Gate Leakage Suppression and Contact Engineering in Nitride Heterostructures

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We present a self-consistent approach to examine current flow in a general metal-polar heterostructure junction. The approach is applied to examine properties of two classes of junctions that are important in devices: (i) GaN/AlGaN/high-κ insulator structures for potential applications in very small gate devices to suppress gate tunneling current; (ii) GaN/AlGaN/$LiNbO_3$ junctions for both n-type and p-type semiconductors with practical application for low source resistance regions. The physical parameters used for high-κ dielectrics and polarization charges reflect values typically found in ferroelectric materials. Our studies indicate that tailoring of junction properties is possible if polar oxides as thin as ~ 20Å can be achieved.

I. INTRODUCTION

GaN/AlGaN heterostructure field effect transistors (HFETs) have attracted considerable interest owing to their potential use in high power, high voltage and high temperature, electronic and optoelectronic devices[1, 2]. The nitride based structures are different from other semiconductor heterostructures since there is a large spontaneous polarization in the nitrides[3, 4]. Additionally, the piezoelectric effect is also very strong. As a result, there is a strong fixed polarization charge at the heterointerface[5], which can introduce very large electric fields ($\sim 10^6$ V$\cdot$ cm^{-1}) and band bending, and induce a two dimensional electron gas (2DEG) ($\sim 10^{13}$ cm^{-2}) in the heterostructure interface grown on Ga-faced structures. For N-faced grown designs, a two dimensional hole gas (2DHG) can also be induced. Advances in nitride heterostructure technology have attracted careful studies into junction properties of metal-polar heterostructure combinations where dopants are replaced by built-in polar fixed charges. Very large band bending caused by interface fixed charges permits the tailoring of the current-voltage ($I-V$) relations[6] by simply controlling the AlGaN layer thickness. It is important to develop a theoretical model that can predict the $I-V$ relationship in a general metal-polar heterostructure system.

In this paper, we will present such a model and apply it to two classes of junctions that are important for device technologies: (i) A GaN/AlGaN/high-κ dielectric insulator junction. We examine if such junctions can reduce gate tunneling without significantly influencing gate control of the channel; (ii) A GaN/AlGaN/$LiNbO_3$ (or other similar polar materials) junction for application in very low resistance junctions. We will examine both n-type and p-type junctions. Such junctions could be useful as tunneling junctions or as junctions for very low source resistance in HFETs.

In a previous work[6], we have demonstrated how the polar charge and the resultant band bending can affect tunneling probabilities and $I-V$ relations in a metal heterostructure junction. In order to apply that model to more involved cases, we need to determine the current flow inside the entire device, which can be expressed by the drift-diffusion current model, as well as effects arising out of hysteresis exhibited by ferroelectric materials[7]. The

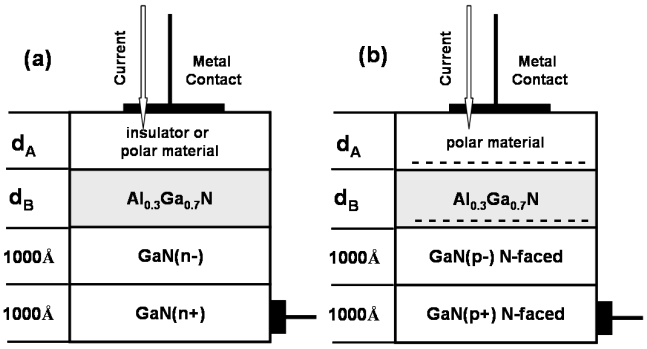

FIG. 1: (a) A schematic of the n-type structures considered is shown; (b) A schematic of the p-type structures considered is shown.

drift-diffusion current model has been applied to numerical simulation for many decades [8, 9]. Very early work[8] first used the drift-diffusion model in numerical simulation on bipolar junction transistors (BJTs).

In this work, the tunneling current was considered as the dominant factor in the current at the heterointerface. The drift-diffusion current model was then included in our charge control model to simulate the current flow in bulk region. It addresses charge control as well as transport through tunneling and drift diffusion. With this model, we examine the $I-V$ characteristics and sheet charge density. In Sec. (II), we will discuss the formalism that constitutes the theoretical basis of this work. Results are presented in Sec. (III). We conclude in Sec. (IV).

II. FORMALISM

In this section, we provide the formalism for the drift diffusion charge control model. To develop the model, we need several steps :(i) Solution of Poisson and Schrödinger equations to get the band profiles[10, 11], (ii) Use of the drift-diffusion current model to get quasi-fermi levels, and (iii) Set the tunneling current to be the boundary condition of drift-diffusion current model.

