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Characterization of interface states in Al2O3/AlGaN/GaN structures for improved performance of high-electron-mobility transistors

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Characterization of interface states in Al$_2$O$_3$/AlGaN/GaN structures for improved performance of high-electron-mobility transistors

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We have investigated the relationship between improved electrical properties of Al$_2$O$_3$/AlGaN/GaN metal-oxide-semiconductor high-electron-mobility transistors (MOS-HEMTs) and electronic state densities at the Al$_2$O$_3$/AlGaN interface evaluated from the same structures as the MOS-HEMTs. To evaluate Al$_2$O$_3$/AlGaN interface state densities of the MOS-HEMTs, two types of capacitance-voltage (C-V) measurement techniques were employed: the photo-assisted C-V measurement for the near-midgap states and the frequency dependent C-V characteristics for the states near the conduction-band edge. To reduce the interface states, an N$_2$O-radical treatment was applied to the AlGaN surface just prior to the deposition of the Al$_2$O$_3$ insulator. As compared to the sample without the treatment, the N$_2$O-radical treated Al$_2$O$_3$/AlGaN/GaN structure showed smaller frequency dispersion of the C-V curves in the positive gate bias range. The state densities at the Al$_2$O$_3$/AlGaN interface were estimated to be $1 \times 10^{12}$ cm$^{-2}$ eV$^{-1}$ or less around the midgap and $8 \times 10^{12}$ cm$^{-2}$ eV$^{-1}$ near the conduction-band edge. In addition, we observed higher maximum drain current at the positive gate bias and suppressed threshold voltage instability under the negative gate bias stress even at 150°C. Results presented in this paper indicated that the N$_2$O-radical treatment is effective both in reducing the interface states and improving the electrical properties of the Al$_2$O$_3$/AlGaN/GaN MOS-HEMTs.

I. INTRODUCTION

GaN and related-material high-electron-mobility transistors (HEMTs) are promising for high-power and high-frequency device applications, owing to their good physical properties such as high-breakdown electric field and high-saturation electron velocity. In particular, high-density and high-mobility two dimensional electron gas (2DEG) generated at the AlGaN/GaN interface enables us to realize power switching transistors having extremely low on-state resistance applicable to next generation power conversion systems. To achieve normally-off operation, metal-oxide-semiconductor (MOS) gate structures are absolutely required for suppressing gate leakage current under a forward gate bias operation. For realizing a good insulated gate, we should consider material properties of insulators: wide bandgap leading to large band offset against GaN-based-materials, high breakdown field, and high permittivity. In addition, low-density electronic states at the insulator/GaN-based-material interfaces are also necessary because interface states may cause various operational stability and reliability issues in GaN-based MOS-HEMTs such as threshold voltage instability and current collapse phenomenon. To address these issues, it is essential to investigate not only the densities of electronic states at the insulator/GaN-based-material interfaces but also the various process conditions to control them.

Al$_2$O$_3$ is one of the leading candidates for gate insulators in GaN-based devices. GaN-based MOS-HEMTs using an Al$_2$O$_3$ as the insulator have been demonstrated by many groups. The typical values of bandgap and permittivity reported for the Al$_2$O$_3$ film are 7–9 eV and 8–10, respectively. The Al$_2$O$_3$ film prepared by atomic layer deposition (ALD), in particular, showed relatively low electronic state densities in the Al$_2$O$_3$/n-GaN system. However, in the MOS-HEMT structures, the insulator/semiconductor interface is usually formed on the AlGaN/GaN heterostructures, resulting in the existence of two interfaces under the gate electrode. In this case, because those two interfaces make potential control rather complicated during capacitance-voltage (C-V) measurements, it is difficult to characterize interface states in the MOS-HEMTs compared with MOS structures having a single semiconductor layer (e.g., the Al$_2$O$_3$/n-GaN structure). Moreover, the wide bandgap of GaN-based materials also leads to extremely low emission rate of electrons captured at the interface states, making the evaluation of interface state densities difficult. For example, a typically used AlGaN with an Al composition ratio of around 25% has a bandgap of approximately 4.0 eV. Accordingly, the time constant for thermal electron emission from its midgap ($\sim 2.0$ eV) is estimated to be several years at room temperature. It means that only a limited number of the interface states can be detected during the standard C-V measurements. Although several groups have proposed new methods to characterize electronic states in the MOS-HEMT structures, there have been few reports on MOS interface state densities of the GaN-based MOS-HEMTs and their relationship to the resulting electrical properties has not been discussed in detail.

