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Exponential dependence of capture cross section on activation energy for interface traps in Al$_2$O$_3$/AlN/AlGaN/GaN metal-insulator-semiconductor heterostructures

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This paper presents a systematic study on the interface traps in AlGaN/GaN metal-insulator-semiconductor (MIS) heterostructures with an atomic layer deposited Al$_2$O$_3$/AlN gate stack. The interface trap density in MIS heterostructures with and without recess gate is estimated to be $2.76 \times 10^{13}$ eV$^{-1}$ cm$^{-2}$ and $2.38 \times 10^{13}$ eV$^{-1}$ cm$^{-2}$, respectively, by using the conductance method. The capture cross section, extracted from Arrhenius fitting, shows an exponential increase from $1.73 \times 10^{-18}$ cm$^2$ to $1.07 \times 10^{-16}$ cm$^2$ with an increase in trap activation energy from 0.21 eV to 0.47 eV for MIS heterostructures with recess gate, while the exponentially related capture cross section and activation energy for the case without recess gate are $1.19 \times 10^{-18}$–$2.36 \times 10^{-12}$ cm$^2$ and 0.15–0.82 eV, respectively. The voltage-dependent measurement enables different interface traps detectable which are continuously distributed within the bandgap, and the exponential dependence of the capture cross section on activation energy is attributed to the entropy change accompanying electron emission from interface traps to the conduction band. The comparison between devices with and without recess gate shows that recess etching leads to a decrease in the linear dependence factor of activation energy on gate voltage from 0.61 to 0.52 and also slightly reduces the influence of atomic vibration on electron emission. Published by AIP Publishing.

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GaN-based metal-insulator-semiconductor high-electron-mobility transistors (MIS-HEMTs) have attracted increasing interest in power and RF applications due to the suppressed leakage current and enlarged gate swing compared with the conventional Schottky-gate HEMTs. Gate dielectrics are of vital importance to MIS-HEMTs, and various insulators have been studied, such as SiO$_2$ grown by plasma enhanced chemical vapor deposition (PECVD),$^1$ SiN grown by plasma enhanced atomic layer deposition (PEALD) or low-pressure chemical vapor deposition (LPCVD),$^{2,4}$ Al$_2$O$_3$ and HfO$_2$ grown by atomic layer deposition (ALD),$^{5,8}$ and AlN grown by PEALD.$^{9,10}$ Oxide gate dielectrics exhibit excellent electrical insulation properties but simultaneously bring in high-density interface trap states ($>10^{13}$ cm$^{-2}$ eV$^{-1}$)$^{7,8}$ which are induced by the native interfacial oxide layer, structural damage, or dangling bonds. The charging/discharging effect of interface traps will cause device degradation and reliability problems, such as threshold voltage ($V_{th}$) instability.$^{11,12}$ The use of nitride gate dielectrics will improve interface quality due to the absence of oxygen atoms, but SiN may cause interdiffusion and interaction of Si and Al,$^5$ and PEALD-grown AlN suffers from the electrical insulation property.$^{10}$

Accurate characterization of interface traps is of great importance to the development of high-quality gate dielectrics. Several approaches such as deep level transient spectroscopy,$^{8,13}$ pulsed current-voltage (PIV),$^{14}$ frequency-dependent capacitance method,$^{15}$ and conductance method$^{7,16}$ have been developed to study the interface traps in GaN-based MIS heterostructures (MIS-HEMTs). The emission time constant (or activation energy) and mapping of trap density for MIS heterostructures with different gate dielectrics were investigated in the previous reports, while the capture cross section of interface traps, another critical variable, was rarely involved.

In this paper, the capture cross section and the activation energy and density map of interface traps in AlGaN/GaN MIS heterostructures were studied by using the temperature- and voltage-dependent conductance method. The Al$_2$O$_3$/AlN stack was adopted as the gate dielectric, where the upper Al$_2$O$_3$ was used as an electrical-insulation layer and the AlN interfacial layer contributed to improving the interface quality.$^{17}$ Recess etching was commonly used in MIS-HEMTs to enhance the gate controllability or realize normally OFF operation, so this work was focused on the MIS heterostructures with recess gate, and the impact on interface traps was also discussed. Interface traps with activation energies of 0.21–0.47 eV and 0.15–0.82 eV were detected for devices with and without recess gate, respectively, and the exponential dependence of the capture cross section on activation energy was observed, which was attributed to the entropy change accompanying electron emission from interface traps to the conduction band.

