Role of Electrochemical Reactions in the Degradation Mechanisms of AlGaN/GaN HEMTs

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Abstract

The nature of structural degradation in AlGaN/GaN high electron mobility transistors (HEMTs) are investigated in this work. Moisture from the environment and/or adsorbed water on the III-N surface were found to play an important role in the formation of surface pits during OFF-state electrical stress. The mechanism of this water-related structural degradation is explained by an electrochemical cell formed at the gate edge where gate metal, the III-N surface and the passivation layer meet.

INTRODUCTION

The unique combination of the high critical electric field of wide band gap materials and the existence of a high mobility two-dimensional electron gas (2DEG) allows AlGaN/GaN transistors to be the most promising candidates for high power and high frequency applications [1]. The main structural degradation mechanisms studied to date for AlGaN/GaN HEMTs are related to the formation of physical defects (pits and cracks) during high drain OFF-state stress. It has been argued in the past that the field-induced inverse piezoelectric effect of AlGaN material may play a role in causing surface cracking and gate leakage (I_g) degradation above a critical voltage [2-3]. In addition, the pits could also be caused by electrochemical reactions at the surface due to the combination of high electric field and oxygen [4-6]. Despite these proposed degradation models, direct experimental evidence of the nature of the structural and electrical degradation in AlGaN/GaN HEMTs is still lacking.

The goal of this work is to fully understand the nature of the structural degradation in GaN HEMTs. The results described in this study have been reproduced in more than 75 devices across 15 different wafers, both from industry and academia

DEVICE STRUCTURES

Prototype AlGaN/GaN HEMTs made by an industrial collaborator were used in this study. Similar results were achieved in transistors fabricated at MIT [5]. The HEMT structure consisted of a 3 nm GaN cap, 14 nm AlGaN barrier, 1 nm AlN interlayer and a thick GaN buffer layer epitaxially grown on a semi-insulating SiC substrate. A T-shape Pt/Au gate with a length L_g of 250 nm was deposited via metal evaporation. The device surface was passivated by a thick SiN_y layer deposited using plasma enhanced chemical vapor deposition (PECVD).

EXPERIMENTAL RESULTS

The impact of moisture on the structural degradation of AlGaN/GaN HEMTs was studied in an atmosphere-controlled probe station. Two chips from the same wafer with five identical AlGaN/GaN HEMTs on each chip were stressed at high drain OFF-state bias (V_{gs} = -7 V and V_{ds} = 43 V, which is much lower than the breakdown voltage) for 3000 s (at room temperature in darkness), one in ambient air and the other in a 1×10^{-7} Torr vacuum.

After the removal of the gate metal, the exposed surface in the gate area of these electrically-stressed HEMTs was investigated using scanning electron microscopy (SEM) and atomic force microscopy (AFM). Fig. 1 shows the top view and depth profile of the surface area around the gate of the HEMTs that were stressed in ambient air and in vacuum. It can be seen that the mean size and density of the surface pits were significantly higher in the HEMTs stressed in ambient air than those stressed in vacuum.

A different set of two HEMTs (one in each chip) was imaged using cross-sectional transmission electron microscopy (TEM) to study the pits without etching the

passivation and gate metals. A smaller pit size was again found in the devices stressed in vacuum when compared with those stressed in ambient air as shown in Fig. 2 (a) and (b), respectively. In addition, the material in the surface pits was characterized using energy dispersive X-ray analysis (EDX). A low concentration of gallium and aluminum and a high concentration of oxygen were observed inside the pit, as shown in Fig. 2 (c) and (d), indicating the important role of oxygen in the structural degradation of AlGaN/GaN HEMTs.

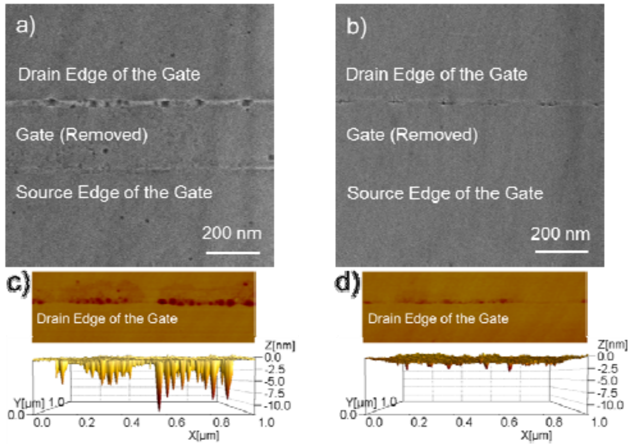


Fig. 1. SEM and AFM analysis of the AlGaN/GaN HEMTs stressed at V_{gs} = -7 V and V_{ds} = 43 V for 3000 s after gate metals were removed: SEM top view (a) and AFM depth profile (c) in ambient air; SEM top view (b) and AFM depth profile (d) in vacuum of 1×10^{-7} Torr.

