Study of Interfacial Charge Properties and Engineering of ALD dielectric/III-Nitride Interfaces

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Keywords: III-Nitride, ALD dielectric, interface, MISHEMT

Abstract

Atomic layer deposited Al_2O_3/III-nitride interfacial charge properties were investigated for III-nitride layers of different polarity. On all the orientations of GaN and Ga-polar AlGaN, substantial amount of positive sheet charge density is induced at the Al_2O_3/III-Nitride interface, and post-metallization anneals (PMA) is one of the methods which can significantly alter this sheet charge. It is proposed that the charges are originated from defects at surface that can be passivated and neutralized through a H_2 based anneal. The interface charge density engineering described here can be used to improve performance of device such as gate leakage and electron transport. Lateral electrostatic engineering is also capable to be achieved.

Introduction

III-Nitride-based high electron mobility transistors (HEMTs) have been investigated widely for applications in high power and high frequency electronics due to the large bandgap and high electron velocity of GaN. Metal-insulator-semiconductor HEMTs (MISHEMTs) structures can efficiently suppress gate leakage in vertically scaled transistors with ultra-thin gate barriers needed for higher frequency (mm-wave) operation, and could enable ultra-low leakage for loss-sensitive applications such as power switching circuits. In this work, we discuss the presence of fixed interface charges at the dielectric/semiconductor interface, their effect on the energy band profile and electron transport, and methods to reduce this fixed interface charge density.

While the interface trap density and related dispersion in ALD/III-nitride interfaces is less than that seen in III-As semiconductors[1], recent work[2,3] has shown that a high density of *fixed* charges (~ 1 $\mu C/cm^2$) is induced at ALD-grown Al_2O_3/GaN and Al_2O_3/AlN structures. It was shown that this charge is not modulated by electric field, and therefore does not lead to hysteresis, but it does significantly modify the electrostatics in the system. The high interfacial fixed charges reduce the mobility of the 2-dimensional electron gas (2DEG)[4] through remote ionized impurity scatter, and induce high electric fields in the oxide thus increasing tunneling-related leakage currents. This fixed-charge-induced electric field can also lead to substantial leakage for gate dielectric in N-polar III-Nitride HEMTs.

Simulation

Theoretical investigation of remote impurity scattering for dielectric/AlGaN/GaN structures and the effect 2DEG concentration, and AlGaN thickness are shown in Figure 1 and 2. Remote impurity scattering was found to be the dominant mechanism when the 2DEG density is below $5x10^{12}$ cm^{-2} and dielectric/AlGaN interface charge density is above $5x10^{12}$ cm^{-2}. The interfacial charge has significant effect on the mobility as the AlGaN cap layer thickness is scaled down below 5nm. We will report experimental transport data for highly scaled dielectric/AlGaN/GaN structures with different fixed interface charge density, and compare results with the theoretical predictions.

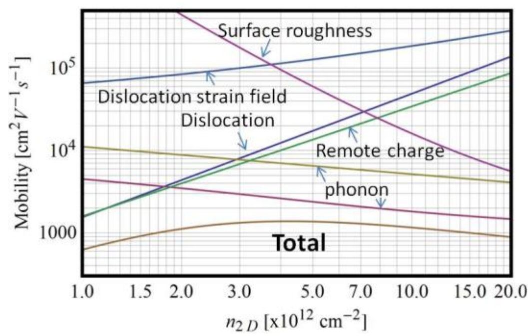

Fig.1. Simulation results – scattering models.

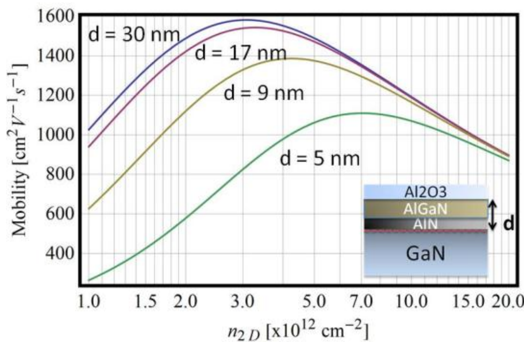

Fig.2. Simulation results – Mobility vs. 2DEG density.

