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Polarization engineered 1-dimensional electron gas arrays

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(Received 23 October 2011; accepted 30 January 2012; published online 27 February 2012)

One-dimensional electron gas based devices are of great interest due to their promise in high-performance electronics and future device applications. However, synthesis and patterning of arrays of nanowires is a challenge in all material systems. Here we demonstrate a novel system based on vicinal AlGaN/GaN heterostructures that enables direct electrostatic tuning of the dimensionality of electrons from 1 D to 2 D. Our approach, based on polarization engineering, enables top-down fabrication of dense arrays of pure 1-dimensional electron channels with carrier confinement equivalent to 90 meV, that are capable of carrying technologically relevant current densities up to 130 mA/mm. A direction-dependent small-signal capacitance-voltage profiling to probe the Fermi occupation function of electron gas was used to demonstrate distinct signatures of 1-dimensional density of states and transport in these structures at room temperature. The system discussed here is based on polarization-induced anisotropic charge in vicinal AlGaN/GaN heterostructures. We developed a 2-sub-band model consisting of 1-D and 2-D sub-bands to describe the behavior of these wires. We find excellent agreement between our model and experimental data, confirming the channel are indeed 1-dimensional. Our demonstration of 1-dimensional electron channel arrays in this system could enable optical, electronic and magnetic devices with added functionalities and performance. © 2012 American Institute of Physics.

I. INTRODUCTION

Semiconductor nanowires, owing to their quantum-confined one-dimensionality, present an excellent system to explore phenomena at the nanoscale and harness them for useful device applications like nanowire based field effect transistors, future device applications, as well as for nanowire photonic devices including microcavity lasers, LEDs, solar cells, and photodetectors. However, achieving controlled assembly of high-density nanowire arrays for large-scale integration, which is crucial for practical applications, is still a major challenge for both top-down and bottom-up approaches. While achieving high quality nanowires with sub-20 nm dimensions becomes a challenge for top-down approach, the bottom-up approach suffers from issues such as poor surface control, poor longitudinal control of doping profiles, and possible metal contamination due to requirement of metal as catalysts for growth initiation.

In our previous work, we showed that the anisotropy in the 2-dimensional electron gas (2DEG) charge introduced by polarization in vicinal AlGaN/GaN heterostructures can lead to lateral confinement along the steps of the vicinal substrate (Fig. 1). Such a vicinal AlGaN/GaN system with anisotropic transport properties is being increasingly investigated in more details recently. In this work, we show that when combined with the vertical confinement (due to a heterostructure conduction band offset), such a system shows signatures of a 1-dimensional electron gas (1DEG) at room temperature. A direction-dependent small-signal capacitance-voltage (C-V) profiling method to probe the Fermi occupation function of the electron gas was used to demonstrate clear signatures of 1-dimensionality. The experimentally obtained data matched excellently with those predicted by a 2-sub-band theoretical model consisting of a 1-D and a 2-D sub-band which we propose here. In addition, we demonstrate electrostatic tuning of the dimensionality of 1-dimensional and 2-dimensional electron gases, and show that these may co-exist in this system depending on the position of the Fermi level. Such an approach can provide both high density self-defined arrays of nanowires, which are not lithographically, but electrostatically obtained, and combines the advantages of both the top-down and bottom-up approaches without having their limitations.

II. EXPERIMENTAL DETAILS

The epitaxial structure used for this study (Fig. 2(a)) was grown by metal organic chemical vapor deposition (MOCVD) on a vicinal sapphire substrate with a miscut of 4° toward the a-direction. The details of the growth of the epitaxial stack grown by MOCVD used here have been reported elsewhere. Due to kinetics of step-flow growth, the atomic terraces and steps characteristic of the vicinal substrate replicate in the AlGaN/GaN epitaxial layers grown by MOCVD as shown by atomic force microscopy (AFM) of the surface of the sample after AlGaN deposition (Fig. 2(b)). For a 4° miscut in GaN, the atomic terraces are expected to be 8-16 nm wide (the variation is due to step-bunching). The
energy band diagram of the N-polar $^{28,29}$ AlGaN/GaN heterostructure described here was obtained using self-consistent 1-dimensional Schrodinger-Poisson (BandEng) $^{30}$ simulations (Fig. 2(c)). A 2DEG is induced at the top interface between GaN and AlN due to fixed spontaneous and piezo-electric polarization. $^{31}$ Ohmic contact pads were fabricated using standard optical lithography by evaporating a metal stack of Ti(20 nm)/Al(120 nm)/Ni(30 nm)/Au(50 nm) and then subjecting to a rapid thermal annealing at 850 °C for 30 s to enable the metals to spike through the top layers to the electron gas. Mesas were defined by using a BCl$_3$/Cl$_2$ based inductively-coupled-plasma/ reactive ion (ICP/RIE) etch chemistry with 30 W of RIE power to etch 100 nm of the epitaxial layer so as to isolate the 2DEGs of individual devices. The Ohmic contacts were fabricated on the sample such that when a bias voltage is applied between two adjacent contacts, the direction of current flow between them would be either parallel or perpendicular (Fig. 2(d)) to the atomic terraces characteristic of the vicinal surface. A contact resistance of 0.6 Ω-mm was extracted from four point transfer length method measurements while sheet resistances in the directions parallel and perpendicular to the atomic terraces were extracted to be 357 and 467 Ωs/square, respectively. This anisotropy in sheet resistance can be attributed to the anisotropy in the 2DEG charge density. $^{22}$ Schottky contacts were defined by evaporating Ni (30 nm)/Au (300 nm)/Ni (50 nm) metal stack to form gates for Schottky diodes to measure C-V.