AlGaN/GaN epitaxial layers used in this paper were grown on SiC substrates by metal-organic chemical vapor deposition, consisting of a 180 nm AlN nuclear layer, 3 μm un-doped GaN buffer layer, 1 nm AlN interlayer, 20 nm
Al$_{0.8}$Ga$_{0.2}$N barrier layer, and 2 nm GaN cap layer from down to top, as shown in Fig. 1. The device process started with Ti/Al/Ni/Au ohmic contacts by electron beam evaporation and rapid thermal annealing at 840 °C in N$_2$ for 30 s. For recess-gate devices, the GaN/AlGaN layers underneath gate areas were partially removed by Cl$_2$-based etching, following 60 nm PECVD-grown SiN passivation and gate definition. The 1 nm AlN interfacial layer and 4 nm Al$_2$O$_3$ insulator layer were grown by PEALD and thermal ALD at 300 °C sequentially. Then, Ni/Au/Ni gate electrodes were fabricated by e-beam evaporation, and post-metallization annealing at 450 °C was carried out to improve the interface quality. Flat field-effect transistor (Fat-FET) structures as shown in Figs. 1(a) and 1(b) were used for the capacitance-voltage (C-V) measurement and trap analysis, with a gate length of 50 μm and a gate width of 100 μm.

Figure 1(c) shows the C-V curves of MIS heterostructures measured at 100 kHz. Recess etching results in a positive voltage shift of 2.4 V and an increase in accumulation-region gate capacitance from 287 to 528 nF/cm$^2$. Note that there exist two sharp rising slopes in C-V curves, where the first one at negative voltage corresponds to the accumulation of electrons at the AlGaN/GaN interface, and the second one at positive voltage corresponds to the response of the insulator/III-nitride interface. In the accumulation region, the gate capacitance of MIS heterostructures can be equivalent to a parallel plate capacitor, whose two plates are the gate electrode and 2D electron gas (2DEG) channel, respectively. Therefore, the distance of the gate electrode from 2DEG for heterostructures with and without recess gate is estimated to be 14.5 nm and 27.1 nm, respectively, indicating a recess-depth of 12.6 nm.

The temperature- and frequency-dependent C-V measurement was carried out to qualitatively evaluate the interface quality between the insulator and nitride layers. Figure 2 shows the C-V results of recess-gate MIS heterostructures. The increase in temperature from 298 K to 473 K causes a positive shift of $V_{th}$ by about 0.5 V, which is attributed to the depletion and redistribution of channel electrons. The $V_{th}$ frequency dispersion at 473 K is within 0.3 V, indicating the well interface quality due to the use of the Al$_2$O$_3$/AlN gate stack. In addition, there exists a sharp drop in C-V curves at 473 K with the gate voltage above 1.5 V. This can be explained by the increased forward thermal electron emission at high temperature.

The quantitative characterization of interface traps was accomplished by using the conductance method. When an ac gate signal is within the second C-V slope region, the charging/discharging process of interface traps can be represented by parallel conductance ($G_p$) in the equivalent circuit model. Interface traps between the insulator and semiconductors are continuously distributed across the bandgap, and the normalized conductance ($G_p/\omega$) is expressed as

$$\frac{G_p}{\omega} = \frac{qD_T}{2\pi\tau_e} \ln \left[ 1 + (\omega\tau_e)^2 \right],$$

where $\omega = 2nf$ is the radial frequency, $q$ is the magnitude of electronic charge, $D_T$ is the interface trap density, and $\tau_e$ is the emission time constant. Figure 3 shows $G_p/\omega$ as a function of radial frequency and the fitting curves using Eq. (1) for recess-gate Al$_2$O$_3$/AlN/AlGaN/GaN MIS heterostructures. With gate biased at a certain voltage, the measurement temperature was increased from 298 K to 473 K with a step of 25 K to derive the activation energy and capture cross section of interface traps. In Fig. 3(a), the temperature-dependent curves with a step of 50 K instead of 25 K were plotted for a more succinct demonstration. Then, the interface traps with different activation energies were studied by varying the gate voltage from 2 V to 2.5 V, as shown in Fig. 3(b).

