A Comprehensive Analysis of AlN spacer and AlGaN n-doping effects on the 2DEG Resistance in AlGaN/AlN/GaN Heterostructures

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1. Abstract

In this paper, several epitaxial variations influencing the bi-dimensional electron gas (2DEG) are investigated. The effects of n-doped AlGaN barrier and AlN spacer thickness are studied by examining the sheet electron density (n_s) and the mobility (μ_s) of the 2DEG using $I_D(V_G)$ and $C(V_G)$ measurements, and 1D Schrödinger-Poisson (1DSP) simulations. Specifically, the correlations between the resistance, μ_s, n_s and the polarization interface charges (σ) are studied. Besides the well-reported benefits of the AlN spacer on n_s, we show that a thicker AlN spacer leads to larger n_s due to the enhancement of the AlN polarization. In addition, we prove experimentally that an n-doped AlGaN barrier does not significantly improve the 2DEG density but leads to the formation of a second channel in the AlGaN barrier for negative gate voltage ($V_G \leq 0V$), driving the overall improvement of the resistance.

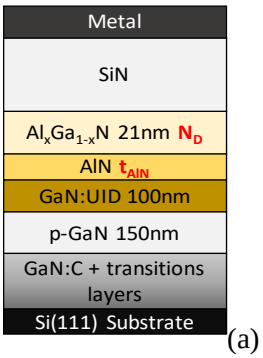
Keywords: AlGaN/AlN/GaN heterostructure; 2DEG; AlN spacer; n-doped AlGaN; Schrödinger-Poisson simulations; Measurements.

2. Introduction

GaN HEMT technology based on AlGaN/AlN/GaN heterostructures on 200 mm diameter Si (111) substrate has aroused a lot of interest for power electronics. Thanks to their crystal and polarization properties, III-N materials are very promising due to high breakdown field and excellent transport properties. To further increase the output power in HEMTs, the resistance of the bi-dimensional electron gas channel (R_{2DEG}) needs to be reduced as far as possible. This improvement can be achieved through either n_s or μ_s enhancement. The AlN spacer between the AlGaN and GaN layer is known to increase the n_s, but its physical root cause is not clearly identified [1,2]. In addition, the effect of n-doped AlGaN on the n_s is investigated [3-6].

3. Experiments

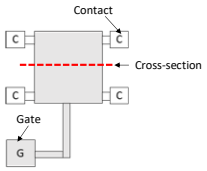
In this work, four different epitaxial-variations grown by MOCVD are investigated. **Figure 1(a)** depicts a cross-section of the studied structure, where the AlN spacer thickness (t_{AlN}) and the n-type AlGaN doping (N_D) are the key parameters of this study. Samples variations are summarized in **Figure 1(b)** and **Figure 1(c)** is a top view of the tested normally-ON Van der Pauw structure.



(a)

	t_{AlN} (nm)	N_D (cm^{-3})
A	0.7	0
B	1.1	0
C	1.5	0
D	0.7	$1x10^{19}$

(b)



(c)

Figure 1: (a) Cross-section of the studied structure (b) Summary table of epitaxial variations (c) Top view of gated Van der Pauw test structure (200µm x 200µm).

In this work, $I_D(V_G)$ and $C(V_G)$ measurements are performed and reported for all the splits (A,B,C,D) in **Figure 2**. The V_{th1} in this article is defined as the gate voltage at which the 2DEG channel is depleted and V_{th2} is the gate voltage required to form a channel inside the AlGaN barrier. $I_D(V_G)$ characteristics show firstly a V_{th1} variation toward negative values when t_{AlN} is increased. Moreover, an n-doped AlGaN barrier leads to an even more negative V_{th1} value and to a higher current density at V_G=0V compared to the undoped cases. Comparison with $C(V_G)$ measurements confirms these electrostatic effects observed on $I_D(V_G)$ curves. **Table 1(a)** reports the extractions of R_{2DEG}, n_s and μ_s, performed from the $I_D(V_G)$ and $C(V_G)$ according to equations 1 to 4. For samples A, B and C, extractions at V_G=0V refer directly to 2DEG parameters, where n_s is calculated by Eq.1 from the $C(V_G)$ and R_{2DEG} with Eq.2 from the $I_D(V_G)$. Finally, μ_s is calculated with Eq.3. As reported in **Table 1(a)**, n_S increases with larger AlN spacer but R_{2DEG} enhancement is limited by mobility degradation, likely due to the rise of surface roughness.

