Study of AlGaN/GaN HEMT Degradation through TCAD Simulations

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***Abstract*— This paper studies, through Three-Dimensional (3D) TCAD simulations, the formation of gate edge pits on the drain-side of GaN high electron mobility transistors (HEMTs) under electrical stress conditions. These pits are believed to be formed due to electrochemical reactions. The simulations predict that holes, which are necessary to initiate the electrochemical reaction but rare under regular HEMT operating conditions, can be generated through trap-assisted, band-to-band tunneling (B2B TAT). The impact of the electrical behavior of the pit (insulator or metal) on the output characteristics (I_D-V_D) of the HEMTs were also studied. Insulator-type pits degrade the ON-resistance, R_D, while metal-types do not. At medium V_D, both types of pit degrade I_D, which will be recovered at higher V_D. But metal-type requires larger V_D to restore the I_D. As the pits grow, the hole generation rate first increases (more with metal pit), then decrease after the pit-to-width ratio exceeds 20%.**

Keywords—AlGaN, GaN, HEMT, Degradation, Pits, 3D, TCAD Simulations

I. INTRODUCTION

AlGaN/GaN HEMTs are promising devices for high power and high frequency applications because they have wider band-gaps, larger breakdown fields, higher electron mobilities, and thus, better theoretical figures of merit than Silicon-based power devices. On the other hand, AlGaN/GaN HEMTs still suffer from poorly understood degradation issues and reliability,, including temporary degradation (e.g. current collapse) and permanent degradation (e.g. pits formation). Their potential thus cannot be fully unfurled until the degradation mechanisms are well understood and under controlled. Traps and pits are commonly believed to be the sources of degradation. They can be well controlled and manipulated in TCAD simulations. Therefore, TCAD simulation provides a versatile and cost-effective way to study the physics of reliability in HEMTs [1].

Gate edge pits due to electrochemical reaction with hydroxyl groups have been proposed as the cause of AlGaN/GaN HEMTs permanent degradation under off-state stress [2]. In that theory, water molecules in the moisture diffuse through the passivation nitride and are reduced to hydroxyl (OH^-) groups by electrons. Holes are then required to decompose AlGaN or GaN under the gate edge, with the decomposed III-N being subsequently oxidized by the hydroxyl group and turning into Al_2O_3 and/or Ga_2O_3 insulator pits.

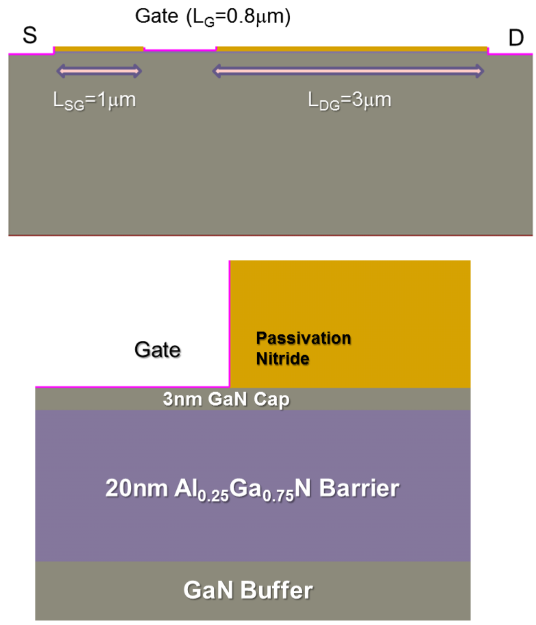

Fig. 1: 2D cross-section (at unpitted region) of the 3D structure used in simulations (Top: Full structure, Bottom: Gate edge on the drain-side).

Various aspects of gate edge pit formation due to the electrochemical reaction are studied and reported here using 3D TCAD simulations [3]. It is shown that trap-assisted, band-to-band tunneling (B2B TAT) in the AlGaN barrier can be responsible for hole generation near the gate, and that electrostatics due to insulator pits provides a possible explanation for the experimentally observed degradation of the ON-resistance, R_D. It is also found that hole generation rates during the pit growth depend strongly on the type of pit and, in general, decreases when the pits are large enough.

