Quantum Capacitance in N-Polar GaN/AlGaN/GaN Heterostructures

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***Abstract*—We investigate the effects of quantum capacitance in an N-polar GaN/AlGaN/GaN heterostructures by directly measuring quantum displacement of the electron wavefunction Δd. A comparison between electrically and microscopically measured thicknesses showed negative quantum displacement effects in the inverted high-electron-mobility-transistor (HEMT) structure. As a result of the quantum capacitance effects, a quantum displacement Δd of ~ -4 nm was extracted from the measurements. Further analysis using 1-D self-consistent Schrodinger–Poisson solver has been done to validate the measured data. Our simulation results, including multiple-subband occupancy, explain the increasing capacitance in the measured C–V profile in N-polar GaN-based HEMTs.**

***Index Terms*—AlGaN/GaN high-electron-mobility transistor (HEMT), capacitance–voltage (C–V), N-polar GaN, negative quantum, quantum capacitance, quantum displacement.**

I. INTRODUCTION

III-NITRIDE high-electron-mobility transistors (HEMTs) have been aggressively scaled down to improve their high-frequency performance. With developments in epitaxial growth and device processing technology, gate lengths as low as 30 nm with gate-channel distance of 6 nm were reported with high cutoff frequencies in the conventional Ga-polar GaN-based HEMTs [1], [2].

To achieve the theoretically estimated high-frequency limits in GaN [3], gate length scaling should be accompanied by minimization of short-channel effects and parasitic elements. N-polar HEMT structures [4]–[6], which have been shown to demonstrate high f_T and $f_{\max}$ recently [7], [8], offer advantages over Ga-polarity devices such as low contact resistance through a narrow gap material [9] and better suppression of short-channel effects due to the inherent back-barrier structure [10]. Among these merits, one key advantage proposed in the N-polar inverted HEMT structure is that the electron wavefunction spread *reduces* the gate–channel distance by forming the 2-D electron gas (2DEG) between the gate metal and GaN/AlGaN heterointerface. This is opposite to normal HEMT (or MOSFET) structures where the wavefunction extension increases the effective gate-channel distance [12] and thereby reduces the capacitance. The quantum mechanical capacitance in the inverted HEMT structure therefore *enhances* the gate-channel capacitance over the geometric capacitance. This effect becomes significant at highly scaled dimensions where the wavefunction displacement is of the same order of magnitude as the physical gate-channel spacing, which, in the case of a normal FET, is the oxide or barrier layer.

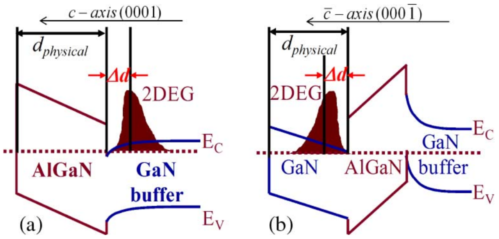

Fig. 1. 2DEG formation and quantum displacement in (a) Ga-polar and (b) N-polar AlGaN/GaN heterostructures.

Due to the finite width of the electron wavefunction along the direction of confinement, a 2DEG manifests itself as a capacitor in series with the geometrical capacitance, with capacitance $C_Q = m^* e^2/(\pi \hbar^2)$, where m^* is the electron mass transverse to the quantum well [11]. This is the quantum capacitance of a 2DEG and is related to the 2-D density of states in the material.

In a typical Ga-polar AlGaN/GaN HEMT [Fig. 1(a)], the gate-channel capacitance $[C_G = 1/(1/C_{\text{geometric}} + 1/C_Q)]$ can be simply written as $C_G = \varepsilon/(d_{\text{physical}} + \Delta d)$, where Δd is the quantum displacement of 2DEG and is known to be $\sim$2 nm for single-subband occupancy in a Ga-polar AlGaN/GaN HEMT [12]. However, 2DEG in N-polar structure is pushed toward the gate [Fig. 1(b)], and the gate capacitance becomes $C_G = \varepsilon/(d_{\text{physical}} - \Delta d)$, thus leading to an *increased* gate-channel capacitance compared to a Ga-polar structure with the same physical thickness.

In this letter, we discuss the negative quantum displacement in an N-polar AlGaN/GaN HEMT with the comparison of physical and electrical measurements of the GaN cap thickness. When the cap thickness *dis similar to*Δd which is the case for highly scaled devices, Δd starts to play a significant and interesting role, and the negative Δd of N-polar HEMTs becomes very critical and advantageous to device performance. This is the first experimental report of this effect in an inverted field-effect device.