$$n_S\,(2DEG) = \frac{1}{q}\int_{V_{th1}}^{V} C.\,dV\Big|_{V=\begin{cases} 0 \text{ if } V_{th2}\geq 0V \\ V_{th2} \text{ if } V_{th2}\ll 0V \end{cases}} \quad (1)$$

$$R_{2DEG,tot} = \frac{\pi}{\ln(2)}.\frac{\Delta V}{I} \quad (2)$$

$$\mu_{S,tot} = \frac{1}{q.R_{2DEG,tot}.n_{S,tot}} \quad (3)$$

Regarding the n-doped AlGaN sample, the extraction of the 2DEG parameters are indirect because n-doping leads to an earlier formation of the second channel in AlGaN (for V_G<<0V, see **Figure 4(d)**). Consequently, the extraction at V_G=0V accounts for the 2DEG and the AlGaN channel as details in **Table 1(b)**. n_s(total) refers to the value extracted at V_G=0V corresponding to the sum of both channels (Eq.4). R_{2DEG} is extracted at V_{th2} before the formation of the n-AlGaN channel and R_{AlGaN} is deduced using Eq.5, where R_{tot} is the resistance at V_G=0V.

$$n_S\,(total) = \frac{1}{q}\int_{Vth1}^{0} C.\,dV \quad (4)$$

$$R_{AlGaN} = \frac{R_{tot}.R_{2DEG}}{R_{2DEG} - R_{tot}} \quad (5)$$

Surprisingly, the n_s(2DEG) barely increases with doping and the R_{2DEG} reduction is caused by a mobility degradation, likely induced by the high level of doping near the 2DEG channel. Depicted in Figure 4, the simulations of the electron density as a function of the depth for the four-studied samples explain and validate this weak rise of n_S for the doped AlGaN. Indeed, since the onset of charge density in the AlGaN barrier occurs near the AlGaN/AlN interface and thus near the 2DEG channel, a variation of the gate voltage will induce a simultaneous variation of both channels. We attribute the difference between the doped and undoped sample

to the enhance electric field in the AlGaN near the interface induced by the high level of donors. Hence, the overall resistance improvement is only attributed to the high n_s in the AlGaN barrier.

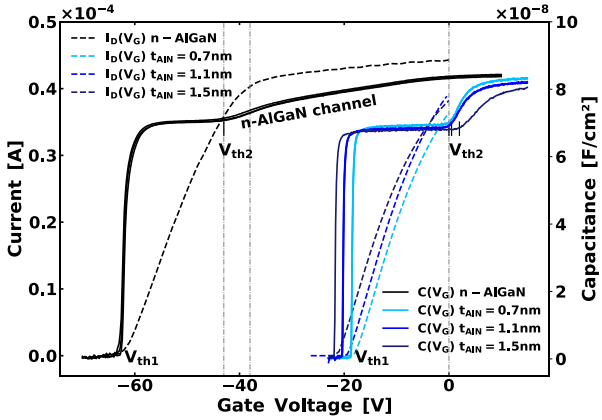


Figure 2: $I_D(V_G)$ and $C(V_G)$ measurements at 1kHz respectively on B1500 device analyzer and HP4284 LCR meter.

	$n_S\,(cm^{-2})$	R_{2DEG} (Ω/□)	μ_s (cm².V⁻¹.s⁻¹)
A	7.9x10¹²	371	2123
B	8.2x10¹²	344	2145
C	8.4x10¹²	351	1981
D	8.2x10¹²	441	1728

(a)

D	$n_S\,(cm^{-2})$	R (Ω/□)	μ (cm².V⁻¹.s⁻¹)
AlGaN channel	2.1x10¹³	1207	216
2DEG (V_G~-43V)	8.2x10¹²	441	1728
Total (V_G=0V)	2.9x10¹³	323	663

(b)

Table 1: (a) Extracted 2DEG parameters R_{2DEG}, n_s and μ_s at V_G=0V for samples A, B, C and at V_{th2} for sample D, (b) AlGaN and 2DEG detailed channel parameters for sample D.

	t_{SiN} (nm)	$\sigma_{AlGaN/AlN}$ (cm^{-2})	$\sigma_{AlN/GaN}$ (cm^{-2})
A	73.5	-6.00x10¹²	1.57x10¹³
B	74.5	-8.00x10¹²	1.82x10¹³
C	75.5	-1.42x10¹³	2.5x10¹³
D	73.5	-6.00x10¹²	1.57x10¹³

Table 2: 1DSP simulated parameters for all samples. The fitting parameters are the interface charges $\sigma_{AlGaN/AlN}$ and $\sigma_{AlN/GaN}$ and the fitting references are V_{th1} and V_{th2}.