II. HOLE GENERATION IN HEMTS

Holes are rare at room temperature in regular AlGaN/GaN HEMTs without the presence of non-thermal electron-hole pair generation processes. Holes can be generated through impact ionization or direct band-to-band tunneling. However, very high electric fields are required to initiate the hole generation process in AlGaN/GaN due to their wide bandgaps. As suggested in [2], under regular biases, the most probable source of holes near the gate is B2B TAT. So, the presence of traps is required in order to initiate the hole generation process.

Traps in the AlGaN barrier have been studied extensively in the literature, with different trap energy levels and trap concentrations being reported [4]-[7]. According to [4], there may be a substantial density of traps with energy levels within 0.5eV from the conduction band (CB) edge of the AlGaN barrier. Reference [5] shows that, there are more than 10^{12} cm^{-2} donor traps in the barrier layer at 0.5±0.1eV below the CB. Reference [6] shows that the traps are 0.45eV below the CB, while reference [7] argues for a high trap density about 1eV above the valence band (VB) edge.

In our simulations, single energy level traps are placed at 0.45eV below the CB. Fig. 1 shows the structure simulated while Fig. 2 describes the parameters used for B2B TAT simulations and schematically illustrates the B2B TAT process. The drain voltage, V_D, and the gate voltage, V_G, were biased at 43V and -7V respectively. Fig. 3 shows that the vertical electric field peaks at the gate edge on the drain-side and holes are generated in excess of 2×10^{18} $cm^{-2}s^{-1}$. This agrees with experiments where most of the pits are observed at the gate edge on the drain-side [2] for a positive V_{DS} value.

According to the TEM pictures in [2], the pit size is in the order of 15nm and stress time is about 3000s. To check if the hole generation rate is enough to form the pits, we assume a continuous trench needs to be formed along the gate edge with depth and width both equal to 15nm. If the structure is stressed for 3000s, the number of holes required to convert GaN (following [2]'s approach) to pits per cm width of device is

$$3\ V \rho N_A / M$$

where V is the volume of the pit (15nm×15nm×1cm), ρ is GaN density (6.15g/cm^3), N_A is the Avogadro's Number (6.02×10^{23} mol^{-1}) and M is the molar mass of GaN (83.73g/mol). This equals to 3×10^{11} holes per cm width of device. For the simulation corresponding to Fig. 3, the device generated more than 10^{14} holes per cm width in 3000s, which is more than enough to form the continuous trench.

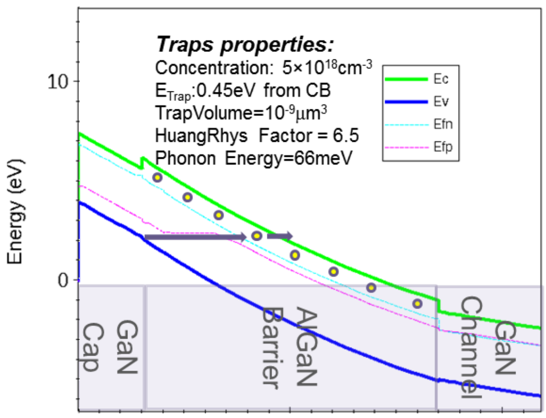

Fig. 2: Schematic diagram illustrating the BTB TAT process (vertical cut under the gate edge on the drain-side).

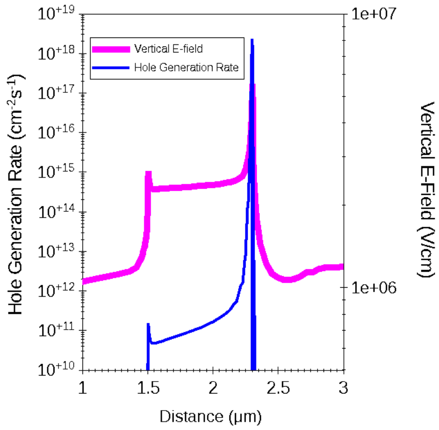

Fig. 3: Horizontal cut along cap/barrier interface showing vertical electric field, which peaks at the gate edge on the drain-side. Hole generation rate due to B2B TAT per unit area along the interface is also shown.