Experiment

Ga-polar GaN samples were grown using a Veeco GEN 930 plasma molecular beam epitaxy system (PAMBE), on Fe-doped semi-insulating GaN/sapphire templates[5]. The N-polar samples were grown by PAMBE on n-doped free standing GaN template[5]. The epitaxial layer consisted of 200 nm unintentionally doped GaN followed by 100 nm silicon-doped GaN ([Si] ~ 1x10^{18} cm^{3}]. As-received bulk m-plane GaN samples ([Si] ~6x10^{16} cm^{3}) were used[6]. A 29 nm $Al_{0.3}Ga_{0.7}N$/1 nm AlN/GaN HEMT[7] sample on Si substrate with 2DEG sheet carrier density of 1.1x10^{13} cm^{2} (as-received) was used in the study. The $Al_{0.3}Ga_{0.7}N$ layer was then recessed to 9 nm. Three Al_2O_3 layers of nominal thickness 6 nm, 12 nm, and 18 nm were deposited by atomic layer deposition (ALD) on each Ga-polar, N-polar GaN, and m-plane GaN sample at 300˚C, using trimethylaluminum (TMA) and H_2O as precursors. For the case of Al_2O_3 on AlGaN, 17nm Al_2O_3 was deposited by ALD. Six times of H_2O pulses (0.1 sec for each) were used at the beginning of deposition, and then followed by TMA precursor. The difference between estimated and measured Al_2O_3 thickness was less than 0.3 nm as confirmed by ellipsometry. Post-deposition anneal (PDA) consisted of 700˚C in forming gas for 1 minute. Gate patterns were defined by optical contact aligner, and a Ni/Au/Ni (30/200/30 nm) stack was deposited using an e-beam evaporator. Large contacts for ohmic contact were patterned using contact lithography, and buffered oxide etch (BOE) 10:1 was used to locally remove the oxide layer for large features in order to get ohmic contacts. After gate metallization, PMA was carried out in the forming gas (5% H_2, 95%N_2) in a rapid thermal annealing system at temperatures varying from 400˚C, to 550˚C.

Results and Discussion

A quantitative analysis of the interface barrier of Ni/Al_2O_3/GaN capacitors was carried out to determine conduction band discontinuity, electric field in the dielectric layer, and interface fixed charge from capacitance voltage (C-V) measurements for each polarity. A linear relationship between the flat-band voltage and oxide thickness was observed, indicating absence of Fermi-level pinning at the Al_2O_3/GaN interface, and non-zero electric field in the oxide, even during flat band conditions in the GaN. The energy band diagram and electrostatic chart are shown in figure 3(a). A simple analytical expression relating the applied flat band gate voltage to the interfacial parameters can be derived as

$$qV_{gi} = \left(\varphi_b - \Delta E_c - \varphi_s\right) - qF_{ox}t_{oxi}$$

where φ_b is the Ni/Al_2O_3 conduction band barrier height, F_{ox} the electric field in the oxide, φ_s is the energy difference between conduction band and Fermi level in GaN, ΔE_c is the conduction band offset between Al_2O_3 and GaN, and V_{gi} is the flat band gate bias for Al_2O_3 thickness t_{oxi}. The conduction band offset (ΔE_C) was estimated by the equation to be 2.1 eV for Al_2O_3/Ga-polar GaN interface. Successively higher post-metallization anneals, were found to decrease the interface charge . The field in the oxide under flat band conditions in GaN was reduced from 1.92 to 0.22 MV/cm (Figure 3b) corresponding to a large decrease in the interface net charge density from 1x10^{13} cm^{-2} to 1x10^{12} cm^{-2}. The

gate leakage current was also suppressed due to the reduction in the electric field (Figure 4). The reduction of interface charge density using post-metallization anneal was found to occur not only in Ga-polar GaN, but also in N-polar GaN, non-polar GaN (Figure 3b), and AlGaN/GaN structures (Figure 5).

The high interface fixed charges can act as remote scattering centers and decrease electron mobility especially when gate oxide thickness is scaled[4], and the channel is close (several nm) from the fixed charges. The results described here provide a method to reduce the interface charge density, thereby eliminating mobility degradation due to remote ionized impurity scattering. Perhaps unique to the III-nitride system, the ability to tune high dielectric/semiconductor charge densities (of the order of 10^{13}) can provide a new way to engineer lateral band structures and charge density in semiconductor devices.