4. Simulations

To understand the physical root causes leading to the enhancement of the 2DEG properties, the previous $C(V_G)$ measurements are compared to 1DSP simulations and reported in **Figure 3**. The Poisson and Schrödinger equations are solved self-consistently under the parabolic mass approximation for the Γ-valley. The material parameters used in the simulations are based on Ref.7. The AlGaN polarization charge at the SiN/AlGaN interface is assumed to be completely compensated by a positive charge [7]. Polarization charges at the AlGaN/AlN and AlN/GaN interfaces ($\sigma_{AlGaN/AlN}$ and $\sigma_{AlN/GaN}$) are determined to account for the

experimental V_{th1} and V_{th2} and reported in **Table 2**. These charges are found to be lower than the theoretical values induced by AlN with complete polarization [8]. Indeed, theoretical charges are calculated according to the Ambacher's works [1,3,8], by considering two heterojunctions: the AlN/GaN heterojunction resulting in a positive polarization interface charge responsible for the well-known 2DEG, and the AlGaN/AlN heterojunction resulting in a negative polarization interface charge. The interface charges calculations take into account for the spontaneous (P_{sp}) and the piezoelectric polarization (P_{pz}). GaN is considered as a fully relaxed material. The theoretical charges values are very high ($\sigma_{AlGaN/AlN}$ = -5.42x10^{13} cm^{-2} and $\sigma_{AlN/GaN}$=6.56x10^{13} cm^{-2}) and they induce a much more large shift on both V_{th1} (towards more negative voltage values) and V_{th2} (towards more positive voltage values) compared to the experimental results. In addition, not enough V_{th1} dependency with the AlN thickness is observed by considering these theoretical charges. Thereby, these results suggest that the polarization of AlN is attenuated for very thin layers. **Figure 4** illustrates the decrease of n_s with thinner AlN spacer. To take into account this reduction, we introduce a factor PR (polarization rate) in our calculations of polarization charges see Eq.6 and Eq.7. Interestingly, as depicted in **Figure 5**, using the same PR for the top and bottom charges, these calculated charges are similar to the ones extracted in **Table 2**, for the different t_{AlN}.

$$\sigma_{Al_xGa_{1-x}N/AlN}(x) = \{P_{tot}(AlN) \times PR - [\, P_{sp}(Al_xGa_{1-x}N) + P_{pz}(Al_xGa_{1-x}N)]\}/q \quad (6)$$

$$\sigma_{AlN/GaN} = \{\, P_{sp}(GaN) - P_{tot}(AlN) \times PR\}/q \quad (7)$$

These results support our assumption regarding the attenuation of the AlN polarization for very thin layer. Indeed, the theoretical charges calculation was demonstrated for thickness from 30nm [8]; in this work the studied thicknesses are approximately a few atomic layers considering that the lattice parameter c of the AlN is around 4.98Å. Another hypothesis is that this effect can also, in part, be due to a reduction of the Al fraction in AlN, which becomes an Al-rich AlGaN for very thin layers. However, this assumption seems not sufficient to explain the experimental observations. Indeed, both charges are interdependent and by decreasing the Al content and assuming a complete polarization, the simulated capacitance well reproduces the effect on the V_{th2} but not on V_{th1}. In addition, the Al molar fraction to account for the AlN/GaN polarization interface charge (**Tab.2**) are found to be too low, about 0.305, 0.35 and 0.46 respectively for the AlN 0.7nm, 1.1nm and 1.5nm and do not reproduce the V_{th1} variations.

Going back at **Table 2**, we can notice that for samples D and A, which differ only by AlGaN doping, the same interface charges are determined despite the very different V_{th1} and V_{th2} values obtained on the two samples. This is consistent and corroborates our estimations of $\sigma_{AlGaN/AlN}$ and $\sigma_{AlN/GaN}$. **Figure 6** outlines the polarization rate reduction with thinner t_{AlN} through an empirical model. This simple model gives good approximation for simulations and it seems in accordance with Berdalovic's work, which supposes a 65% of polarization in a 3.5nm AlN layer.

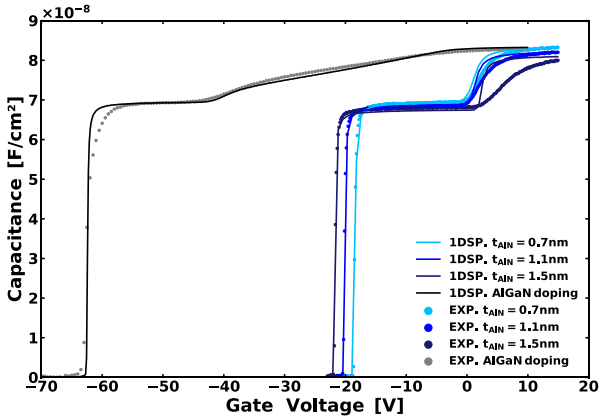


Figure 3: $C(V_G)$ simulations (lines) and comparison with the experimental $C(V_G)$ (dots) for samples A, B, C and D.

