

The effects of gate work functions on the gate breakdown of the $E$-mode device are investigated by simulating distribution of electric field at drain voltage of 5 V, as shown in figure 6. The equivalent circuit of the gate region can be modeled as a Schottky-metal/Ga$_2$O$_3$ junction, and under forward gate bias conditions, the Schottky metal/Ga$_2$O$_3$ diode has forward bias. As can be indicated from the figure 6(a), with the same forward gate bias of 8 V, the peak electric-field is buried within the Schottky metal/Ga$_2$O$_3$ diode and the strength of the electric field in the Ga$_2$O$_3$ layer decreases with increase of the gate work functions. Thus, the device with gate work function of 5.7 eV exhibits the lowest electric field in the Ga$_2$O$_3$ layer. Figure 6(b) shows distributions of electric field with a gate work function of 5.7 eV at gate voltages of 3, 4 and 5 V. It can be found out from figure 6(b) that the strength of electric field in Ga$_2$O$_3$ layer increases as the forward gate voltage increases. Then, the increasing forward gate voltage of the device will reach the gate breakdown voltage when the strength of electric field in the Ga$_2$O$_3$ layer is large enough. In addition, the forward bias gate breakdown has known to be related with avalanche breakdown mechanism [30], and the rate of avalanche breakdown is positive correlation with electric field. Thus, the device with gate work function of 5.7 eV is the last to be broke with increasing gate voltages due to the lowest electric field in the Ga$_2$O$_3$ layer, resulting in the largest gate breakdown, as shown in figure 5(a).

Figure 7 presents the distribution of electric field with the three gate work functions, where the gate and drain voltages are both 0 V, in which the strength of electric field in the Ga$_2$O$_3$ layer of gate work function of 4.6 eV is $2.9 \times 10^6$ V m$^{-1}$ and decrease as the gate work functions increase. The off-state gate leakage can be ascribed to the tunnel current, as the strength of electric field of the device is high and the Ga$_2$O$_3$ layer is sufficiently thin. This tunneling of carriers in the presence of
Data availability statement

The data generated and/or analyzed during the current study are not publicly available for legal/ethical reasons but are available from the corresponding author on reasonable request.

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4. Conclusions

Electrical performances of the proposed E-mode AlGaN/GaN HEMTs with n-type β-Ga2O3/p-GaN gate stack under gate work functions of 4.6, 5.1 and 5.7 eV were studied by TCAD device simulations. There is a trade-off between threshold voltage and saturation drain current of the device with different gate work functions. The simulation results indicate that with increasing of gate work functions, the threshold voltage increases, whereas the saturation drain current decreases. This can be attributed to the larger Schottky barrier height owing to the higher gate work function, which regulate band diagrams at off-state and change electron concentrations in the potential well at on-state of the device. In addition, the device with a gate work function of 5.7 eV shows the largest gate breakdown voltage of 12.7 V, which can be ascribed to the lowest strength of electric field in the Ga2O3 layer. Moreover, the device with a gate work function of 5.7 eV shows the lowest off-state gate leakage current of $1 \times 10^{-34}$ A mm$^{-1}$, whose magnitude is 20 orders smaller than the device with a gate work function of 4.6 eV. This can be attributed to the largest strength of electric field in the Ga2O3 layer at drain voltage of 0 V deduced by the Fowler-Nordheim equation.

where $E$ is the electric field in the Ga2O3 layer, and $A$ and $B$ are constants. As shown in figure 7, the device with gate work function of 4.6 eV exhibits the largest strength of electric field in the Ga2O3 layer, thus, this device obtains the largest tunnel current according to the formula above. Therefore, the device with gate work function of 4.6 eV shows the largest off-state gate leakage, as shown in figure 5(b).

Figure 7. Distributions of electric field with gate work functions of 4.6, 5.1 and 5.7 eV. The gate and drain voltage are both set as 0 V.
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