The interface trap density and emission time constant, as mapped in Fig. 4, were obtained by numerical fitting of the experimental data using Eq. (1). The trap density for MIS heterostructures with and without recess gate is estimated to be $2.76 \times 10^{13}$ eV$^{-1}$ cm$^{-2}$ and $2.38 \times 10^{13}$ eV$^{-1}$ cm$^{-2}$, respectively. The density fluctuation resulting from error is within 3%, and the sharp drop at temperature above 448 K is the underestimation of trap density due to thermal electron emission leakage current. Ramanan et al. reported that the conductance method used in AlGaN/GaN HEMTs may lead to severe underestimation error of trap density due to the existence of the AlGaN barrier resistance, especially for the case with an AlN interlayer. The high-temperature capacitance method and pulsed current-voltage (PIV) method were immune to the barrier resistance, so comparison among these...
three methods was made to confirm the accuracy of the conductance method used in this work. The frequency-dependent capacitance method at 373 K showed an interface trap density in the range of $2.30 \times 10^{13} \text{eV}^{-1} \text{cm}^{-2}$ for MIS heterostructures without recess gate, and $1.55 - 3.50 \times 10^{13} \text{eV}^{-1} \text{cm}^{-2}$ was derived by the PIV method, both confirming the reasonable accuracy of the conductance method used in this work. The inconsistence of our results with those in Ref. 14 is attributed to the sample difference in gate dielectric materials, which has been demonstrated in Ramanan’s previous work. According to the bonding constraint theory, high-k dielectrics are prone to creation of high-density dielectric/nitride interface traps due to a high average atomic coordination state and the resulting bond strain. In this work, the 1 nm AlN interfacial layer between the nitride epilayer and ALD-grown oxide effectively improves the interface quality, for which case the conductance method used in MOS-HEMTs exhibits reasonable accuracy. For high-k HfAlO and HfO2 gate dielectrics, however, the use of the conductance method causes large underestimation error of interface trap density for the case with high trap density.  

With an increase in temperature and gate voltage, the derived emission time constant for recess-gate MIS heterostructures decreases exponentially-like from 7.1 ms to 0.45 $\mu$s, as shown in Fig. 4(b), and that for the case without recess gate is from 0.24 ms to 0.32 $\mu$s. The exponential-like dependence of emission time constant on temperature and gate voltage can be explained by Shockley-Read-Hall statistics, allowing the emission time constant to be written as the Arrhenius equation

$$\tau_e = \frac{1}{\gamma_n \sigma_n} \exp \left( \frac{\Delta E_A}{kT} \right),$$

where $\sigma_n$ is the capture cross section, $N_C$ represents the effective density of states in the AlGaN conduction band, $v_{th}$ is the electron thermal velocity, $\Delta E_A$ is the trap activation energy, $k$ is Boltzmann’s constant, and $T$ represents the temperature. With devices biased at different gate voltages, the activation energy of detectable interface traps varies, so gate voltage and temperature lead to an exponential-like variation of emission time constant.

By taking the temperature dependence of $N_C$ and $v_{th}$ into consideration, the activation energy and capture cross section of interface traps can be derived from the $s_e^2/kT$ curves. The electron thermal velocity and effective density of states in the conduction band are

$$v_{th} = \sqrt{3kT/m_n}, \quad N_C = 2\left(2\pi m_n kT/h^2\right)^{3/2},$$

allowing the emission time constant to be written as the Arrhenius equation

$$\tau_e T^2 = \left(\gamma_n \sigma_n^{-1}\right) \exp \left(\Delta E_A / kT\right),$$

with $\gamma_n = \left(v_{th} T^{3/2}(N_C h^2)^2 \right) = 3.25 \times 10^{21} \text{cm}^{-2} \text{s}^{-1} \text{K}^{-1}$, where $m_n = 0.284 m_0$ is the effective mass of electrons in the AlGaN barrier, $h$ is Planck’s constant, and $m_0$ is the electron mass in free space. Figure 5(a) shows the $\tau_e T^2 \sim 1/kT$ curves of recess-gate MIS heterostructures, fitting well with the Arrhenius plots. With the gate voltage increasing from 2 V to 2.5 V, the shallower interface traps are detectable, as shown in Fig. 5(b), where $\Delta E_{A1}$ and $\Delta E_{A2}$ are the activation energies of interface traps with gate voltage at $V_1$ and $V_2$, respectively, $E_C$ is the conduction band of the GaN buffer layer.  