II. GROWTH, FABRICATIONS, AND MEASUREMENTS

An N-polar AlGaN/GaN HEMT structure was grown on 4H-SiC substrate using plasma-assisted molecular beam

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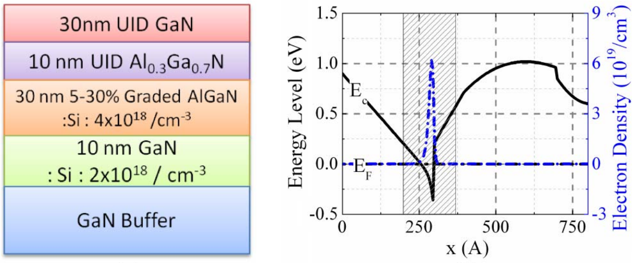
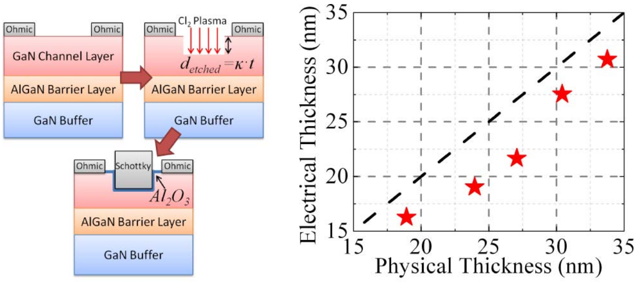


(a) (b)

Fig. 2. (a) Epitaxial structure and (b) energy-band diagram of an N-polar AlGaN/GaN heterostructure.



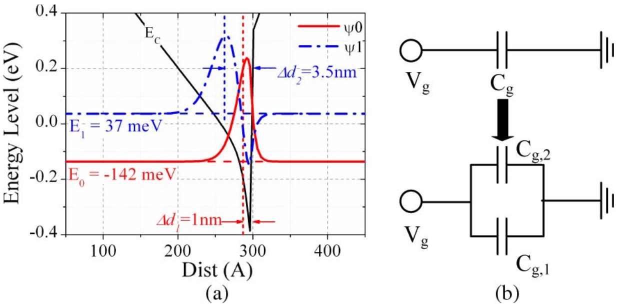
(a) (b)

Fig. 3. (a) Fabrication process of Schottky diode for a thickness series. (b) Measured physical cap thickness versus elecstrical cap thickness which includes 5 nm of Al_2O_3 layer ($\varepsilon_r = 9$) [20].

epitaxy for the measurements of the negative quantum displacement. The two-step GaN buffer layer was grown on 45 nm of AlN nucleation layer to minimize buffer leakage, dislocation density, and impurity incorporation [13]. To keep the valence-band edge far away from the Fermi level to avoid charge trapping by the donorlike trap found near the valence-band edge [5], [14], the barrier layer grown on GaN buffer consists of 10 nm of Si-doped ($N_D = 2 \times 10^{18}$ cm^{-3}) GaN layer and 31.5 nm of linearly graded n-doped ($N_D = 4 \times 10^{18}$ cm^{-3}) AlGaN layer in which the Al composition was graded from 5% (bottom) to 34% (top). Then, 30 nm of GaN channel layer was grown on top of the structure (Fig. 2).

To measure capacitance–voltage (C–V) characteristics, circular metal-oxide-semiconductor capacitors of 90-μm radius were fabricated on the epistructure. Ti/Al/Ni/Au alloyed ohmic contacts were formed by rapid thermal annealing, and the contact resistance was found to be $0.4–0.5\ \Omega \cdot \mathrm{mm}$ by TLM method. The GaN channel layer was etched down using low-power Cl_2-based inductively coupled-plasma reactive-ion etching for different durations. Five nanometers of Al_2O_3 thickness (measured independently using ellipsometry) was deposited using atomic layer deposition (ALD) to suppress the gate leakage from thin GaN cap layer. Finally, Ni was evaporated to form Schottky contacts on the etched surface [Fig. 3(a)].

For samples with different etch durations, C–V measurements (using Agilent B1500 parameter analyzer) and physical thickness measurements (using Zeiss Ultra 55 Plus FE-SEM) were taken to find the quantum displacement Δd. From the zero-bias capacitance of the C–V measurements, the electrical cap thickness was calculated as $d_{\mathrm{cap,electrical}} = \varepsilon / C_{C-V}$ for each etch duration (each physical thickness). Then, the calculated cap thickness is shown in Fig. 3(b) as a function of the physical thickness.



(a) (b)

Fig. 4. (a) First- and second-subband wavefunctions in the quantum well and (b) equivalent circuit diagram of the given N-polar AlGaN/GaN heterostructure.

The physical cap thickness as a function of the etch duration can be written as

$$d_{\mathrm{cap,physical}}(t) = d_0 - \kappa \cdot t + d_{\mathrm{ALD}} \tag{1}$$

where t, d_0, κ, and d_{ALD} are the etch duration, initial cap thickness, etch rate, and deposited ALD oxide thickness, respectively. Similarly, the calculated cap thickness is

$$d_{\mathrm{cap,electrical}}(t) = d_0 - \kappa \cdot t + \Delta d + d_{\mathrm{ALD}}. \tag{2}$$

From (1) and the measured initial cap thickness $d_{\mathrm{physical}}(t = 0)$, the etch rate κ was found to be 0.9 Å/s by linear fitting of the measured physical thickness (standard deviation $= 0.3\%$).

Since both two equations share the same components except for the quantum capacitance, the averaged Δd value of ~ -4 nm for N-polar AlGaN/GaN HEMT structure was found from Fig. 3(b). This experimentally confirms that the electron wavefunction spread in the inverted HEMT determines the gate-to-channel spacing, effectively making it smaller than the physical GaN cap thickness.