III. Effects of Pits

Pits have been observed after off-state stresses in various experiments [2][8]. Both, insulator [2] and metal pits [8] have been proposed. 3D simulations with pits filled with Al_2O_3 (insulator pit) or with a metal that produces a 0.55 eV Schottky barrier to GaN or 1.35 eV to $Al_{0.25}Ga_{0.75}N$ (metal pits) are conducted to understand their electrostatic effects on I_D-V_D curves. Pits are represented by hemispheres located under the gate edge on the drain-side, centered around where most holes are generated. Due to reflective boundary conditions, a unit cell domain as depicted in Fig. 4 can be chosen so that the pit diameter to simulated width ratio (pit-to-width ratio) determines the linear pit density. Different pit-to-width ratios (20%, 50%, and 80%) and pit radii (r = 10nm and 20nm) were simulated.

Fig. 5 shows the simulated I_D-V_D curves at V_G=0V for HEMTs with different pit sizes. The pinch-off voltage of the HEMTs without pits is about -5V. Simulations indicate that pitting has to be close enough to the barrier-channel interface in order to produce significant impact on I_D-V_D curves. Pits with r = 10 nm, i.e. with pit bottom 13nm away from the

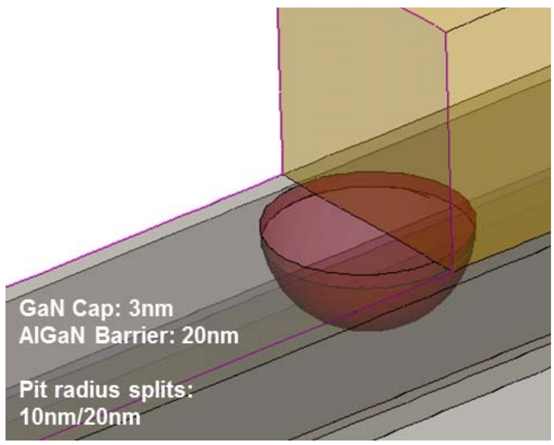

Fig. 4: Structure for simulating HEMT with pits (showing gate edge region on the drain-side). The hemisphere is the Al_2O_3 pit. For metal pit, the hemisphere is replaced by gate contact.

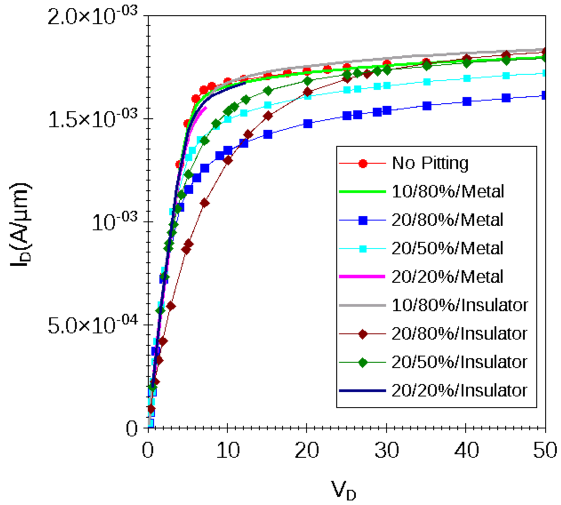

Fig. 5: I_D-V_D curves of HEMT with different pitting radii (in nm) and pit-to-width ratio. "Metal": Metal pits; "Insulator": Insulator pits

barrier-channel interface, have little effect on I_D-V_D's, while pits with r = 20 nm, i.e. with pit bottom 3 nm from the barrier-channel interface, significantly affect I_D-V_D's when the pit-to-width ratio is larger than 20%, for both metal and insulator pits.