FIG. 3. (a) Temperature- and (b) voltage-dependent $G_p/\omega_0$ as a function of radial frequency for MIS heterostructures with recess gate. Geometries and solid lines represent the experimental data and fitting curves, respectively.

FIG. 4. (a) Interface trap density and (b) emission time constant as a function of temperature and voltage for recess-gate Al2O3/AlN/AlGaN/GaN MIS heterostructures.
and $E_F$ represents the Fermi energy level. According to the exponential-like dependence of emission time constant on gate voltage, we conclude that the activation energy is linearly dependent on gate voltage, as expressed by the empirical formula in Fig. 5(b), where $\Delta E_{F0}$ is the relative Fermi energy below the conduction band at the equilibrium state (biased at 0 V) and $\alpha$ is the linear factor related to the partial voltage across the AlGaN barrier layer.

Figure 6 shows the activation energy and capture cross section of interface traps at different gate voltages. The trap activation energy as a function of gate voltage fits well with the empirical formula for both devices with and without recess gate. The use of recess gate leads to a decrease in $\Delta E_{F0}$ from 1.97 eV to 1.49 eV, i.e., raises the equilibrium-state Fermi energy level at the interface by 0.48 eV. The linear factor is also decreased from 0.61 to 0.52 by recess etching due to the reduced partial voltage across the AlGaN barrier layer. Similar to the reports in Ref. 22, the capture cross section of interface traps in Al$_2$O$_3$/AlN/AlGaN/GaN MIS heterostructures is exponentially dependent on activation energy. For recess-gate devices, the capture cross section increases from $1.73 \times 10^{-18} \text{ cm}^2$ to $1.07 \times 10^{-16} \text{ cm}^2$ with the activation energy varying from 0.21 eV to 0.47 eV. For devices without recess gate, the capture cross section and activation energy of detectable interface traps are $1.19 \times 10^{-18}–2.36 \times 10^{-12} \text{ cm}^2$ and 0.15–0.82 eV, respectively. The $\Delta E_A$-dependent capture cross section is attributed to the entropy change accompanying electron emission from interface traps to the conduction band, which can be expressed as:

$$\sigma_n = \sigma_0 X_n = \sigma_0 g_n \exp (\Delta S_{na}/k),$$

(5)

where $\sigma_0$ is the “true capture cross section” independent of the entropy change and activation energy, $X_n$ is an “entropy factor,” $g_n$ represents the change due to electronic degeneracy, and $\Delta S_{na}$ represents the atomic vibrational changes. The degeneracy and entropy factors are not well known for deep level traps, making it difficult to quantitatively study on the exponential dependence of the capture cross section, but it is obvious that the atomic vibration varying with the trap energy level makes contribution to the exponential dependence, and recess etching slightly reduces the influence of atomic vibration.

In conclusion, the interface traps in Al$_2$O$_3$/AlN/AlGaN/GaN MIS heterostructures were systematically studied in this paper by using the temperature- and voltage-dependent conductance method. The emission time constant of interface traps in MIS heterostructures with and without recess gate is estimated to be 0.45 μs–7.1 ms and 0.32 μs–0.24 ms, respectively, and the 12.6 nm recess etching results in a slight increase in trap density from $2.38 \times 10^{13} \text{ eV}^{-1} \text{ cm}^{-2}$ to $2.76 \times 10^{13} \text{ eV}^{-1} \text{ cm}^{-2}$. Numerical fitting using Arrhenius plots showed the capture cross section and the activation energy of interface traps. The interface traps with the activation energy ranging from 0.15 eV to 0.82 eV are detectable for MIS heterostructures without recess gate, where the activation energy is linearly dependent on gate voltage, with a linear factor of 0.61. For the case with recess gate, however, the linear factor is 0.52 with the activation energy ranging from 0.21 eV to 0.47 eV. An exponential increase in the capture cross section (from $1.73 \times 10^{-18} \text{ cm}^2$ to $1.07 \times 10^{-16} \text{ cm}^2$ for MIS heterostructures with recess gate and from $1.19 \times 10^{-18} \text{ cm}^2$ to $2.36 \times 10^{-12} \text{ cm}^2$ for that without recess gate) with an increase in activation energy is achieved, which is attributed to the entropy change accompanying electron emission from interface traps to the conduction band, and recess etching slightly reduces the influence of atomic vibration.

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