Full-Quantum Study of AlGaN/GaN HEMTs with InAlN Back-Barrier

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***Abstract*—A full-quantum simulation of the electron transport in the two-dimensional electron gas (2DEG) of a AlGaN/GaN/InAlN/GaN heterostructure is carried out using the non-equilibrium Green function (NEGF) approach. The introduction of the InAlN back-barrier and the use of a ultra-thin GaN layer for the charge transport considerably entangles the physics of the device. A full-quantum approach is then deemed necessary to shed light on the transport properties of these devices. Gate-length and channel-thickness scaling are studied to assess the impact of confinement effects on the elctrostatic integrity of the device.**

I. Introduction

GaN is a promising wide-band-gap semiconductor due to its high saturation velocity, high breakdown field and high mobility. And most notably in virtue of the high 2D electron gas (2DEG) density that can be induced by polarization at the AlGaN/GaN hetero-interface [1], [2].

Even though electric, optical and mechanical properties of a nitride based heterojunction are well understood, a number of device improving techniques like the use of ultra-thin layers as in gate recess, the use of advanced materials such as the high-k dielectrics, or the introduction of back-barriers, are complicating the physical modeling. Accurate numerical simulations that correctly take into account for quantum physical effects are indeed crucial to gain physical insight on non-trivial devices. It is then very likely that TCAD approaches to simulate charge transport in GaN based devices will experience the same relentless evolution that silicon simulators underwent in the last twenty years as technology moved from sub-micrometer MOS devices and drift diffusion to FinFET and full-quantum approaches.

By using 2D self-consistent Poisson-Schrödinger simulations, we focus on a AlGaN/GaN heterojunction transistor featuring an ultra-thin GaN channel, a stress-free InAlN back-barrier and a high-k dielectric as gate barrier layer as sketched in Fig. 1. Such a device is a case study of an improved GaN device architecture in which quantum confinement effects are non-negligible. Importantly, in this study the quantum-mechanical effects in the electron transport layer are accounted for both in the quantization and in the transport direction.

The studied devices features an ideal gate with a work-function Φ_{M} =5.1 eV and ideal reflection-less Source/Drain contacts. Gate stack is formed by complete recess of the AlGaN barrier layer replaced by 2 nm HfO_2 and a 2 nm AlN layer that is known to maximize the GaN channel electron

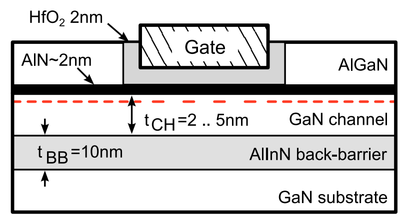

Fig. 1. Schematic representation of a GaN device featuring InAlN back-barrier, High-k dielectric and AlN barrier inter-layer. InAlN is lattice matched to GaN, *i.e.* 82% Al content. Device has a recessed Ni-based metal gate (work-function Φ_{M} =5.1 eV) and a source/drain access barrier made of 18 nm undoped AlGaN with 20% Al content. If not specified otherwise, gate length is L_G=300 nm, source and drain access regions are L_S=L_D=300 nm wide.

charge [3]. The use of high-k materials in GaN devices was proposed in [4]. The 10 nm thick back-barrier Indium content is chosen to be 18% to match the GaN lattice constant and assure a mechanical stress-free heterojunction. The feasibility of a ultra-thin GaN channel (few nano-meters) over a InAlN back-barrier has been recently demonstrated in [5].

We then address the issues originated by the scaling of the channel thickness and of the gate length, identifying the length at which short channel effects (SCE) may be non-negligible.

II. The Model

The origin of the 2DEG at the (Al,In,Ga)N/GaN hetero-junction is now well understood [6]. The 2DEG is formed at the interface to compensate the polarization charges induced by to the strong gradients of spontaneous (P_{sp}) and piezo-electric (P_{pz}) polarization present in nitride materials [7]. By exploiting a finite element method (FEM), we implemented piezo and spontaneous polarization charges at the interfaces following the non-linear model in [7].