There are two distinct simulated signatures in the I_D-V_D's from metal and insulator pits. The presence of insulator pits can result in significant R_D degradation. This can be explained by the additional large negative piezo-electric charge that forms between the insulator and the III-N underneath and depletes the two-dimensional electron gas (2DEG) under the gate edge (Fig. 6). Conversely, for metal pits, the Schottky barrier contact shifted closer to the channel is not electrostatically as effective in depleting the 2DEG (Fig. 7).

The second clear signature in simulation results is that the degraded ON-current at medium V_D recovers at a lower V_D values for insulator pits than for metal pits. This seems to be consistent with metal pits reducing the average barrier thickness and leading to better capacitive coupling and hence control over the channel charge. As a result, devices with metal pits would require higher V_D to lower the band at the gate edge and consequently raise the on current (Fig. 8). Based on the

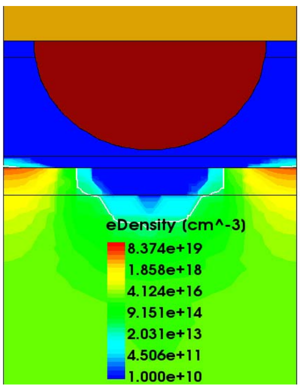

Fig. 6: 2D cross-section of HEMT (20/80%/Al_2O_3) showing depletion of 2DEG due to negative PE charge at AlGaN/insulator interface at low V_D

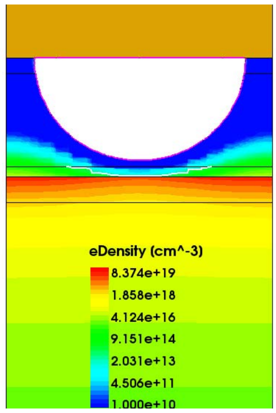

Fig. 7: 2D cross-section of HEMT with a metal pit (20/80%/metal) at low V_D

experimental data given in [2], it is more plausible that the pits are formed by an insulator such as Al_2O_3 because of the degradation of R_D.

IV. Pit Growth and Hole Generation

As the pits start growing, the electrostatic of the HEMT is expected to change significantly as indicated in Fig. 6 and Fig. 7, due to the increase in and redistribution of PE charge and/or change of gate geometry. Therefore, HEMTs with various sizes of pits are simulated to investigate how the BTB TAT is affected during pit growth.

The width of the simulated device is fixed at 0.046µm and pit radius is varied from 3nm to 21nm, which means the pit hemisphere diameter is varied from 6nm to 21nm (i.e. the pit-to-width ratio from 13% to 91%). Pit with r=3nm represents the initial stage of pit formation while r=21nm represents the final stage of pit formation (Fig. 9).

Fig. 10 shows that when metal pits start growing, hole

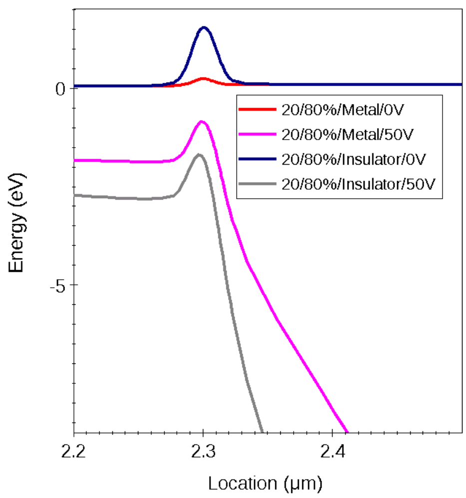

Fig. 8: 1D cut along GaN channel (from source to drain) of conduction band edges of metal and Al_2O_3 pits devices around gate edge on the drain-side (where the peaks are) at different drain biases.