III. RESULTS AND DISCUSSIONS

A. Capacitance-voltage (C-V) profiling

We are interested in investigating the dimensionality of the channels. Conventionally, the signature of 1-dimensionality for a nanowire is obtained through magneto-transport measurements at cryogenic temperatures or gated conductance measurements (where the conductance is quantized as a multiple of $e^2/h$ for each 1-D channel). However, in...
our system of atomic-terrace defined nanowires, we have a large ensemble ($\sim 0.5 \times 10^6$) of self-aligned 1D channels, and statistical fluctuations make it difficult to observe the traditional 1-D characteristics. However, the electron density populating the ensemble of 1D channels in our system would still have a $1/E$ dependence on energy $E$ due to 1D density of states. This can be investigated by probing the electron density as the Fermi level of the electron gas is tuned. For this, we performed C-V measurements in directions parallel and perpendicular to atomic terraces as shown schematically in Fig. 3(a).

The C-V measurement was done as follows: on a Schottky or gate metal pad ($200 \mu m \times 200 \mu m$), a sinusoidal signal of very small magnitude (30 mV) and a frequency between 100-500 KHz was applied, which rides on a large-signal DC bias also applied on the gate. An Ohmic pad ($200 \mu m \times 100 \mu m$), situated 4 $\mu m$ from the gate pad, is connected to the ground. The charge on the gate metal is reflected in the electron gas populating the channel beneath the gate. For an incremental voltage $\Delta V$ on the gate, the increase in the channel charge $\Delta Q$ is measured. Thus, the small-signal charge flowing between the gate and the Ohmic metals through the electron gas channel provides the value of the capacitance at a particular gate bias as $C = \Delta Q/\Delta V$. However, only those electrons (or charge) whose wave-vectors are not quantized in the direction of gate-to-Ohmic can actually flow between the two contact pads through the channel and hence will contribute toward the capacitance value measured in that direction (i.e., parallel to or perpendicular to atomic terraces). For either direction (parallel or perpendicular), the density of electrons, $n_s$, ($cm^{-2}$) corresponding to a given gate bias $V_{g1}$ can be found by integrating the area under the C-V curve to $V_{g1}$ from pinch-off (i.e., the Schottky bias at which the capacitance starts to rise from zero indicating electrons are starting to populate the electron gas),

$$n_s(V_{g1}) = \frac{1}{q} \int_{V_{pinch-off}}^{V_{g1}} C(V_g)dV_g,$$

where $q = 1.6 \times 10^{-19} C$ is the charge of an electron.

Therefore, irrespective of the actual charge that exists beneath the gate, the measured charge might be different depending on the dimensionality (or quantized state) of the electrons and the measurement direction.

The capacitance (normalized to the area) measured parallel and perpendicular to atomic terraces is shown in Fig. 3(b). It is interesting to observe that the turn-on (or rise) of the capacitances in the two directions is different which manifests as two different zero-bias charge densities in the two directions as extracted using Eq. (1): $7.6 \times 10^{12}$ cm$^{-2}$ parallel to and $5.7 \times 10^{12}$ cm$^{-2}$ perpendicular to atomic terraces. This anisotropy arises from the dependence of the charge on the dimensionality of the electrons and the measurement direction as mentioned before.