In order to shed lights on the electrostatic and transport properties of such devices, we solved self-consistently the 2D Poisson and Schrödinger equations in the non-equilibrium Green's function (NEGF) formalism. To reduce the numerical burden we adopted the coupled mode-space approach, using up to 10 modes. We included piezoelectric, acoustic and optical phonon scattering in the self-consistent Born approximation with parameters from [8].

The deformation potential of acoustic phonons D_{AC} was slightly tuned (see Fig. 2) to reproduce the experimental mobility data. This was evaluated according to the method proposed

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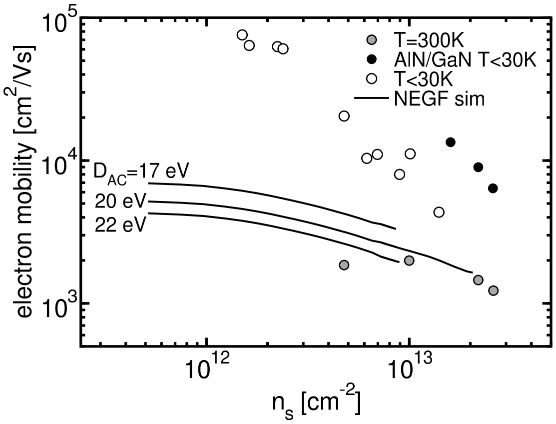

Fig. 2. Measured (symbols) and simulated (lines) electron mobility. For experimental data see [9] and references therein. The acoustic phonon deformation potential D_{AC} used in all simulations was 20 eV.

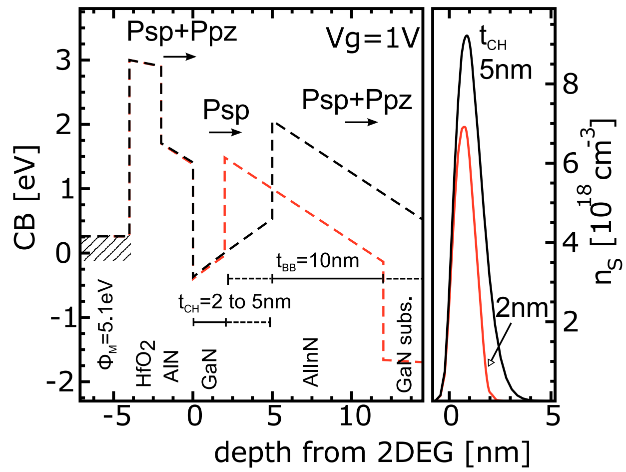

Fig. 3. Conduction band and electron density profile for device with channel thickness of t_{CH} =5 and 2 nm (black and red lines respectively) in a cross-section at the middle of the channel.

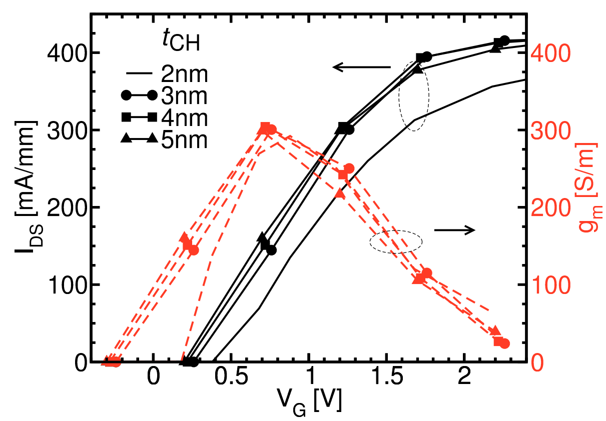

Fig. 4. Transfer characteristics for various t_{CH} at fixed $\mathrm{L_G}$=300 nm. The quantization induced by the presence of the back-barrier acts on the sub-band occupation determining an increase of the threshold voltage V_{T}.

in [10], and a satisfactory fit was found with $D_{\mathrm{AC}} = 20$ eV. We limited the investigations to the gate 'controlled channel', i.e. the barrier/channel interface immediately below the gate material, comprising only the first 300 nm of the drain and source extension areas on the left and right of the gate, as in Fig. 1. In this work, Source/Drain access regions are not simulated. In fact, we considered ideal reflection-less Ohmic contacts, mimicked by including highly doped source and drain regions.