The quasi-fermi levels are then fed back into Poisson equation until the solution goes to convergence. The detail formalism for solving the Poisson and Schrödinger equation can be found in [10]. Once the current was injected into the channel region, the Fermi level splits into two different quasi-fermi levels. In order to accurately calculate the charge density inside the device, we need to use the drift-diffusion model to calculate the quasi-fermi levels in the heterostructure. In the bulk region, excluding the heterojunction interface, the current equation can be expressed by the drift-diffusion equations :

$$J_n = -\mu_n n(z)\frac{\partial E_c}{\partial z} + qD_n\frac{\partial n(z)}{\partial z} \quad (1)$$

$$J_p = \mu_p p(z)\frac{\partial E_v}{\partial z} - qD_p\frac{\partial p(z)}{\partial z}, \quad (2)$$

where μ_n and μ_p are the mobilities of the electrons and holes, and D_n and D_p are the

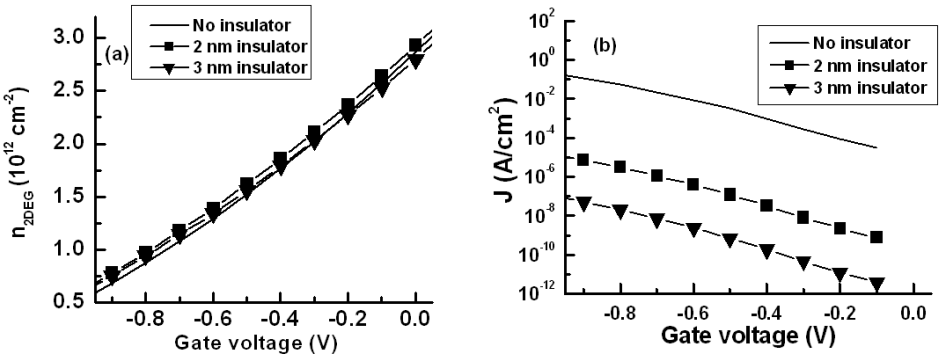

FIG. 2: $I-V$ characteristics and sheet charge densities for the device structure incorporating the insulator. The thickness of the $Al_{0.3}Ga_{0.7}N$ is taken to be 70 Å. Insulator parameters chosen : dielectric constant $\kappa = 29$, band gap, $E_g = 3.74$ eV and Schottky barrier height, $\phi_{SB} = 1.15$ eV.

diffusion coefficients of electrons and holes. Using the continuity equation,

$$\frac{\partial J_n}{\partial z} = qR, \quad \frac{\partial J_p}{\partial z} = -qR, \tag{3}$$

where R represents the Schottky-Read-Hall rate. The detail formalism can be found in [12]. As mentioned earlier, we use the Wentzel-Kramer-Brillouin (WKB) approximation to obtain the tunneling probability of the barrier from the metal to the channel region[6].

Once the tunneling current is obtained, we use it at the metal - semiconductor interface. Eqs (1) and (2) are then solved for the quasi-fermi level used in the self-consistent loop.

III. RESULTS

In Fig. 1, we show a generic structure in which either an insulator with high-κ or a polar material (we use the parameter for $LiNbO_3$) with high fixed polarization is incorporated in a $GaN/Al_{0.3}Ga_{0.7}N$ structure. In Fig. 1(a), we show a case where the nitride grown in Ga-faced while for Fig. 1(b), the growth is assumed to N-faced. As a result, in Fig. 1(a) there is an electron gas formed at the AlGaN/GaN interface while for Fig.1(b) a hole gas is formed. A fixed polar charge density, 1.68×10^{13} cm^{-2}, exists at the heterointerface between AlGaN and GaN due to the spontaneous polarization and piezoelectric effect. The GaN (n-) layer is assumed to be doped at 2×10^{16} cm^{-3}, and the GaN (n+) layer is doped at 5×10^{16} cm^{-3}. The doping values are chosen to be quite low to illustrate the ability of polar layers to create ohmic behaviors. The thicknesses of both layers are 1000Å. A fixed polar charge density, 1.68×10^{13} cm^{-2} and -1.68×10^{13} cm^{-2}, exists at the heterointerface between AlGaN and GaN for Ga-faced and N-faced cases,respectively. The GaN (p-) layer is doped at 5×10^{17} cm^{-3}, and the GaN (n+) layer is doped at 1×10^{18} cm^{-3}. The thicknesses of both layers are 1000Å. Our first simulations address the issue to gate tunneling suppression. It is well known that one way to reduce gate tunneling in FETs is to add a high dielectric constant region between the gate and the channel[13]. Such approaches have been successfully demonstrated in Si MOSFET where $BaTiO_3$ has been added. In Fig. 2(a), we show results of calculation for structures where a material with $E_g = 3.74$ eV and $\kappa = 29\epsilon_0$ has been added between the metal and AlGaN. The high-κ material is assumed to be non-polar. Our results indicate