### B. Two sub-band model: Tuning of dimensionality and comparison with experimental data

To explain the direction-dependence of the C-V profile and the charge, as well as to establish the 1-dimensional nature of the system, we propose a 2-sub-band theory with a sub-band $E_0 < E_{bar}$ and a sub-band $E_1$ just above $E_{bar}$, where $E_{bar}$ is the lateral confinement energy corresponding to the saw-tooth profile (simplified representation in Fig. 3(c)). Electrons populating $E_0$ are quantized in two dimensions ($x$ and $z$) and can carry current in only one dimension (momentum wave-vector $k_y$) leading to 1-dimensional channel transport. The electrons populating $E_1$ have only wave-vector $k_z$ quantized due to heterostructure

![FIG. 3. (Color online) Capacitance measurement and 2-sub-band model. (a) Schematic showing orientation of Schottky and Ohmic contacts for C-V measurements parallel and perpendicular to atomic terraces. (b) Normalized capacitance as a function of applied gate bias when probed for transport parallel and perpendicular to atomic terraces. (c) Saw-tooth energy band profile (simplified as triangular wells) in the lateral direction along atomic terraces (as shown in Fig. 2(b)). Electrons in sub-band $E_0$ have wave-vectors non-quantized in $y$-direction only and hence are purely 1-dimensional. Sub-band $E_1$ consists of pure 2-dimensional electrons with only $k_z$ wave-vector quantized in $z$-axis (growth direction).]
confinement in vertical direction but can carry current in the other two directions (momentum wave-vectors $k_x$ and $k_y$) (as shown in Fig. 3(c)), thus contributing to pure 2-dimensional transport.

When the gate voltage is lower than pinch-off voltage of the channel (−7 V in this case), the capacitance is zero indicating the entire charge is depleted. At pinch-off voltage which is $\sim$−6 V and $\sim$−5 V for transport parallel and perpendicular to atomic terraces, respectively, the capacitance starts to rise indicating that electrons start populating the first sub-band. As gate-bias is increased, the Fermi level $E_F$ rises from below sub-band $E_0$ to above $E_1$ to account for the gradually increasing electron density populating the two sub-bands. At any given position of $E_F$, electrons populating only $E_1$ (or electrons with non-quantized wave-vector $k_y$) are sensitive to (or measured by) C-V profiling in the direction perpendicular to atomic terraces while C-V profiling in the parallel direction will measure electrons populating both $E_0$ and $E_1$ (or electrons with wave-vector $k_y$). Thus, the capacitance shown in Fig. 3(b) corresponding to perpendicular direction is a direct measurement of a pure 2DEG density while that corresponding to parallel direction gives the total of 1DEG and 2DEG densities. The difference of the capacitances measured in the two directions is the capacitance for the 1-dimensional charge populating the $E_0$ sub-band only.

Thus we have

$$n_{1D}(V_g) = n_{parallel}(V_g) - n_{perpendicular}(V_g).$$  \hspace{1cm} (2)

Evaluating the area under this C-V curve gives the pure 1-dimensional charge density in dimensions of cm⁻² which can be converted to effective 1-dimensional charge density in unit of cm⁻² or m⁻¹ by multiplying it with the nanowire pitch or in this case, the average atomic terrace width.

Theoretically, at any position of Fermi level $E_F$, the total number of electrons populating the $E_0$ sub-band, which are purely 1-dimensional, is given by the integration of the product of the 1-D density of states and the Fermi occupation function,

$$n_{1D}(E_F) = \int_{E_0}^{\infty} \frac{\sqrt{2m^*}}{\pi \hbar \sqrt{E}} \frac{1}{1 + \exp \left( \frac{E - E_F}{kT} \right)} dt_{\text{terrace}}. \hspace{1cm} (3)$$

where $m^*$ is the effective electron mass in GaN ($= 0.2$ times free electron mass), $k$ is Boltzmann constant ($= 1.38 \times 10^{-23}$ SI units), $T$ is room temperature ($= 300$ K) where measurements are performed and $\hbar = 1.054 \times 10^{-34}$ SI units) is the reduced Dirac constant. The expression is divided by the average atomic terrace width $t_{\text{terrace}}$ in order to normalize the 1-dimensional density of electrons (cm⁻¹) in units of cm⁻². Similarly, at any Fermi level, electrons occupying the $E_1$ sub-band, which are purely 2-dimensional, is given by integrating the product of 2-D density of states and the Fermi occupation function

$$n_{2D}(E_F) = \int_{E_0}^{\infty} \frac{m^*}{\pi \hbar^2} \frac{1}{1 + \exp \left( \frac{E - E_F}{kT} \right)} \frac{1}{t_{\text{terrace}}} \exp \left( \frac{E - E_F}{kT} \right) dE. \hspace{1cm} (4)$$