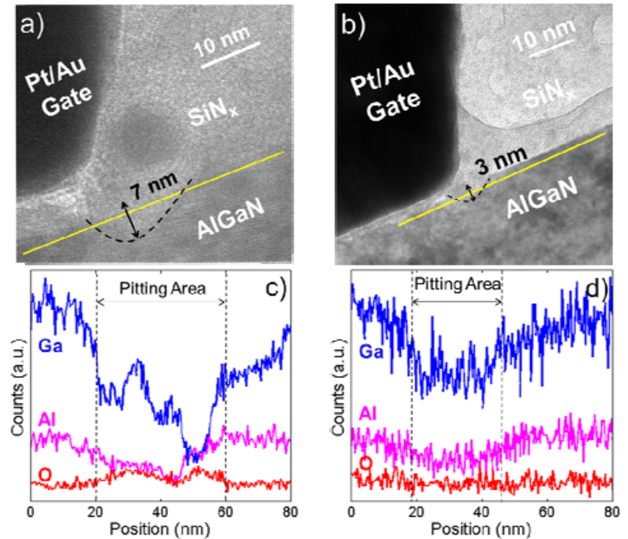


Fig. 2. Cross-sectional TEM images at the drain edge of the gate in the AlGaN/GaN HEMTs stressed at V_{gs} = -7 V and V_{ds} = 43 V for 3000 s in ambient air (a) and in a vacuum of 1×10^{-7} Torr (b); EDX line analysis across the pitting area for the above HEMTs stressed in ambient air (c) and in vacuum (d). The EDX line scan is indicated as the yellow line in (a) and (b).

Given that surface pitting is reduced when the devices are electrically stressed in vacuum conditions, the oxygen in the pits is most likely from the oxygen gas O_2 and/or moisture H_2O present in ambient air. In order to discriminate between these two options, another two chips of five identical AlGaN/GaN HEMTs were stressed in the chamber at the same OFF-state bias and duration in water-saturated Ar and in dry Ar. As shown in Fig 3, the surface pitting was significantly accelerated by water-saturated Ar with respect to dry Ar, which directly supports the water molecules as the cause of the surface pitting.

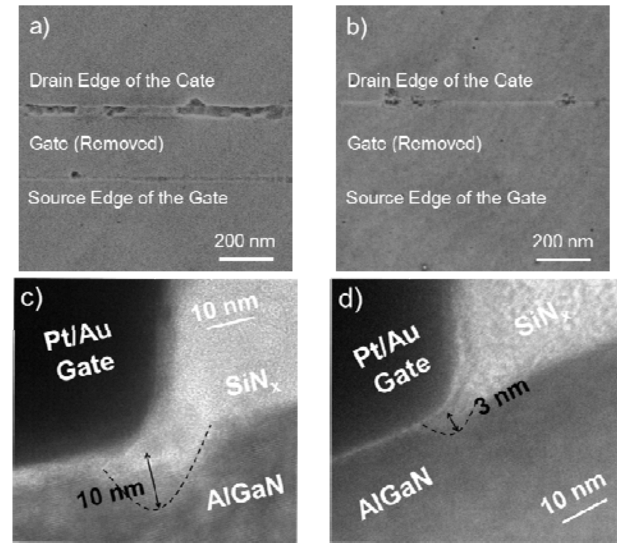


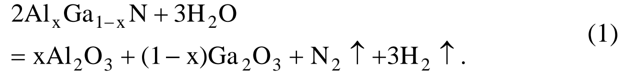
Fig. 3. SEM images of AlGaN/GaN HEMTs stressed at Vgs = -7 V and Vds = 43 V for 3000 s in water-saturated Ar (a) and in dry Ar (b), after gate metals and passivations were removed; Cross-sectional TEM images at the drain edge of the gate in AlGaN/GaN HEMTs stressed in water-saturated Ar (c) and in dry Ar (d) before etching.