III. Back-barrier

Among the various technological booster options available, different back-barriers design comprising AlN [11], AlGaN [12], InGaN [13], or InAlN [5] have been recently proposed in order to increase the confinement of the 2DEG. Adoption of a InGaN back-barrier [13] for example significantly improved RF figures of merit of the device by shifting the conduction band of the GaN channel lower than the conduction band of the buffer.

In another approach an InAlN back-barrier [5] possibly in conjunction with a N-polar crystal growth [14] was proposed and allowed a scaling down of the gate to sub 100 nm lengths without any decrease of channel charge density (n_{s}) or electron mobility degradation. In both studies the presence of the back-barrier improved the short-channel effects caused by gate length scaling in the quest for optimal RF device. In any case, presence of a back-barrier could be in principle beneficial for power devices also, as a mean to control the V_{T} of the device, suppress the substrate leakage and improve the device reliability.

A conduction-band cross-section of our studied device is shown in Fig. 3 with a profile of the electron charge for channel thickness t_{CH}= 5 and 2 nm and gate length of $\mathrm{L_G}$=300 nm. Charge profile along the vertical direction slightly depends on t_{CH} *i.e.* a thinner channel results in a smaller electron density. Electron density is maximal at a close distance of about 1 nm from the AlGaN/GaN interface, sign of a strong vertical quantization. As can be seen also in the I-V trans-characteristics plotted in Fig. 4, spatial deformation of the 2DEG have no substantial effect on device transport properties, while thinning the channel thickness down to as much as $t_{\mathrm{CH}} < 3$ nm. Consequently, phonon-limited mobility is not affected by sub-band charge re-partition down to t_{CH}= 2 nm (see the transconductance in Fig. 5). The decrease of the t_{CH} has only a limited impact on the threshold voltage V_{T}. This is true of course for the case of a perfect interface with no thickness spread or roughness. In such a case quantum confinement effects would not significantly degrade device performance even with channels as thin as 3 nm.

IV. Gate-length Scaling

Further, we focused on the device with minimum thickness, t_{CH}= 2 nm, which is expected to present the best electrostatic integrity, and studied its transport properties as the gate length L_G is scaled down from 300 nm to 25 nm. Fig. 6 presents the transfer characteristics and the g_m for different gate lengths, showing both a current increase and a small V_{T} reduction for shorter L_G. As shown in the energy-resolved current density

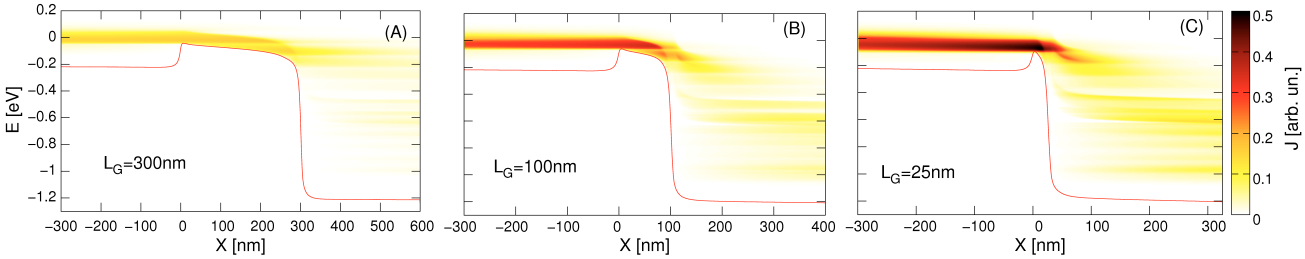

Fig. 8. Lowest Conduction sub-band profile along the transport direction and energy-resolved current density at $V_G = 0.7$ V and $V_{DS} = 1$ V for the device with $t_{\rm CH}$ =2 nm and with L_G =300 nm (A), L_G =100 nm (B) and L_G =25 nm (C). The efficient device electrostatics results in similar barrier heights for the three gate lengths. In the saturation regime the current in the drain region is energetically redistributed by the emission of optical phonons with energy $\hbar\omega_{op} = 90$ meV.