In this paper, we have attempted to determine interface state density distributions of Al$_2$O$_3$/AlGaN/GaN MOS-HEMTs using two types of C-V analysis, the photo-assisted measurement for the...
measurement and the frequency dispersion characterization. We then discuss the relationship between the interface states and resulting electrical properties including threshold voltage instability of the MOS-HEMTs.

II. FABRICATION PROCESS

Figure 1 schematically shows the structure of the fabricated Al2O3/AlGaN/GaN MOS-HEMT. We used an Al0.23Ga0.77N/GaN heterostructure grown on a sapphire substrate by metal organic chemical vapor deposition. Sheet resistance and electron mobility of the heterostructure were estimated to be 440 Ω/sq and 1770 cm²/Vs, respectively. In this study, we employed the “ohmic-first” process to prevent damage to the Al2O3 film during ohmic annealing.11 After the pretreatment of the sample surface in a 30%-HF solution for 5 min, we deposited a 10 nm SiN as a surface protection layer by electron cyclotron resonance chemical vapor deposition. Ti/Al/Ti/Au (20/50 nm) source and drain electrodes were then deposited on the AlGaN surface, followed by ohmic annealing at 800 °C for 1 min in N2 ambient. Device isolation was performed in a reactive ion beam etching chamber using CH4-based plasma. After removing the SiN layer with a buffered HF, we applied an N2O-radical treatment prepared on the same chip as the pretreatment of the MOS-HEMTs. We then discuss the relationship between the interface states and resulting electrical properties including threshold voltage instability of the MOS-HEMTs.

III. EXPERIMENT

A. Typical C-V characteristics of Al2O3/AlGaN/GaN diode structures

Figure 2 shows the C-V characteristics of the Al2O3/AlGaN/GaN diode structures without and with the N2O-radical treatment. As indicated by the solid line in Fig. 3(a), the ideal C-V curve shows a two-step capacitance change which is also observed in the experimental data. C2DEG is also in agreement with those in Fig. 2. The two broken lines show an example of the C-V calculation assuming the two typical interface state density D1 and D2 distributions, shown in Fig. 3(b). In the plots, C2DEG, the charge neutrality level Ecnl is a branch point for acceptor- and donor-like interface states having a U-shaped distribution.
C. Frequency dispersion $C$-$V$ characteristics

Figure 4 compares the frequency dispersion of the $C$-$V$ characteristics of the MOS-HEMTs without and with the N$_2$O-radical treatment. The measurement frequencies were 1 kHz, 10 kHz, 100 kHz, and 1 MHz. In the positive bias range, we clearly observed frequency dispersion for the both samples probably caused by electron capture and emission at the Al$_2$O$_3$/AlGaN interface states. For the N$_2$O-radical treated sample, in particular, the smaller dispersion between those frequencies indicates the reduction of interface states. The relationship between the time constant $\tau_1$ and the frequency $f_1$ is given by Eq. (2)

$$\tau_1 = \frac{1}{2\pi f_1},$$

and the trap energy depth $E_1$ corresponding to $f_1$ is expressed by the SRH statistics as follows:

$$E_1 = kT \ln \left( \frac{\sigma N_C v}{2\pi f_1} \right).$$
As schematically shown in Fig. 5, the interface states distributed within the bandgap can be divided into two parts by $E_1$. In the upper energy range which has faster time constants than the measurement frequency ($\tau < 1/2\pi f_1$), electron capture and emission at the interface states can respond to the ac gate signal. In this case, the interface trap capacitance $C_{it}$ and resistance $R_{it}$ associated with electron capture and emission at the interface states are connected parallel to the depletion capacitance (the AlGaN capacitance $C_{AlGaN}$ in this case). Consequently, that leads to the overestimation of the measurement capacitance at the smaller gate bias, causing a leftward on-set voltage shift for the lower frequencies in the positive bias region. Note that such overestimation of the capacitance increasing with $D_{it}$ is not observed in the $C$-$V$ calculation shown in Fig. 3(a) because the present calculation does not take into account the frequency response of the interface states. To estimate $D_{it}$ from the experimental data, we then focused on the on-set voltage shifts in the frequency dependent $C$-$V$ curves.

Fig. 6(a) compares the $C$-$V$ characteristics of the sample without the treatment measured at 100 kHz and 1 MHz in the positive bias range. The on-set voltage difference $\Delta V$ between two frequencies ($f_1, f_2$) corresponds to the interface charge density $\Delta Q_{it}$ in the energy range of $E_1$ to $E_2$ as schematically shown in Fig. 6(b). $E_1$ and $E_2$ were estimated to be 0.17 and 0.23 eV, respectively, using Eq. (3), where $f_1, f_2, \sigma$ are 1 MHz, 100 kHz and $1 \times 10^{-16}$ cm$^2$, respectively. In this energy range, $D_{it}$ can be estimated from the following equation:

$$D_{it}(E = E_{AVG}) = \frac{C_{AlGaN} [V_2 - V_1]}{q} \frac{E_2 - E_1}{\Delta E} = \frac{C_{AlGaN}}{q} \Delta V,$$

where $V_1$ and $V_2$ are the on-set voltages for $f_1$ and $f_2$, respectively.$^{21}$ $E_{AVG}$ is the average energy between $E_1$ and $E_2$, as described by Eq. (5)

$$E_{AVG} = E_1 + \frac{E_2 - E_1}{2} = E_1 + \Delta E/2.$$

In this energy range, the interface states do not respond to the ac signal. Using a lower frequency $f_2$, the trap energy depth $E_2$ at which $C_{it}$ starts to be detected becomes deeper. This leads to the overestimation of the capacitance at the smaller gate bias, causing a leftward on-set voltage shift for the lower frequencies in the positive bias region. Note that such overestimation of the capacitance increasing with $D_{it}$ is not observed in the $C$-$V$ calculation shown in Fig. 3(a) because the present calculation does not take into account the frequency response of the interface states. To estimate $D_{it}$ from the experimental data, we then focused on the on-set voltage shifts in the frequency dependent $C$-$V$ curves.

FIG. 4. Frequency dispersion of the $C$-$V$ characteristics of the Al$_2$O$_3$/AlGaN/GaN MOS diode structures without and with the N$_2$O-radical treatment in the positive bias range.

FIG. 5. Equivalent circuit of the interface states in Al$_2$O$_3$/AlGaN/GaN structures during the $C$-$V$ measurement.

FIG. 6. (a) $C$-$V$ curves of the sample without the surface treatment measured at frequencies of 100 kHz and 1 MHz. (b) Schematic illustration of $D_{it}$ energy ranges corresponding to measurement frequencies.
Although we have to assume a value of $\sigma$ in $E_i$ (as suggested in Eq. (3)) to determine the energy position of $D_{it}$, the energy difference $\Delta E$, which is also used in Eq. (4), is independent of $\sigma$ but dependent on $T, f_1$, and $f_2$, as described by Eq. (6)

$$\Delta E = E_2 - E_1 = kT \ln \left( \frac{\sigma N_{CV}}{2\pi f_2} \right) - kT \ln \left( \frac{\sigma N_{CV}}{2\pi f_1} \right) = kT \ln(f_1/f_2).$$

Therefore, $D_{it}$ can be evaluated using Eq. (4) without assuming a value of $\sigma$. Supposing that $\sigma$ is constant for both samples without and with the N$_2$O-radical treatment, we can compare the $D_{it}$ distributions of both samples in the same energy range.