The difference in the pit sizes between water-saturated and dry Ar was also reproducible in other gas environments including air, oxygen gas (O_2), nitrogen gas (N_2) and carbon dioxide gas (CO_2). The very small surface pitting observed in dry O_2 and dry CO_2 further confirms that the oxygen found in the surface pits comes mainly from water.

WATER-ASSISTED ELECTROCHEMICAL REACTIONS

We therefore propose that a water-assisted electrochemical reaction or corrosion process is a significant contributor of the surface pitting observed after OFF-state degradation in AlGaN/GaN HEMTs. The gate-SiN_y-$Al_xGa_{1-x}N$ region at the gate edge forms an electrochemical cell which causes anodic oxidation of the $Al_xGa_{1-x}N$ layer (Fig. 4). The reaction starts at the GaN cap surface and then proceeds into the AlGaN barrier during the electrical stress. For simplicity, we use $Al_xGa_{1-x}N$ to indicate both the GaN

cap (x=0) and the AlGaN barrier. The proposed reduction-oxidation (redox) reaction between $Al_xGa_{1-x}N$ and water is:

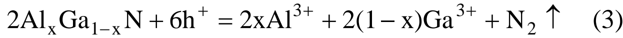


$$2Al_xGa_{1-x}N + 3H_2O = xAl_2O_3 + (1-x)Ga_2O_3 + N_2\uparrow + 3H_2\uparrow . \quad (1)$$

In the electrochemical cell, the gate metal acts as the cathode, which provides electrons to the water at the interface between SiN_y and $Al_xGa_{1-x}N$ when the gate-to-drain diode is reversed biased. The corresponding reduction reaction for the water is:

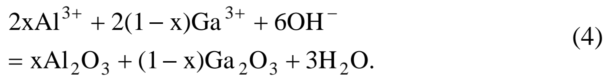
$$2H_2O + 2e^- = H_2 + 2OH^- . \quad (2)$$

The electrons contribute to the total gate current. On the other hand, the $Al_xGa_{1-x}N$ layer acts as the anode and is decomposed and subsequently anodically oxidized in the presence of holes and hydroxyl ions (OH^-) following:



$$2Al_xGa_{1-x}N + 6h^+ = 2xAl^{3+} + 2(1-x)Ga^{3+} + N_2\uparrow \quad (3)$$

And



$$2xAl^{3+} + 2(1-x)Ga^{3+} + 6OH^- = xAl_2O_3 + (1-x)Ga_2O_3 + 3H_2O. \quad (4)$$

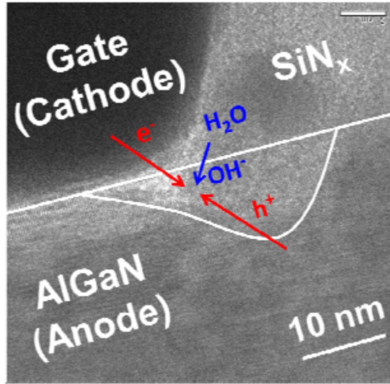


Fig. 4. An electrochemical cell formed at the drain edge of the gate in AlGaN/GaN HEMTs under high OFF-state drain bias.

The decomposition of the $Al_xGa_{1-x}N$ (the GaN cap and the AlGaN barrier) causes the surface pitting that was observed in the SEM, AFM and TEM analyses. The subsequent formation of the aluminum and gallium oxides explains the origin of the high concentration of oxygen in the pitting area.

In summary, for the proposed corrosion process to happen, it is necessary that:

1) Holes are available at the top III-N surface at the gate edge during the high OFF-state drain bias condition.
2) Water from the ambient diffuses/permeates through the bulk SiN_y passivation layer and reaches the III-N surface.

THE SOURCE OF HOLES

In principle, holes can be generated under high electric field by two mechanisms: i) impact ionization, and, ii) inter-band tunneling.

1) Impact ionization

Most of the impact ionization occurs in the region with the maximum electric field ($E_{\max}$), following the equation [7]:

$$j_{hole}^{ion} \approx \alpha \exp(-\frac{E_i}{E_{\max}}) j_g L_{eff} , \quad (5)$$

where α is a constant coefficient, E_i is a characteristic electric field for the impact ionization and L_{eff} is the effective length of the high field region.

2) Inter-band Tunneling

Under a high electric field, electrons from the valence band in the AlGaN barrier could also directly tunnel through the barrier into the conduction band. This process leaves holes in the valence band that can migrate to the surface.

