Available online at www.sciencedirect.com
SCIENCE DIRECT®
Solid-State Electronics 47 (2003) 2155–2159
SOLID-STATE ELECTRONICS
www.elsevier.com/locate/sse

Examination of $LiNbO_3$/nitride heterostructures

Madhusudan Singh *, Yuh-Renn Wu, Jasprit Singh

Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, MI 48109, USA

Received 15 October 2002; accepted 2 January 2003

Abstract

Oxides such as $LiNbO_3$, $PbTiO_3$, etc. have large polarization effects arising from the ferroelectric and piezoelectric effects. Recent work on nitride heterostructures has shown that polar charge can be used to substitute for dopant charge and controlled to create a two-dimensional electron (and hole) gas, resulting in ohmic contacts and diode like current–voltage characteristics. In this paper, we examine the potential of using ferroelectrics with traditional semiconductors for applications in novel electronic devices. In particular, we examine their use in creating very high sheet charge densities of mobile charge and tailorable current–voltage characteristics. It is seen that owing to hysteresis based effects in the ferroelectric layer, the direction of variation of voltage has a marked effect on the charge induced as well as the variation of that charge with voltage.

Keywords: Ferroelectrics; Hysteresis; Piezoelectric charge; Spontaneous polarization; Hybrid $LiNbO_3$–nitride devices

1. Introduction

The ability to fabricate high quality semiconductor heterostructures has revolutionized semiconductor device technology. Quantum well lasers, modulation doped field effect transistors, etc. have been made possible by heterostructures. Traditional semiconductor heterostructures have no polarization except for strained structures such as InGaAs/GaAs grown along (1 1 1) orientation. Nitride heterostructure are being actively studied for applications in blue light emission and high power microwave devices. It is now known that for (0 0 0 1) growth, there are strong spontaneous and piezoelectric related polarization effects at nitride interfaces. As a result of interface fixed charge, two interesting effects occur: (1) In structures like AlGaN/GaN, a large two-dimensional electron (and hole) gas can be induced. This mobile charge can be used to design undoped heterostructure FETs. (2) Polar charge causes a strong band bending in InGaN/GaN quantum wells used for blue light emission. This strong band bending reduces the electron–hole overlap and thus negatively impacts device performance.

In nitride heterostructures, the polarization values are determined by material compositions and strain, and cannot be altered once the structure is fabricated.

In ferroelectric materials, it is known that the value of polarization can be altered and in particular, the spontaneous polarization can be switched by poling. If ferroelectric semiconductor junctions are fabricated will there be novel physical effects that can then be exploited for device design? This paper will attempt to address this issue. Since ferroelectric semiconductor heterostructure junctions are in their infancy, there are many unknown parameters. This study will provide guidance on some improvement. We will examine the following issues:

(1) Can ferroelectric layers be used to induce band bending and free carrier density in semiconductors?
(2) Are there interesting junction transport characteristics that can be exploited for non-linear devices?

* Corresponding author. Tel.: +1-734-763-6466; fax: +1-734-763-9324.
E-mail address: chhabra@eecs.umich.edu (M. Singh).

0038-1101/$ - see front matter © 2003 Elsevier Ltd. All rights reserved.
doi:10.1016/S0038-1101(03)00189-8

2. Formalism

There are two sources of polar charge at the heterointerfaces of nitride heterostructures. The strain due to coherent epitaxy (below critical thickness) results in piezoelectric effect induced charge. In addition, the shift in the cation and anion sub-lattices in the grown crystal leads to spontaneous polarization [2,3]. The magnitude and direction of the electric fields associated with spontaneous polarization and piezoelectric effect depend on the substrate, the growth orientation and the nature of the surface (cation terminated or anion terminated). For the results given here we will assume the most common growth conditions employed for the nitride systems where growth is on sapphire and is along the (0 0 0 1) direction with Ga terminated surface. The effective substrate is defined by the a thick buffer that is grown on the starting substrate (sapphire). Once dislocations are generated the thick buffer forms its own lattice and acts as a substrate for the next layers as long as the growth is coherent i.e., buffer thickness is small enough to generate no dislocations.

