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Interface charge engineering on an *in situ* SiN /AlGaN/GaN platform for normally off GaN MIS-HEMTs with improved breakdown performance ©

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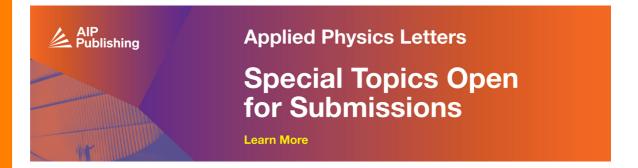
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ABSTRACT

This work adopts interface charge engineering to fabricate normally off metal–insulator–semiconductor high electron mobility transistors (MIS-HEMTs) on an *in situ* $SiN_x/AlGaN/GaN$ platform using an *in situ* O_3 treatment performed in the atomic layer deposition system. The combination of *in situ* SiN_x passivation and an O_3 -treated $Al_2O_3/AlGaN$ gate interface allows the device to provide an excellent breakdown voltage of 1498 V at a low specific on-resistance of $2.02 \, \text{m}\Omega \, \text{cm}^2$. The threshold voltage is increased by 2 V by significantly compensating the net polarization charges by more than five times with O_3 treatment as well as reducing the interface traps and improving the high-temperature gate stability. Furthermore, a physical model of fixed charges at the $Al_2O_3/AlGaN$ interface is established based on dielectric thickness-dependent linear fitting and numerical calculations. The matched device performance and simulated energy band bending elucidate the O_3 -treated fixed-charge modulation mechanism, providing a practical method for producing normally off GaN MIS-HEMTs.

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GaN metal-insulator-semiconductor high electron mobility transistors (MIS-HEMTs) are potential candidates for the next generation of high-power electronics. Generally, the two-dimensional electron gas (2DEG) properties and device performance can be compromised by process-induced damage at the interface of the dielectric/ AlGaN barrier. To mitigate this issue, the *in situ* SiN_x insulator layer, which is continuously grown on the AlGaN barrier by metal-organic chemical vapor deposition (MOCVD), has been extensively studied as a means of protecting the AlGaN surface from air and process-induced damage. In addition, compared with *ex situ* SiN_x deposition methods, such as plasma-enhanced chemical vapor deposition (PECVD) or low-pressure chemical vapor deposition (LPCVD), *in situ* SiN_x has a lower growth rate and higher growth temperature,

which is favorable for reducing dielectric defects, thus suppressing the gate leakage current. 5

Generally, a large number of positive fixed charges at the *in situ* $SiN_x/AlGaN$ interface induces a high 2DEG density at the AlGaN/GaN heterojunction, and the GaN MIS-HEMT based on the *in situ* $SiN_x/AlGaN/GaN$ platform features a negative threshold voltage (V_{th}) and a low on-state resistance (R_{on}). For in commercial product applications, the normally on *in situ* $SiN_x/AlGaN/GaN$ MIS-HEMT is usually integrated with a normally off SiMOSFET in a cascode connection to simplify circuit design and build a fail-safe system. The intrinsic parasitic problem in a cascode structure restricts its application to high-frequency and high-voltage fields. As a result, individual etching-free normally off SiMOSFET of SiMOSFET in a cascode structure restricts its application to high-frequency and high-voltage fields. As a result, individual etching-free normally off SiMOSFET of SiMOSFET in a cascode structure restricts its application to high-frequency and high-voltage fields. As a result, individual etching-free normally off SiMOSFET of SiMOSFET in a cascode structure restricts its application to high-frequency and high-voltage fields. As a result, individual etching-free

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engineering and ultrathin-barrier (UTB) techniques by depleting the 2DEG at the gate region.^{8–10} It has been reported that the positive fixed charges at the Al₂O₃/GaN interface were decreased by post-dielectric/gate annealing ¹¹ and can also be reduced by a CF₄ or O₂ plasma. ^{12,13} However, the positive fixed charge at the *in situ* SiN_x/AlGaN interface persists after dry etching unless the underlying AlGaN barrier is simultaneously etched or thinned. ¹⁴ Therefore, there are limited reports regarding normally off MIS-HEMT on *in situ* SiN_x/AlGaN/GaN platforms.