The choice of $E_0$ and $E_1$ is explained as follows: As a simplified approximation, let us consider $E_0$, the 1st sub-band, as reference, i.e., $E_0 = 0$. There is no absolute or universal relation between $E_0$ and $E_1$, because that depends on the total charge in the system. Depending on how much 1-dimensional and 2-dimensional charge exists in the system, the position of $E_1$ will be different. The further $E_1$ is from $E_0$, the more is the 1-dimensional and less is the 2-dimensional charge for a given total charge. In our system investigated, we have a total 1-dimensional charge of $\sim 2 \times 10^{12}$ cm⁻² and total charge (1-D + 2-D) of $\sim 7.5 \times 10^{12}$ cm⁻² as obtained from C-V measurement. These charges will determine the position of sub-band $E_1$ relative to $E_0$. Of course, the total charge in the system will determine the position of Fermi Level ($E_F$) relative to $E_0$ (or to $E_1$, once $E_1$ is determined) at zero gate bias. The dependence of $E_F$ on gate bias also needs to be calculated at this point to estimate the relative position of $E_1$. To do this, we calculate the total electron density of the system as a function of Fermi level, which is simply given by $n_{\text{Total}}(E_F) = n_{1D}(E_F) + n_{2D}(E_F)$, where $n_{1D}$ and $n_{2D}$ are obtained from Eqs. (3) and (4), respectively. Dividing the total charge $Q_{\text{Total}}(E_F) = q(n_{1D} + n_{2D})$ by the zero-bias capacitance of the system gives the voltage shift needed to apply on the gate to achieve the given amount of charge. This voltage shift is required to be added to the pinch-off voltage to obtain the true gate bias corresponding to any given charge and hence the Fermi level. The normalized zero-bias capacitance is given by the ratio of the di-electric constant of GaN ($= 8.9$) and the separation between gate and the electron gas (which is $\sim 30$ nm in this case). For a total charge of $\sim 7.5 \times 10^{12}$ cm⁻² in our system, we found that a position of $E_F$ approximately $\sim 0.18$ eV above $E_0$, is consistent with the total charge at zero gate bias. Subsequently, a position of $E_1$ $\sim 0.09$ eV above $E_0$ gives a reasonably accurate value of pure 1-dimensional charge close to $\sim 2 \times 10^{12}$ cm⁻² which we observe experimentally. Thus, the positions of $E_1$ and $E_F$ relative to $E_0$ are purely dependent on the system under investigation and hence behave like fitting parameters.

It is noteworthy that while the 1-D density of states has an inverse dependence on $\sqrt{E}$, the 2-D density of states is a step function and hence has no dependence on energy. This implies that at higher energies, 1-dimensional electrons have a decreasing number of states of energy available for occupation while for 2-D electrons, energy level is immaterial since its density of states is a step function of a particular sub-band. This fundamental difference in the dependence of 1-D and 2-D density of states on energy is clearly observable in Fig. 4 which shows the theoretically calculated variation of both 1-D and 2-D electron densities as the gate bias is increased. While 1-D electron density tends to increase very slowly at higher energies, 2-D electron density continues to increase sharply at higher energy. The experimentally obtained values for the same as extracted from Eq. (2) and preceding discussions are also plotted in the Fig. 4.
It is interesting to note that till the Fermi level reaches the sub-band $E_1$, the total electron density in the system is mostly contributed by purely 1-D electrons (occupying sub-band $E_0$). As the Fermi level rises past $E_1$, the contribution from 2-D electrons starts to dominate as (1-D) electrons occupying $E_0$ have a decreasing availability of energy states on account of the $1/\sqrt{E}$ dependence of the 1-D density of states.

Two important observations are, firstly the theoretical and experimental values for both 1D and 2D electrons match up excellently, both in their bias-dependent behavior and in the...
magnitudes. This proves the 1-dimensionality of the electrons existing in the system at room temperature besides providing a concrete proof to our 2-sub-band model. Secondly, depending on the position of the Fermi level, 1-D and 2-D electrons co-exist in the system. While for $E_F > E_1$, transport is purely due to 2-D electrons in direction perpendicular to atomic terraces, for $E_F < E_1$, transport is purely due to 1-D electrons in direction parallel to atomic step. This system therefore enables direct electrostatic tuning of the dimensionality of electron gases and can provide an excellent platform to explore physics of low-dimensional systems even at room temperature.