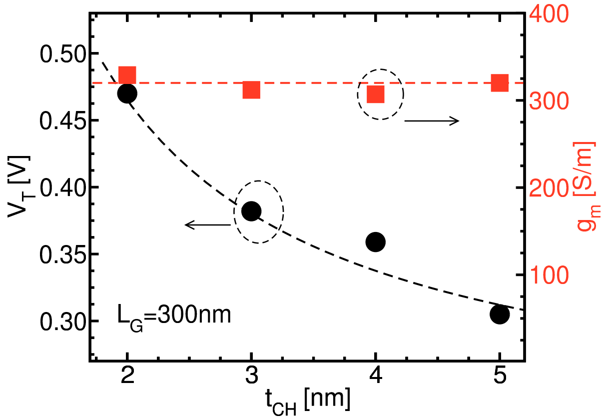

Fig. 5. Threshold voltage ($V_{\rm T}$) and transconductance (g_m) evolution as a function of the channel thickness. Symbols are data, dashed lines are a guide to the eye. The increase of quantum confinement results in a small positive $V_{\rm T}$ shift without changing g_m.

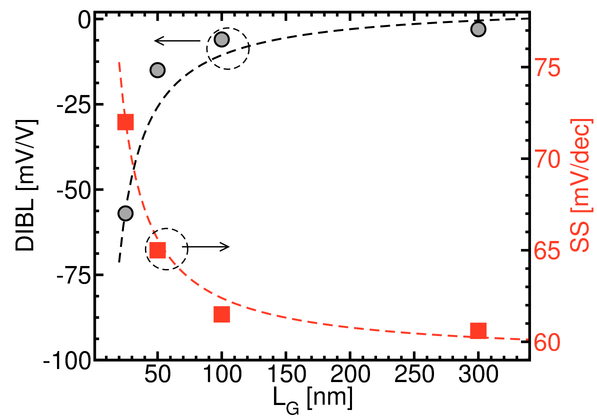

Fig. 7. Sub-threshold slope (SS) and drain induced barrier lowering (DIBL) between $V_{DS} = 50$ mV and $V_{DS} = 1$ V as a function of channel length for $t_{\rm CH} = 2$ nm device. Symbols are data, dashed lines are a guide to he eye. Down to a channel length of 25 nm, the device features good SCE immunity.

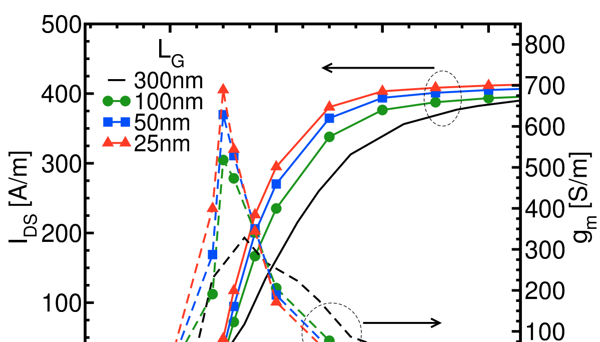

Fig. 6. Transfer characteristics and transconductance at $V_{DS} = 50$ mV for the devices with different gate lengths. No appreciable $V_{\rm T}$ shift is found down to L_G =25 nm due to the minimization of the SCE provided by the back-barrier.

plots of Fig. 8, the L_G reduction slightly decreases the channel barrier even in the saturation regime, where electron transport is dominated by optical phonon emission in the drain region. Finally, as detailed in Fig. 7, the device exhibits an optimal electrostatics even at the shortest lengths of 25 nm, were DIBL is limited to below 100 mV/V and sub-threshold slope degradation is less than 20%, thus validating the excellent, although theoretical, scaling possibilities of the presented device architecture.

V. Conclusion

Full-quantum self-consistent 2D simulations have been exploited to evaluate and propose feasible design options for aggressively scaled GaN-based transistors that are promising for both power and RF applications. In the presence of a ultra-thin channel and a InAlN back-barrier, devices as thin as $L_G = 25$ nm are still featuring almost undegraded device performance metrics. The study highlights the capability of NEGF methods to analyze the physical properties of such devices.

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