This study fabricates a high-performance normally off GaN MIS-HEMT on an $in\ situ\ SiN_x/AlGaN/GaN\ platform$ with an Al_2O_3 insulating layer by atomic layer deposition (ALD). An $in\ situ\ O_3$ treatment in the ALD system is implemented before the Al_2O_3 deposition to reduce the positive fixed charge on the post- $in\ situ\ SiN_x$ -etching AlGaN surface. This critical step provides the normally off $Al_2O_3/AlGaN/GaN\ MIS-HEMTs$ with $in\ situ\ SiN_x$ passivation, improving the gate and off-state breakdown voltages (BV). The conducted dielectric thickness-dependent fitting and simulated models suggest that the O_3 treatment can significantly increase the device V_{th} by compensating for the fixed charges. In addition, both the interface states and high-temperature gate current leakage instability are suppressed in the fabricated normally off GaN MIS-HEMT.

The MIS-HEMTs were fabricated on a 6-inch in situ SiN_x/ AlGaN/GaN platform. From the bottom to up, it consists of a thick buffer layer, a 300 nm GaN channel layer, a 1 nm AlN spacer, a 5 nm $Al_{0.05}Ga_{0.95}N$ layer, and a 30 nm in situ SiN_x cap layer. Because the in situ SiN_x strongly passivates the wafer, the device process begins with an Ohmic contact. A Ti/Al/Ti/Au metal stack is evaporated through an opened deposition window, followed by an annealing process at 830 °C for 45 s in an N₂ ambient. Next, the in situ SiN_x at the gate region is removed using an inductively coupled plasma reactive ion etching (ICP-RIE) system. After that, the wafer is transferred to the ALD chamber, where it undergoes a pre-gate O₃ treatment at 300 °C. Following this, an 18-nm O₃-based Al₂O₃ insulating layer is deposited, and a Ni/Au metal stack is evaporated as the gate electrode. Subsequently, a 350 °C annealing process is conducted in N₂ ambient for 5 min to improve the Ni/Al₂O₃ contact properties. Finally, a 200-nm SiO₂ layer is deposited by PECVD, and the source field plate is formed to complete the device process.

Figure 1(a) shows the structure of the fabricated GaN MIS-HEMT. The gate width $(W_{\rm G})$, gate length $(L_{\rm G})$, distance of gate-to-source $(L_{\rm GS})$, and distance of gate-to-drain were set to $100/2/3/10~\mu{\rm m}$, respectively, with an extension distance of 3 $\mu{\rm m}$ toward the drain side

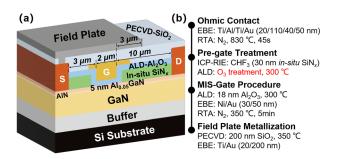


FIG. 1. (a) Schematic of GaN MIS-HEMT on an *in situ* $SiN_x/AlGaN/GaN/Si$ platform; (b) main device fabrication process.

of the source field plate. The main steps of the device process are listed in Fig. 1(b), and an MIS-HEMT without O_3 treatment was also fabricated as a control.

The DC transfer characteristics of the fabricated MIS-HEMTs are plotted in Fig. 2(a) at a bias voltage of $V_D = 10 \text{ V}$. As shown, the O_3 treatment leads to an increase in the device V_{th} from -1.6 to 0.4 V, which is determined using a drain current criterion of 1 μ A/mm. This increase in $V_{\rm th}$ is attributed to the effective reduction of positive fixed charges at the Al₂O₃/AlGaN interface, resulting in a lower net polarization charge density in the gate region. ^{15,16} The performance of the MIS-HEMTs is also characterized by high extrinsic transconductance, with both values greater than 150 mS/mm, which can be attributed to the excellent gate control ability of the UTB structure.¹⁷ As plotted in Fig. 2(b), the *in situ* SiN_x passivation provides numerous positive fixed charges at the in situ SiN_x/AlGaN interface, inducing the high 2DEG density at the UTB Al_{0.05}Ga_{0.95}N/GaN heterojunction and excellent output performance. The $R_{\rm on}$ increases from 9.8 to 11.2 Ω ·mm, showing a depletion of 2DEG at the gate region for the normally off operation.