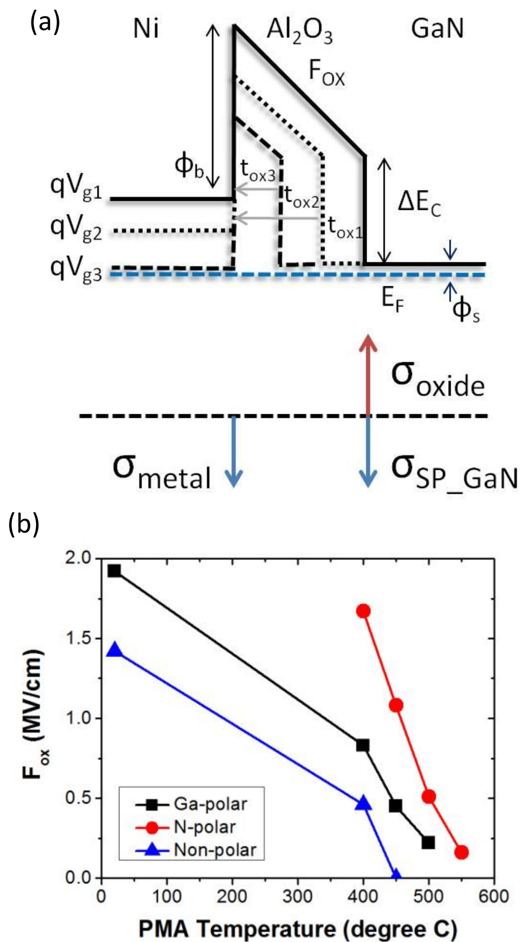

Fig.3. (a) Energy band and charge profile of Ni/Al_2O_3/Ga-polar GaN structure. (b) Electric field in oxide verses PMA temperature with different polarity of GaN.

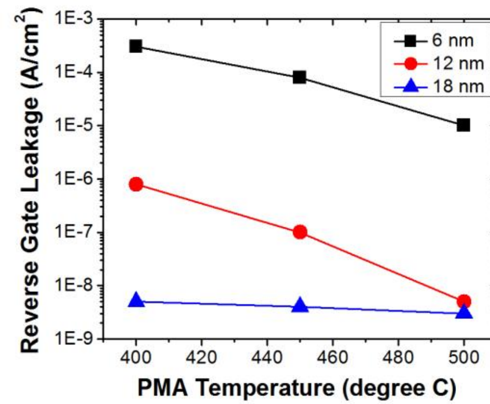

Fig.4. Reverse gate current density (Vg=-4V) vs. PMA temperature with different Al_2O_3 thickness.

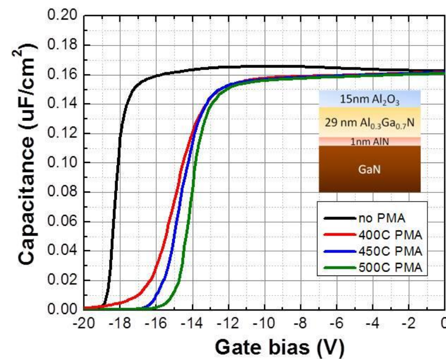

Fig.5. C-V profiles for 15nm Al_2O_3 / 19nm $Al_{0.3}Ga_{0.7}N$ / GaN MISHEMT with different PMA temperature.

Conclusion

Substantial reduction of the Al_2O_3/III-Nitride interface net charges in all polarities of GaN and AlGaN can be effectively done by post metallization anneal in a hydrogen containing ambient. The investigation gives further insight of the origin of the interface fixed charges at ALD dielectric/III-nitride interface, and provides a method to engineer interface charge density. The great suppression of the interface charges leads the reduction the gate leakage in reverse bias and could be critical for electron transport in

GaN-based MISFETs by mitigating remote ionized impurity scattering.

Acknowledgement

This work was funded by the ONR DEFINE MURI (N00014-10-1-0937 Program manager: Dr. Daniel S. Green).

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