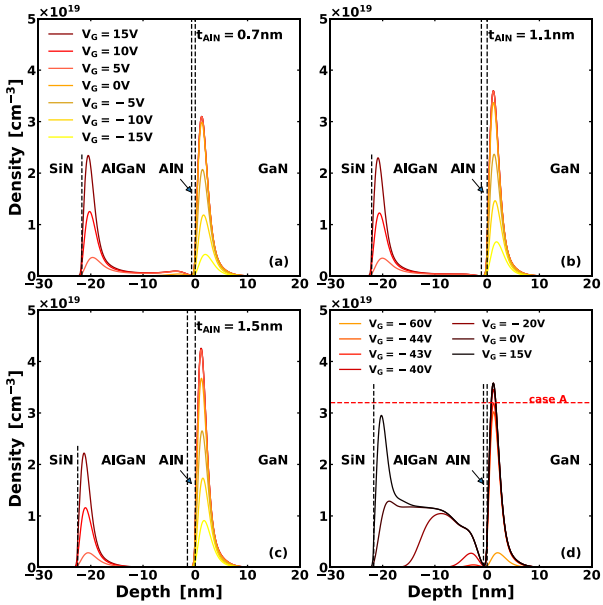


Figure 4: Electron density versus Detph at various V_G obtained from 1DSP simulations, (a) for t_{AlN}=0.7nm, (b) for t_{AlN}=1.1nm, (c) for t_{AlN}=1.5nm, (d) for the n-doped AlGaN, t_{AlN}=0.7nm.

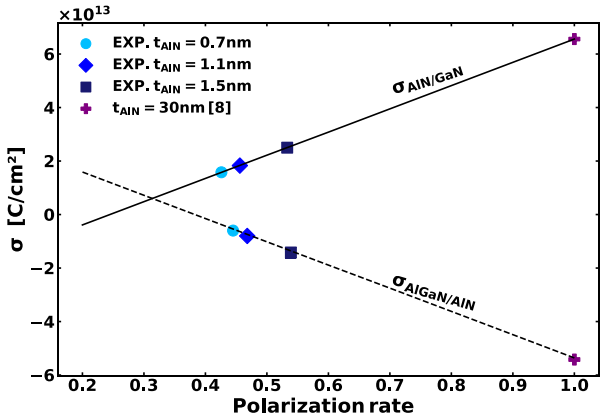


Figure 5: Lines: $\sigma_{AlGaN/AlN}$ and $\sigma_{AlN/GaN}$ vs PR (Eq.6-7). Dots: $\sigma_{AlGaN/AlN}$ and $\sigma_{AlN/GaN}$ extracted from measurements.

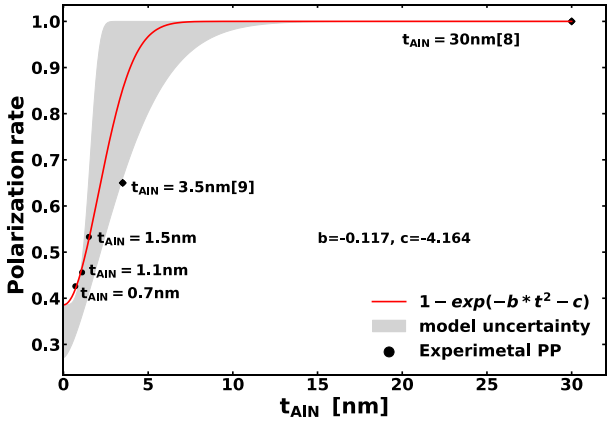


Figure 6: Empirical model predicting the evolution of the polarization rate in the AlN layer as a function of its thickness.

5. Conclusions

In summary, we have demonstrated that n-doped AlGaN improves the on state resistance due to the highly n-doped channel formation in AlGaN for negative voltages. We also showed that the 2DEG density was barely not affected by AlGaN n-doping. Then, we assumed that AlN polarization is attenuated for very thin layers, and increases with thicker AlN layers, resulting in a reduction of R_{2DEG}. This assumption seems the most suitable to explain experimental results. Nevertheless, we find out that R_{2DEG} enhancement with thicker AlN spacer is limited despite the n_S improvement, by mobility degradation for t_{AlN} larger than 1.1nm.

Acknowledgements

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