**IV. RESULTS AND DISCUSSION**

**A. Estimate of $D_{it}$ in Al$_2$O$_3$/AlGaN/GaN MOS-HEMTs**

Figure 7 shows the results of the $D_{it}$ distributions at the Al$_2$O$_3$/AlGaN interface in the MOS-HEMT structures estimated using the combination of the frequency dispersion $C-V$ method and the photo-assisted $C-V$ measurement. In the frequency dispersion method, we assumed $\sigma$ to be $1 \times 10^{-16}$ cm$^2$, giving values of $D_{it}$ in the energy range of $-0.2$ to $-0.32$ eV from $E_C$. For the sample without the treatment, $D_{it}$ near the conduction-band edge was estimated to be $2-3 \times 10^{13}$ cm$^{-2}$ eV$^{-1}$, which is about one order higher than those reported for the Al$_2$O$_3$/n-GaN system. As Ooyama et al. reported in Ref. 23, the defect level densities of AlGaN were about 10 times as high as those of GaN, probably due to high densities of defects related to nitrogen vacancy, oxygen impurity, and their complexes. It is likely that they also led to the higher densities of interface states in Al$_2$O$_3$/AlGaN compared with those in the Al$_2$O$_3$/n-GaN system. We also carried out the photo-assisted $C-V$ measurement using monochromatic lights with photon energies of 1.4–2.2 eV. For the sample without the surface treatment, the minimum state densities around the midgap were estimated to be around $2 \times 10^{12}$ cm$^{-2}$ eV$^{-1}$, which is in good agreement with the data reported for the Al$_2$O$_3$/AlGaN structures.

As already reported in Ref. 18, in comparison, the N$_2$O-radical treated sample showed a lower $D_{it}$ distribution around the midgap with a minimum density of less than $1 \times 10^{12}$ cm$^{-2}$ eV$^{-1}$. Moreover, the state densities near the conduction-band edge were estimated to be $8 \times 10^{12}$ cm$^{-2}$ eV$^{-1}$ for the N$_2$O-radical treated Al$_2$O$_3$/AlGaN interface. Supposing that the $D_{it}$ distributions of both samples are U-shaped as indicated by the broken lines in Fig. 7, the entire acceptor-like state density distribution of the N$_2$O-radical treated MOS-HEMT is expected to be reduced by approximately 40% compared with that of the sample without the treatment. Assuming those entire $D_{it}$ distributions to the numerical solver, the calculated $C-V$ curves reasonably reproduced the experimental data for the two samples at 1 MHz (not shown here). For further consideration of the $D_{it}$ estimation, not only the methods presented here but also other approaches to $C-V$ analyses are necessary. However, the present N$_2$O-radical treatment appears also to be effective in improving the electrical properties of the AlGaN/GaN MOS-HEMTs.

**B. Chemical properties of N$_2$O-radical treated AlGaN surface**

To investigate the chemical bonding properties of the N$_2$O-radical treated AlGaN surface, we carried out X-ray photoelectron spectroscopy (XPS) analysis using a monochromatic Al K$_\alpha$ radiation source ($h\nu = 1486.6$ eV). Figure 8 compares the O 1$s$ and N 1$s$ core-level spectra of the AlGaN surfaces before and after the N$_2$O-radical treatment taken with a photoelectron escape angle of 15$^\circ$. Note that each spectrum was normalized to the Ga 3$d$ peak. As indicated by

![FIG. 7. Al$_2$O$_3$/AlGaN interface state density distributions in the Al$_2$O$_3$/AlGaN/GaN structures without and with the N$_2$O-radical treatment.](image1)