III. ANALYSIS AND DISCUSSION

To understand the physics of the quantum spread Δd, 1-D self-consistent Schrodinger–Poisson simulations [15] were done. At zero bias, two wavefunctions corresponding to the first and second subbands of the structure shown in Fig. 1 were calculated and are shown in Fig. 4(a). The first subband at $T = 300$ K E_0 was found to be 142 meV below the Fermi level with Δd of -1 nm. For the GaN cap thickness of 30 nm, the second subband E_1 (35 meV above the Fermi level) shows Δd of -3.5 nm that agrees well with the measured Δd ($\sim$4 nm). Since E_1 is in proximity to the Fermi level and can be easily occupied at room temperature [16], [17], it can be assumed that the second subband is occupied. Next, we carried out simulation of the C–V curve, including quantum mechanical effects. The equivalent circuit model of the gate capacitor of the given structure with two parallel capacitors associated with the occupied subbands is shown in Fig. 4(b). We consider the case where the barrier layer consists of 5 nm of Al_2O_3 and etched GaN channel layer has an initial thickness of 30 nm. With the variation of the GaN thickness with the etching as in the actual experiments, Δd of the wavefunction was estimated for the first and second subbands.

In Fig. 5(a), the estimated Δd as a function of the GaN cap thickness is shown. The critical GaN cap thickness of 2DEG formation d_{cr} was found to be 6 nm, i.e., 11 nm with

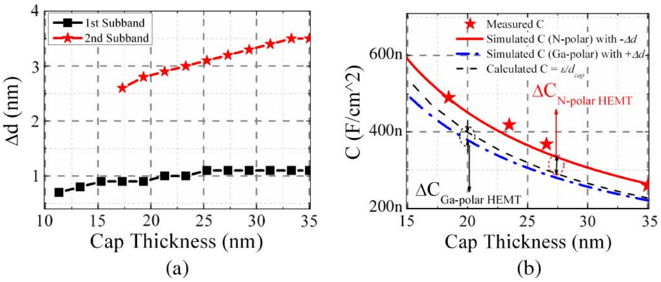


Fig. 5. (a) Quantum displacement Δd of each subband from the heterointerface *toward* the Schottky barrier and (b) total capacitance as functions of the cap thickness which includes 5 nm of Al_2O_3 layer.

5 nm of Al_2O_3. After the GaN layer becomes thicker than d_{cr}, the sheet charge density increases, and the first and second subbands begin to be filled up in the order. Unlike $|\Delta d|$ of the first subband that is $\sim$1 nm even for a thick GaN layer, the value for the second subband increases from 2.5 to 3.5 nm after the onset of the charge accumulation with the increasing GaN thickness. This increasing $|\Delta d|$ of the occupied second subband also explains the increasing C–V profile in N-polar-oriented HEMT structures [18], [19].

The simulated C–V curve with two-subband occupancy matches well with the measured value for the range of cap thickness investigated here, as shown in Fig. 5(b). For comparison, capacitance for a Ga-polar AlGaN/GaN HEMT structure with 5-nm Al_2O_3 varying thicknesses of 34% AlGaN cap layer corresponding to GaN cap thickness of N-polar structure is also shown. As expected from the negative Δd in the N-polar-oriented HEMT structure, there is a significant increase in the gate-channel capacitance $\Delta C_{\mathrm{N\text{-}polar\ HEMT}}$ when compared to the geometric capacitance. The summation of $\Delta C_{\mathrm{N\text{-}polar\ HEMT}}$ and $\Delta C_{\mathrm{Ga\text{-}polar\ HEMT}}$ shows the effective difference of C_g between Ga-polar-oriented and N-polar-oriented HEMT structures for the same physical barrier thickness. With the difference in Δd between Ga- and N-polar HEMT structures, which is approximately 5–6 nm, the N-polar AlGaN/GaN HEMT structure can obtain additional gate capacitance value against the Ga-polar HEMT structures for the same cap thickness. In Fig. 5(b), the additional capacitance value is about 15%-20% over the cap thickness of 15-35 nm. However, for millimeter-wave and higher frequencies, the cap thickness will be reduced further, and the effects of this enhancement will be more pronounced. For example, for a physical cap thickness of 6 nm, there is more than two times enhancement in the gate–source capacitance between N-polar and Ga-polar structures and, consequently, a higher device transconductance. We expect that this will lead to direct reduction in the parasitic delays such as the delay related to the gate–drain capacitance C_{gd}.

IV. CONCLUSION

In this letter, we have investigated the negative quantum capacitance effects in N-polar GaN/AlGaN/GaN heterostructures. Negative quantum displacement of ~ -4 nm was found from the measurements. Through further analysis with simulations, this quantum displacement and the increasing C–V profile in N-polar HEMT structure are found to be mainly due to the second-subband occupancy. Enhancement of the gate–source capacitance of N-polar HEMTs shown here is expected to be significant as N-polar HEMTs are scaled to shorter gate length and smaller gate-channel distance. Our observations apply not only to III-nitride N-polar HEMTs but also to an inverted FET structure in any material system.

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