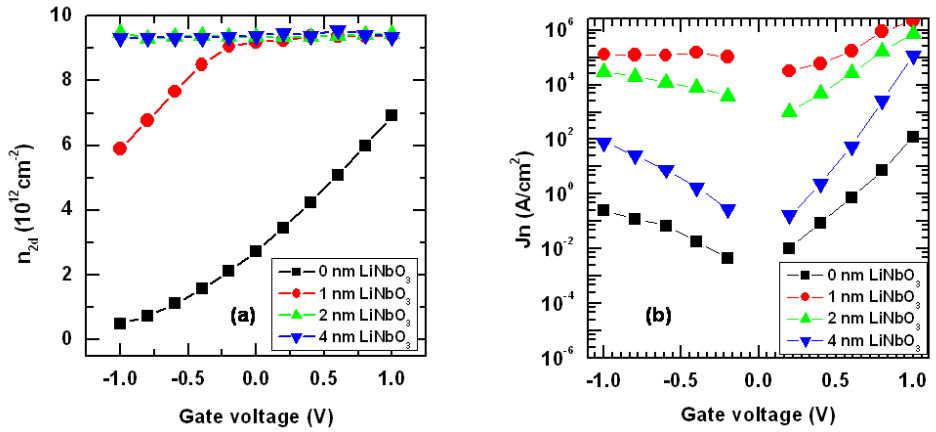

FIG. 3: (a) Dependence of $I-V$ characteristics and sheet charge densities on thickness, d_A, of the polar layer. The barrier thickness of $Al_{0.3}Ga_{0.7}N$ is 50 Å. The dielectric constant, band gap, and Schottky barrier height are 29 ϵ_0, 4.0 eV, and 1.2 eV, respectively.

that 2DEG sheet charge density is relatively insensitive to increase in insulator thickness. However, tunneling current is reduced at least by a factor of 10^4 with introduction of an insulator layer of thickness, $d_A = 30$Å. Thus, a high-κ insulator layer can be used to decouple the relationship between barrier layer thickness and 2DEG sheet charge density.

It is also worthwhile to note that the gate control of channel properties of a FET described above (such as transconductance, g_m) is relatively unaffected due to the high capacitance of the polar layer. Consider the structure to be composed of two capacitors in series. The capacitance of gate ,C_g, would be similar to the capacitance of a similar FET structure, C_B, without additional polar or insulator layer because $C_g = C_A C_B/(C_A + C_B) \approx C_B$. where C_A is the capacitance of either the polar or the insulator layer. This makes it amply clear that the introduction of the polar or insulator layer does not affect the transconductance, which is still adequately described by the relation, $g_m = C_g v_{sat} \approx C_B v_{sat}$, which may be seen to be the same transconductance as that of a structure without either a polar or an insulator layer(v_{sat} is the saturation velocity of the carriers in FET channel region). Since g_m is the main figure of merit in description of FETs, its apparent that characteristics of circuits employing the proposed structure would not be affected much.

Our next set of results focuses on how a polar oxide can be exploited to increase the tunneling current to create low resistance contacts or tailorable $I-V$ characteristics. It is well known that in semiconductor technology, one way to convert a rectifying contact into an ohmic contact is to heavily dope the semiconductor in the region of the contact. Another way to achieve the same result is to use polar materials[11] in the region of the contact. In the nitride system, the interfacial polar charge results from spontaneous polarization and piezoelectric effect, which cannot be altered once the crystal is grown. In ferroelectrics like $LiNbO_3$, $SrTiO_3$, etc., polarization values can be much larger than what is possible in nitrides and can also be controlled by external fields. Ferroelectrics have been grown on nitrides and other semiconductors although their junction properties have not been reported. We examine the $I-V$ characteristics of a structure where a thin layer of $LiNbO_3$ with $\sigma = +2.84 \times 10^{14}$ cm^{-2} is present between a metal and the AlGaN/GaN structure. Results are shown in Fig. 3. As we can see, a very strong band bending can be induced, which leads to a very high tunneling current. In absence of "gate" bias, the barrier becomes very thin and

the tunneling current density is increased by a factor of nearly 10^5 (in either bias condition) when compared to the case without any polar layer. Increase in the polar material's thickness initially increases the tunneling current and the 2DEG sheet charge density. It can be seen that the positive polar charges at the AlGaN/polar material heterointerface lead to higher band bending when d_A increases from 0 Åto 20 Å. However, when the thickness d_A is over 20 Å, the induced 2DEG charge at the AlGaN/polar material heterointerface starts to annul the band bending. Then the barrier thickness, $d_A + d_B$, dominates the tunneling probability. Hence, there exists an optimal thickness ($\simeq 20$Å) that corresponds to the highest tunneling current. Therefore, adding a polar material layer basically forms the ohmic junction without heavy doping, traditionally difficult to obtain in large band gap materials [14–16].