The $I_{\rm G}$ – $V_{\rm G}$ curve in Fig. 2(c) illustrates that the O₃ treatment allows for a maximum positive $V_{\rm G}$ of 16 V, while the controlled device shows a limit of only 14.3 V. This slight increase in gate BV can be attributed to the lower concentration of oxygen vacancy ($V_{\rm O}$) defects resulting from pre-gate O₃ treatment. A similar improvement is seen in the off-state BV, which increases from 1278 to 1498 V due to the O₃-treated Al₂O₃/AlGaN interface, as shown in Fig. 2(d). The high-quality in situ SiN_x passivation, along with an optimized source field plate, also contributes to the excellent breakdown performance. A 1.5 μ m transfer length for each Ohmic contact is included when

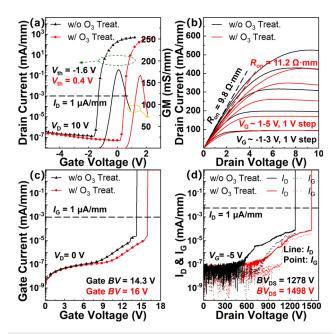


FIG. 2. (a) Semi-log transfer, (b) output, (c) I_G – V_G , and (d) OFF-state characteristics of fabricated GaN MIS-HEMTs on an *in situ* SiN_x/AlGaN/GaN platform without and with O $_3$ treatment.

calculating specific on-resistance ($R_{\rm on,sp}$), where the optimized device features a high BV_{DS} of 1498 V with a low $R_{\rm on,sp}$ of 2.02 m Ω cm².

The reasons for the improved device performance from the O₃ treatment are studied by detecting the microstructure. Figure 3(a) demonstrates the top view and surface profile of the etching trench of in situ SiN_x/AlGaN by atomic force microscopy (AFM). Following the removal of in situ SiNx by dry etching, the underlying AlGaN surface displays a root mean square (RMS) roughness of 0.82 nm, while an improved surface morphology with an RMS of 0.54 nm is observed in Fig. 3(b). The O_3 treatment helps to decrease the V_O defects, showing a better pre-deposition surface. Surface X-ray photoelectron spectroscopy (XPS), shown in Fig. 3(c), reveals that Si atoms are present in the top few atomic layers of the AlGaN surface after in situ SiN_x etching. The incorporated Si atoms may act as surface donors that significantly impact interface charges and channel scattering. 19 Additionally, after strong oxidization by O₃ treatment, most of the Ga-N and Si-N bonds are replaced by Ga-O and Si-O bonds to form an O-terminated AlGaN surface. Following the Al₂O₃ deposition, scanning transmission electron microscopy [STEM, Fig. 3(d)] shows an apparent local transition layer at the Al₂O₃/AlGaN interface and crystalline grains in the Al₂O₃ bulk, while the cross section of the O₃-treated sample shows

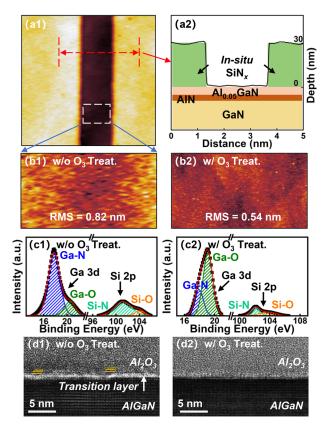


FIG. 3. (a1) AFM top view and (a2) surface profile of *in situ* SiN_x/AlGaN trench; (b) morphology of exposed AlGaN surface after etching and O_3 treatment; (c) XPS analysis of AlGaN surface composition; (d) STEM cross-view of Al₂O₃/AlGaN interface, showing the transition layer (indicated by white arrow) and crystalline grains (highlighted with orange guidelines along the local crystalline orientation) without O_3 treatment

a sharp interface and amorphous Al_2O_3 . The O_3 -treated Al_2O_3 /AlGaN interface with fewer V_O defects and crystalline grains may suppress the trap-assisted tunneling, 20,21 indicating the improved breakdown performance of GaN MIS-HEMTs in this work.