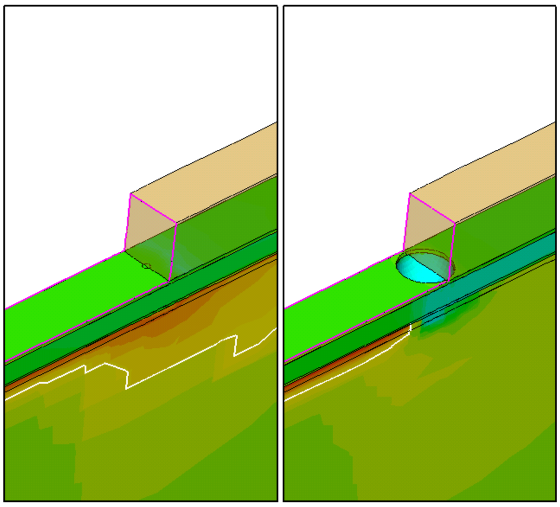

Fig. 9: Structures for simulating metal pit size effects on BTB TAT. Left: r=3nm, Right: r=21nm. Electron density is shown (at V_G=-6V, V_D=43V). The hemispheres are filled with Al_2O_3 in insulator pit case.

generation rate can increase by 3 orders of magnitude. This is because of the increase in electric field due to the irregularity formed by the small initial pits. On the other hand, insulator pits do not lead to substantial increase in hole generation.

The hole generation starts reducing substantially at about r=10nm (or when pit-to-width ratio is larger than 20%). This is because 3D effect kicks in that the unpitted regions are affected by the pits laterally and the band diagram is altered such that the electric field is much smaller for BTB TAT (Fig. 11).

V. Conclusions

3D TCAD simulations were performed to study the physics of pit formation in AlGaN/GaN HEMT. It is showed that BTB TAT can be responsible for hole generation, which is required to initiate the electrochemical reaction proposed in the literature. Metal and insulator pits have different effects on I_D-V_D curves. During pit formation, hole generation rate initially

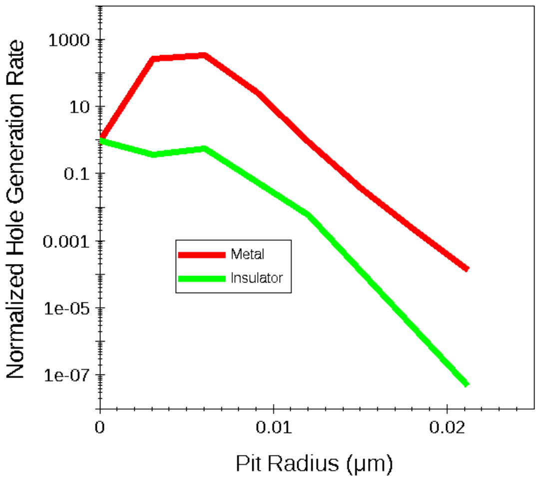

Fig. 10: Hole generation rates of HEMTs with different pit sizes normalized to that of HEMT without pits (r=0nm).

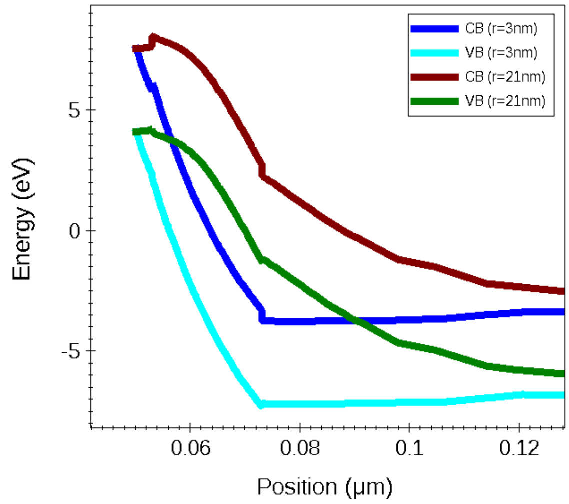

Fig. 11: 1D vertical cut of band diagram at un-pitted region at gate edge on the drain-side for r=3nm and r=21nm in Fig. 9

increases for metal pit and is almost constant for insulator pits. However, both slow down as the pits grow larger due to 3D effects of pits on unpitted regions.

VI. Acknowledgements

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