![FIG. 8. (a) O 1$s$ and (b) N 1$s$ core-level spectra obtained from the AlGaN surfaces before and after the N$_2$O-radical treatment.](image2)
the broken line in Fig. 8(a), the increase of the AlGaOx peak was observed for the N2O-radical treated AlGaN surface, probably arising from the oxidation of the AlGaN due to the treatment. We also confirmed chemical shifts in the Ga 3d and Al 2p core-level spectra (not shown here). In the N 1s spectra shown in Fig. 8(b), however, the AlGaN peak at 397.0 eV is decreased for the N2O-radical treated sample but still remains and overlaps with the broadened Ga LMM Auger spectra. The broader linewidth and the chemical shift of Ga Auger signal were also observed in the GaOx layer prepared by photoelectrochemical oxidation of GaN. That is, the XPS spectra obtained from the N2O-radical treated surface contain those of the AlGaN and AlGa-oxide layers, suggesting the oxidation layer was very thin (1 nm or less). Bae et al. reported that an ultra thin Ga-oxide layer prepared by the remote plasma-assisted oxidation process is effective in reducing interface states for the SiO2/n-GaN system. Tajima et al. compared the oxidation processes for access regions in AlGaN/GaN HEMTs using O2- and N2O-plasma treatments. In their report, N2O plasma promoted the oxidation of the AlGaN surface with an N-O bonding network, which probably suppressed the defect formation in the AlGaN layer during the oxidation process. As shown in Fig. 8(b), we also confirmed the small presence of the N-O bonding peak at around 402.5 eV for the N2O-radical treated AlGaN surface. Although the mechanism is not clear yet, it is likely that the monolayer-level formation of the AlGa-oxide layer prepared by the N2O-radical treatment is effective in reducing electronic states at the Al2O3/AlGaN interface.

C. Electrical properties of Al2O3/AlGaN/GaN MOS-HEMTs

Figure 9 shows the drain current-voltage ($I_{DS}-V_{DS}$) characteristics of the Al2O3/AlGaN/GaN MOS-HEMTs without and with the N2O-radical treatment. We used Agilent B1500A Semiconductor Device Analyzer with B1525A High Voltage Semiconductor Pulse Generator Unit for pulsed current-voltage measurements. Pulse width and period were 5 $\mu$s and 0.5 s, respectively. The drain-source and gate-source base-voltages were set to 0 V, “no-stress” condition. At the gate-source voltage $V_{GS} = 0$ V, both samples show almost the same current density, indicating no pronounced degradation of the 2DEG channel due to the N2O-radical treatment. At $V_{GS} = +4$ V, in contrast, the N2O-radical treated MOS-HEMT shows higher current density than the MOS-HEMT without the treatment. This tendency was also confirmed in the transfer characteristics in the saturation region, as indicated by the solid lines in Fig. 10. For the MOS-HEMT without the treatment, a marked decrease of transconductance was observed at high gate bias range. When the gate bias is positive, electron transfer from the AlGaN/GaN interface to the Al2O3/AlGaN interface occurs, which can be confirmed in the C-V results in Fig. 2, resulting in the parasitic channel formation at the Al2O3/AlGaN interface. In this case, the relatively high-density interface states caused the degradation of electron mobility, leading to the decrease of transconductance. In comparison, the improvement of transfer characteristics of the N2O-radical treated MOS-HEMT in the positive gate bias region is due to the reduction of interface states, also as confirmed in Fig. 7.