For p-type nitride based materials, it is even harder to form an ohmic contact due to its large Schottky barrier height and difficulty in achieving for heavy doping. One way to overcome this problem is to use with high metal work function materials. However, it is hard to find a suitable metal. Therefore, by adding a polar material to enhance the valence band bending would be a choice to form an ohmic contact. It is well known that for ferroelectric materials, we can easily reverse the polarization by applying electrical field. Figure 4 shows the $I - V$ characteristic of p-type Ga-faced and N-faced with different $LiNbO_3$ layer thickness. It is known that Ga-faced nitride based materials would have higher mobility in the channel region. However, it also introduces a fixed positive polar charge at the GaN/AlGaN heterostructure interface which basically form a large barrier height for the hole current. Figure 4(a) shows that by adding a $LiNbO_3$ layer, we can significantly increase the tunneling current, and we can get an optimal thickness of 30 Åfor this cases. However, by comparing the the n-type Ga-faced GaN/AlGaN devices, the current density is still relatively lower. unlike Ga-faced nitride based materials, N-faced nitride based materials has a large fixed negative polar charge at the AlGaN/GaN heterostructure interface, which enhances the band bending of the valence band. Figure 4(b) shows the results of N-faced GaN devices. It is shown that the current density increases a factor of 100 compared to the Ga-faced GaN devices. An optimal $LiNbO_3$ layer thickness of 20 Åis obtained in this case. It is shown that by adding a polar material for p-type nitride based materials, one can be more easily to form an ohmic contact, which would be very useful to design optoelectronic devices.

IV. CONCLUSIONS

In this work, we have examined vertical transport in GaN/AlGaN/insulator, and GaN/AlGaN/$LiNbO_3$ polar material junctions. Introduction of the insulator layer shows that we can significantly reduce the tunneling current density without affecting the sheet charge density or changing the circuit characteristics of the device significantly. This is of use in designing low gate leakage structures in the gate region of HEMT's without affecting sheet charge density or transconductance in the channel region.

We have examined use of a strongly polar layer, which can allow the formation of ohmic junctions. Also we have found that there exists an optimal thickness of the polar material that yields the highest possible tunneling current. This is likely to be of considerable use in design of low resistance contacts. Further, the direction of the polarization in the polar material can be changed at growth time by using poling. This can be used to form self-insulating regions and suggests a new growth method by using laterally varying electric fields during crystal growth. This work was supported by grant F004815 and F001681 from the

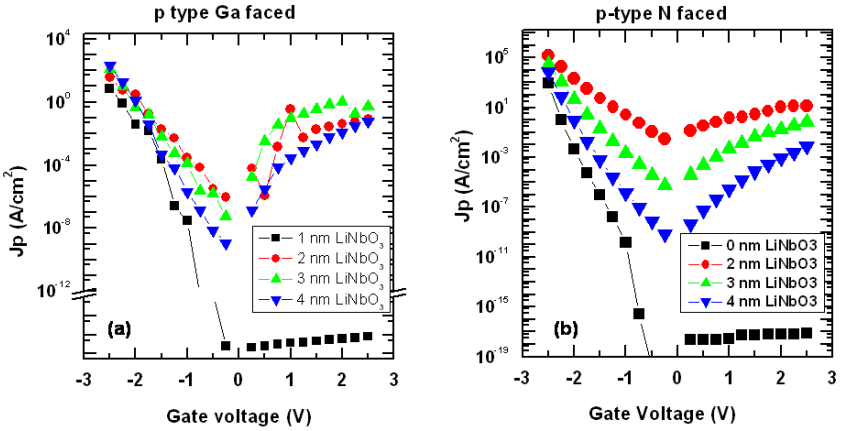

FIG. 4: (a) Dependence of $I-V$ characteristics on thickness, d_A, of the polar layer for the p-type N-faced nitride based devices; (b) Dependence of $I-V$ characteristics on thickness, d_A, of the polar layer for the p-type Ga-faced nitride based devices. The barrier thickness of $Al_{0.3}Ga_{0.7}N$ is 50 Å.

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