A series of GaN Schottky HEMTs and MIS-HEMTs with step-graded Al_2O_3 thicknesses were fabricated to confirm the fixed charge variation induced by the O_3 treatment. The V_{th} shift between the GaN MIS-HEMT and Schottky HEMT (no gate dielectric) in this work can be described as 22

$$\Delta V_{\rm th} = (\Delta \Phi_{\rm m} - \Delta E_{\rm c})/e + (\sigma_{\rm F} - \sigma_{\rm pol-})/\varepsilon_{\rm Al2O3} \times t_{\rm Al2O3}, \quad (1)$$

where $\Delta\Phi_{\rm m}$ represents the difference in Schottky barrier height between the Ni/Al₂O₃ and Ni/AlGaN interfaces, $\Delta E_{\rm c}$ is the conduction band offset for Al₂O₃/AlGaN, and $\sigma_{\rm F}$ and $\sigma_{\rm pol.}$ are the Al₂O₃/AlGaN interface fixed charge density and the GaN net negative spontaneous polarization charge density (1.8 × 10¹³ cm⁻²), respectively. ε and t are the permittivity and thickness of gate Al₂O₃. The linear fitting in Fig. 4(a) shows that the GaN MIS-HEMT $\sigma_{\rm F}$ values with and without O₃ treatment extracted from different slopes are 1.92 and 2.44 × 10¹³ cm⁻², respectively. The net polarization charge densities at the Al₂O₃/AlGaN interface are calculated as 1.2 and 6.4 × 10¹² cm⁻², indicating that the fixed-charge-induced 2DEG density can be decreased by more than five times by O₃ treatment.

Figure 4(b) plots the double-sweep capacitance–voltage (C–V) curves of the $Al_2O_3/Al_{0.05}GaN/AlN/GaN$ MIS-diodes fabricated using the same process as the MIS-HEMTs. The $V_{\rm FB}$ shifts from -1.2 to 0.8 V after O_3 treatment, where the $V_{\rm FB}$ increment of 2 V is in accordance with the MIS-HEMT performance. Furthermore, the C–V hysteresis decreases from 0.55 to 0.04 V, and this remarkable improvement is attributed to the improved $Al_2O_3/AlGaN$ interface quality from the O_3 treatment. The dielectric and interface charges can be extracted from the following equation:

$$Q_t = C_{\rm ox} \times \Delta V_{\rm FB},\tag{2}$$

where $Q_{\rm t}$ is the sum of the dielectric bulk and interface trap charges, $C_{\rm ox}$ is the oxide capacitance, and $\Delta V_{\rm FB}$ is the flatband voltage shift. The $Q_{\rm t}$ at the Al₂O₃/AlGaN interface without O₃ treatment is calculated as $1.22\times10^{12}\,{\rm cm^{-2}\cdot eV^{-1}}$, while the counterpart O₃-treated interface is $8.62\times10^{10}\,{\rm cm^{-2}\cdot eV^{-1}}$. It is confirmed that the bulk and interface traps in the Al₂O₃/AlGaN structure are effectively reduced by more than one order of magnitude by the O₃ treatment. Furthermore, the gate current leakage increases with increasing test temperature. The gate BV degenerates from 14.3 to 12 V at 200 °C, while the O₃-treated device features a stabilized gate current leakage with the maximum gate voltage decreasing by less than 1 V, as plotted in Fig. 4(c). Thus, the temperature-dependent, trap-assisted tunneling or Poole–Frenkel emission is suppressed in the O₃-treated interface, demonstrating high-temperature gate stability for the fabricated GaN MIS-HEMT.

According to the microstructure and device characteristics, the atom arrangements of the $in\ situ\ SiN_x/AlGaN$ interface and Al_2O_3 fabricated on the post- $in\ situ\ SiN_x$ -etching AlGaN surface are illustrated in Figs. 5(a)–5(c). V_O defects and substitutional Si atom dangling bonds at the O₃-treated Al₂O₃/AlGaN interface are both compensated, reducing the traps and positive fixed charges. The decreased interface charges (Q_{tt}) and oxide bulk charges ($Q_{ox,\ bulk}$) trapped in the MIS

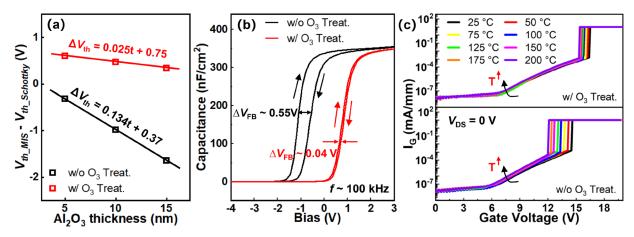


FIG. 4. (a) Experimental V_{th} shift and linear fitting between GaN MIS-HEMT and Schottky HEMT vs various gate Al_2O_3 thicknesses; (b) double-sweep C-V characteristics of $Al_2O_3/Al_{0.05}GaN/AlN/GaN$ MIS-diode at f=100 kHz; and (c) temperature-dependent gate current leakage.

structure contribute to improving the breakdown performance, while the reduced positive fixed charge ($\sigma_{\rm F}$) increases the $V_{\rm th}$ of GaN MISHEMT.