This direct inter-band tunneling would generally obey the Keldysh equation [8-9]:

$$j_{tunnel} = CE^2 \exp(-\frac{E_t}{E}) , \quad (6)$$

where j_{tunnel} is the tunneling current density, C is a constant, E is the electric field, and E_t is a characteristic electric field for direct tunneling in AlGaN .

3) Surface Pitting and Holes

The hole current density in the OFF-state that would be required to explain the structural degradation of AlGaN/GaN HEMTs can be estimated from equation (3), where the decomposition of one mole of AlGaN corresponds to 3 moles of holes. Therefore, to be able to explain the structural defects observed in GaN HEMTs, the average hole current density over the electrical stressing duration should be:

$$\overline{j_h} \propto \frac{3V\rho N_A q}{MAt} = \frac{3\overline{d}\rho N_A q}{Mt} , \quad (7)$$

where V is the volume of the surface pits, ρ is the $Al_xGa_{1-x}N$ density, M is the $Al_xa_{1-x}N$ molar mass, A is the pitting area, t is the electrical stressing duration, N_A is Avogadro's constant and $\overline{d}$ is the average depth of the pits.

$\log(\overline{j_h}/E_{\max}^2)$ as a function of $1/E_{\max}$ using the simulated values of $E_{\max}$ is shown in Fig. 5. It can be seen that $\log(\overline{j_h}/E_{\max}^2)$ follows a linear trend with $1/E_{\max}$ in agreement with equation (6), supporting the hypothesis that hole-generation is caused by inter-band tunneling. At the same time, $\log(\overline{j_h}/\overline{j_g})$ as a function of $1/E_{\max}$ is also plotted in Fig. 5. As can be seen, the hole current needed to feed the growth of the pits is just a very small component of the total gate current. More importantly, $\log(\overline{j_h}/\overline{j_g})$ is an increasing function of $1/E_{\max}$, which opposes equation (5) and indicates that the holes that contribute to pitting are not the result of impact ionization.

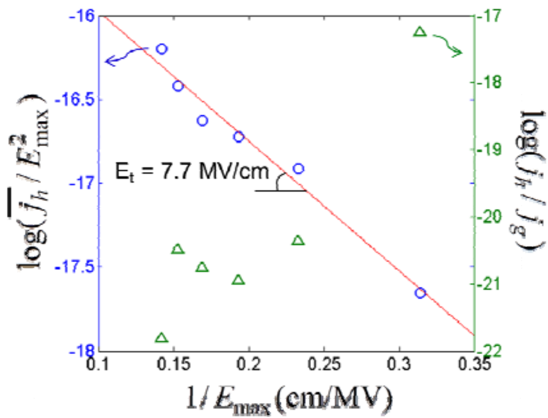


Fig. 5. $\log(\overline{j_h}/E_{\max}^2)$ (blue circles) and $\log(\overline{j_h}/\overline{j_g})$ (green triangles) as a function of $1/E_{\max}$. The number of holes extracted from the volume of the pits seems to follow the inter-band tunneling model – left y axis and not the impact ionization model – right y axis.

The Source of Water

In addition to holes, the proposed electrochemical reaction requires a source of water. In ambient air, there exists a thin layer of adsorbed water on the surface of most solids [10]. Moreover, ambient water can diffuse or permeate through bulk solids with a rate defined as the water vapor transmission rate (WVTR). For a thick (> 100 nm) PECVD SiN_y passivation layer, this rate is on the order of 0.01-0.1g/m^2/day [11-12]. In fact, the WVTR is an important limiting factor on the total electrochemical reaction described in equation (1) and can be estimated by the formation rate of the surface pits using the following formula:

$$WVTR \approx \frac{3}{2}\frac{V\rho M_{H_2O}}{MAt}, \tag{8}$$

where M_{H_2O} = 18 g /mol is the molar mass of water and the rest of the symbols are the same as in equation (7). A calculation based on equation (8) shows that the minimum WVTR needed to cause the observed density and size of the pits is around 0.05-0.1 g/m^2/day, which matches well the typical value of the WVTR for PECVD SiN_y [11-12].

Conclusions

In conclusion, a mechanism involving water-assisted electrochemical reactions at the gate edge has been proposed to explain OFF-state structural degradation (surface pitting) in AlGaN/GaN HEMTs. We show that water from the passivation layer surface and the external atmosphere, as well as holes caused by trap-assisted inter-band tunneling in the AlGaN barrier are likely to play an essential role in forming the surface pits.

Acknowledgements

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