C. Pure 1-D transport: Fermi Level engineering

To demonstrate pure 1-D transport in our system, we are required to reduce the total charge and thus ‘push’ the Fermi Level below $E_1$ sub-band so that only $E_0$ sub-band can contribute to transport. This can be achieved by etching the active layer (GaN) to some critical depth. Since it is not feasible to experimentally obtain the absolute position of $E_F$ with respect to $E_n$, we performed an etch-and-measure study. The region between two adjacent Ohmic pads was etched in steps of 15-30 s and the current between adjacent Ohmic contacts was measured after every etch step. For this, an additional level of lithography was performed where photo-resist was exposed and developed to open a part of the spacing between two such adjacent pads. Thus, on exposing the sample to ICP-RIE chamber with standard plasma-etch recipe, only the region opened by photo-resist between two adjacent Ohmic pads would be etched.

The epitaxial structure for the as-grown N-polar GaN/AlN/AlGaN/GaN heterostructure was shown in Fig. 2(a). Since AlN in our structure is less than 1 nm and its primary purpose being to enhance the mobility, it can be ignored for simplicity in explanation. Hence, it is not shown in Fig. 5(a), where we only consider a simple N-polar GaN/AlGaN/GaN heterostructure. The schematic of its energy band diagram along the red-dotted line (indicated in the structure) is shown to its right. Current is measured on such structures between adjacent Ohmic contacts source (S) and drain (D). However, if we etch the active region between them (as shown in Fig. 5(b)) to reduce the thickness of the GaN channel layer, the vertical electric field in it increases as shown in the energy band diagram to its right (due to constant Fermi pinning of the surface). This lowers the charge existing at the top interface of GaN and AlGaN.

To investigate dependence of current levels in the two directions on etch depth, a controlled etch recipe which gives an etch rate of $\sim$6 nm/min for N-face GaN was used to etch the sample in steps of 15-30 s. As the top GaN thickness starts to decrease with increasing etch time leading to a decreasing charge (in both directions), we would expect to measure a decreasing current level between two pads for the same applied bias. Since the exact epitaxial structure used in this study had a 5 nm SiNx passivation layer and a 2 nm Al$_{0.2}$Ga$_{0.8}$N on top of the active GaN channel layer, the etching would initially result in a ‘dead’ time in which the SiNx and Al$_{0.6}$Ga$_{0.4}$N would be etched without any appreciable effect on the current levels (Figs. 6(a)–6(c)). After 6 mins of total etch time as shown in Fig. 6(d), current in the direction perpendicular to atomic terraces starts to drop significantly although that in the parallel direction stays nearly the same. With further etching, the current in both directions starts to decrease (Fig. 6(e)), indicating a gradual lowering of the charge as expected. At a critical etch depth corresponding to a total etch time of 6 mins and 45 s when the Fermi level has been ‘pushed’ below $E_1$ but above $E_0$ as shown in Fig. 7(a), we observe current up to 130 mA/mm in the parallel direction but negligible current in the direction perpendicular to atomic terraces (Fig. 7(b)) implying achieving a 1-dimensional condition. This observation of 1-D transport is consistent and repeatable for Ohmic contacts separated by various spacing levels (6 μm to 22 μm) and across various regions of the sample. To our knowledge, this is the first demonstration of 1-D transport without lithographically synthesized, designed or fabricated nanowire structures.

IV. SUMMARY AND CONCLUSION

We demonstrated the co-existence of 1-D and 2-D electron gases in a polarization-engineered vicinal AlGaN/GaN hetero-structure system. We also showed that C-V profiling can be used as a tool to probe as well as to tune the dimensionality of electron gas between 1-D and 2-D. We proposed a two sub-band model to explain the dimensionality-dependence of electron gases on Fermi level position which we verified with experimentally measured data. Finally, using our model, we engineered the Fermi Level to show clear and sharp signatures of pure 1-D transport (parallel to atomic terraces) at room temperature. Each atomic terrace, characteristic of the vicinal substrate, defines one 1-D channel at the GaN/AlGaN interface when transport is considered parallel to the terraces. The terrace width and hence channel dimension ($\sim$10-20 nm) is defined by the miscut angle of the
vicinal substrate and these 1-D channels are not lithographically, but electrostatically defined. Since our approach using this novel system enables us to achieve self-defined, regularly-spaced dense arrays of 1-D channels of electrons, it holds lot of promise for practical electronic and optical device applications and to provide a unique platform to probe low-dimensional systems.