To investigate the operational stability of the MOS-HEMTs, we also performed negative-gate-bias-induced $V_{th}$ instability measurements. In Fig. 10, the broken lines (“gate-stress”) show transfer characteristics pulsed from...
negative-gate-bias stress condition, \( V_{GS} = -8 \, \text{V} \) and \( V_{DS} = 0 \, \text{V} \). For the sample without the treatment, we observed a threshold voltage shift \( \Delta V_{th} \) of 0.7 V toward the negative bias direction, which is probably due to the negative-gate-bias-induced electron emission from the Al\(_2\)O\(_3\)/AlGaN interface. Figure 11 shows the potential profile of the Al\(_2\)O\(_3\)/AlGaN/GaN structure calculated by using the numerical Poisson solver. At \( V_{GS} = -8 \, \text{V} \), \( E_F \) is located far below the valence-band edge at the Al\(_2\)O\(_3\)/AlGaN interface. In this case, electron at the shallow states which have shorter time constants can be emitted, resulting in the \( V_{th} \) shift toward the negative bias direction. Using Eq. (1) and the pulse period of 0.5 s, \( E_{Tm} \) for the pulsed measurement can be estimated to be 0.6 eV. When we integrated the expected \( D_h \) distribution determined in Fig. 7 from \( E_C \) to \( E_{Tm} \), the resulting charge density is in good agreement with the charge difference \( \Delta Q_{Al2O3} = C_{Al2O3} \Delta V_{th}/q \), \( 3.2 \times 10^{12} \, \text{cm}^{-2} \), corresponding to 0.7 V-shift. In contrast, the suppressed \( V_{th} \) shift for the N\(_2\)O-radical treated MOS-HEMT is clearly due to the reduction of the interface states. For this sample, \( \Delta Q_{th} \) was estimated to be \( 1.4 \times 10^{12} \, \text{cm}^{-2} \) with \( \Delta V_{th} \) of 0.3 V, which is approximately 40%-less compared with that of the MOS-HEMT without the treatment.

Figure 12 shows the results on the negative-gate-bias-induced \( V_{th} \) shifts of the MOS-HEMTs measured at room temperature (RT), 100 \(^\circ\)C, and 150 \(^\circ\)C. For both samples, the amount of \( V_{th} \) shifts increased with increasing temperature. Because \( E_{Tm} \) is proportional to the temperature as described in Eq. (1), the larger amount of electron emission caused larger \( V_{th} \) shifts toward the negative bias direction. For the N\(_2\)O-radical treated MOS-HEMT, however, we observed the smaller \( V_{th} \) shift of less than 0.5 V even at 150 \(^\circ\)C. The N\(_2\)O-radical treated MOS-HEMT shows more stable \( V_{th} \) under negative-gate bias stress at high temperatures due to the reduction of interface states. The results presented in this paper are the first report on the relationship between electrical properties of GaN-based MOS-HEMTs and experimental \( D_h \) distributions evaluated for the same structures. The N\(_2\)O-radical treatment is one of the effective processes for reducing the Al\(_2\)O\(_3\)/AlGaN interface states and improving the electrical properties of the GaN-based MOS-HEMTs.

V. CONCLUSION

We have estimated the Al\(_2\)O\(_3\)/AlGaN interface state density distributions in the Al\(_2\)O\(_3\)/AlGaN/GaN MOS-HEMTs using the combination of the frequency dependent and photo-assisted \( C-V \) methods. The N\(_2\)O-radical treated MOS-HEMT showed smaller frequency dispersion of the \( C-V \) curves than that of the sample without the treatment, indicating the reduction of the interface states. The state densities were estimated to be \( 1 \times 10^{12} \, \text{cm}^{-2} \, \text{eV}^{-1} \) or less around the midgap and \( 8 \times 10^{12} \, \text{cm}^{-2} \, \text{eV}^{-1} \) near the conduction-band edge, which is approximately 40% less than those in the MOS-HEMT without treatment. We then investigated the impact of the reduced interface state densities on the electrical properties of the MOS-HEMTs. In the transfer curves, the decrease of transconductance was observed at high gate bias range where the parasitic channel is formed at the Al\(_2\)O\(_3\)/AlGaN interface. In this case, the N\(_2\)O-radical treated MOS-HEMT having the reduced interface states showed higher current density than that of the sample without treatment. We also have performed the negative-gate-bias-induced \( V_{th} \) instability measurements at RT to 150 \(^\circ\)C. For the N\(_2\)O-radical treated MOS-HEMT, the reduced interface states led to more stable \( V_{th} \) even at high temperatures. The results indicated that the N\(_2\)O-radical treatment is effective both in reducing the Al\(_2\)O\(_3\)/AlGaN interface states and improving the electrical properties of the MOS-HEMTs. Control of the MOS interface states is one of the key technologies for improving operational performance and stability of the GaN-based devices.

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