The main charge distribution is demonstrated in Fig. 5(d), considering the polarization charges (σ_{AIGaN} , $\sigma_{AIGaN/AIN}$, and $\sigma_{AIN/GaN}$) in the Al₂O₃/Al_{0.05}GaN/AlN/GaN gate stack. By calculating the heterojunction polarization charges from Vegard's law²⁴ and applying the $\sigma_{\rm F}$ ranging from 2.44 to 1.92×10^{13} cm⁻² in this work, the simulated energy band bending is depicted in Fig. 5(e). The bottom of the conduction band ($E_{\rm C}$) at the AlGaN/AlN/GaN interface rises above the Fermi level ($E_{\rm F}$) by reducing the positive fixed charge, matching the device operation to shift from normally on to normally off. The physical model of the Al₂O₃ thickness-dependent linear fitting and numerical simulation reveals the significance of fixed-charge modulation of $V_{\rm th}$ in GaN MIS-HEMTs.

Using O_3 treatment by ALD, a method for interface charge engineering is adapted to a UTB AlGaN/GaN MIS-HEMT with *in situ*

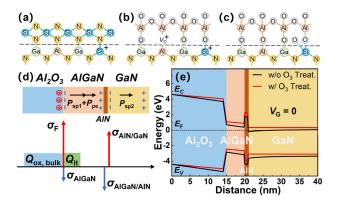


FIG. 5. Illustration of atomic arrangements for (a) *in situ* SiN_x/AlGaN interface. Al₂O₃/AlGaN interfaces (b) without and (c) with O₃ treatment after etching *in situ* SiN_x. (d) Schematic distribution profile of relevant charges in the Al₂O₃/Al_{0.05}GaN/AlN/GaN gate stack. (e) Calculated energy band diagrams for this work considering the σ_F of 1.92 \times 10¹³ (red) and 2.44 \times 10¹³ cm $^{-2}$ (black) at the Al₂O₃/Al_{0.05}GaN interface.

SiN_x caps. A physical relation is established between the interface properties of Al₂O₃/AlGaN and charge variation induced by in situ SiN_x etching/O₃ treatment through XPS analysis, AFM/TEM characterization, C-V measurement, and energy band simulation. The O₃treated Al₂O₃/AlGaN boundary charges are compensated by five times, and the interface traps are reduced by more than one order of magnitude. The fixed-charge modulation resulted in the relatively small positive V_{th} of 0.4 V for normally off operation on GaN MIS-HEMTs. To satisfy the demands of high-power switching system, the $V_{\rm th}$ is assumed to be further increased by optimizing the temperature of O₃ treatment and the post-dielectric/metallization-annealing (PDA/ PMA) processes. Meanwhile, combining a high-quality Al₂O₃/AlGaN gate interface with in situ SiN_x passivation enables the device to display an excellent BV of 1498 V with a low $R_{\text{on,sp}}$ of $2.02 \,\text{m}\Omega \,\text{cm}^2$. The in situ O₃ treatment during the ALD procedure provides a practical method for fabricating normally off GaN power HEMTs with excellent breakdown performance.

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AUTHOR DECLARATIONS Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Jiaqi He: Conceptualization (lead); Formal analysis (lead); Investigation (lead); Methodology (lead); Writing – original draft (lead). Kangyao Wen: Data curation (supporting); Formal analysis (supporting). Peiran Wang: Software (supporting). Minghao He: Formal analysis (supporting); Methodology (supporting). Fangzhou

Du: Resources (supporting). Yang Jiang: Methodology (supporting); Validation (supporting). Chuying Tang: Project administration (supporting). Nick Tao: Writing – review & editing (supporting). Qing Wang: Funding acquisition (supporting); Project administration (supporting); Supervision (supporting); Writing – original draft (supporting). Gang Li: Methodology (supporting); Supervision (supporting); Validation (supporting). Hongyu Yu: Funding acquisition (lead); Project administration (lead); Supervision (lead); Writing – review & editing (lead).

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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