The direction of polarization for ferroelectrics depends upon the direction of poling. Further, its magnitude depends upon the degree of domain formation and thickness [4]. The formalism that we have developed is quite generic and can be applied to a variety of heterostructures. However, for the purposes of this study, we consider $LiNbO_3$/nitride heterostructures. We assume that for the thicknesses of $LiNbO_3$ considered, the spontaneous polarization is close to its maximum value. $LiNbO_3$ has an extremely high spontaneous polarization charge density. The spontaneous polarization charge density for AlN is $\sim$0.081 cm^{-2}. The corresponding value for $LiNbO_3$ is $\sim$0.5 cm^{-2}. Further, the lattice mismatch between nitrides and $LiNbO_3$ is extremely large. This means that the charge contribution due to strain would be absent as the nominal critical thickness for an over-layer is extremely low and the interface is relaxed. Hence, we neglect the additional charge contribution due to piezoelectric effect for $LiNbO_3$ interfaces.

The origin of large amount of polar charge in nitride heterostructures has been discussed earlier [2,3,5]. In the case of $LiNbO_3$, the value of many parameters is less certain.

2.1. Charge control and hysteresis

In the self-consistent approach [1,5], we solve Schrödinger and Poisson equations. This provides us the sub-band levels, their occupation and wavefunctions. Hysteresis effects are included in this treatment by introducing a field dependent correction of the charge at the interface between the ferroelectric and the nitride layers:

$$P^{+}_{\mathrm{sat}}(E) = P_s \tanh\left[\frac{E - E_c}{2\delta}\right] \tag{1}$$

$$P^{-}_{\mathrm{sat}}(E) = P_s \tanh\left[\frac{-E - E_c}{2\delta}\right] \tag{2}$$

$$\delta = E_c \Big/ \ln\left(\frac{1 + P_r/P_s}{1 - P_r/P_s}\right) \tag{3}$$

where the $\pm$ signs refer to the direction of the sweep. P_s and E_c are material parameters [6], as is the remnant polarization ratio, P_r/P_s.

2.2. Tunneling calculation

Once the band profile is known, we use the WKB method to obtain the tunneling probability [1] from the metal to the GaN channel. To obtain the tunneling current [7], we consider the density of states in the GaN substrate. The density of states can be divided into two regimes:

(1) *Within the region of quantum confinement.* The corresponding current density J_{2D} is defined in Eq. (5).
(2) *At energies greater than confinement energy.* The corresponding current density J_{3D} is defined in Eq. (6). Thermionic emission is accounted for by extending the range of energies above the heights of relevant barriers.

The metal contact is considered to be an infinite source of electrons. The expression for the tunneling current is:

$$J_{\mathrm{tunnel}} = J_{2D} + J_{3D} \tag{4}$$

$$\begin{aligned} J_{2D} = q \sum_{n=1}^{n=n_{2D}} & \frac{v(E_n, E_f) D_{2D}(E_n)}{L_n} \\ & \times \int_0^{\infty} (f(E_n + E_t, E_{fs}, T) - f(E_n + E_t, E_{fm}, T)) \\ & \times T(E_n, E_t)\, \mathrm{d}E_t \end{aligned} \tag{5}$$

$$\begin{aligned} J_{3D} = q \int_{E_{n_{2D}}}^{\infty} \int_0^{\infty} & v(E_l, E_f) D_{1D}(E_l) D_{2D}(E_t) \\ & \times (f(E_n + E_t, E_{fs}, T) - f(E_n + E_t, E_{fm}, T)) \\ & \times T(E_l, E_t)\, \mathrm{d}E_t\, \mathrm{d}E_l \end{aligned} \tag{6}$$

where n_{2D} is the total number of bound levels in the 2DEG. E_f is given by,

$$E_f = \min(E_{fs}, E_{fm}) \tag{7}$$

The velocity of carriers in the above equations is a function of E_n and E_l in addition to E_f defined above. Thus, the velocity is a function of the final energies over which the expressions are being summed or integrated.

E_f is defined this way to ensure correct integration ranges for the carrier current.

3. Results

In nitride heterostructures, we have shown [7] that the very high strong band bending caused by polar charge at interfaces allows one to design tailorable diodes where current primarily flows by tunneling. Depending upon the choice of thickness used for the barrier region, one can tailor the turn on voltage, the reverse breakdown voltage and even design the very low resistivity ohmic contacts. In this study, we choose a few representative cases to illustrate the behaviour expected from ferroelectric semiconductor junctions.

We have examined two types of structures. In the first category, we consider some metal/AlN/$LiNbO_3$/GaN layered structures. In the second, we consider a metal/AlGaN/$LiNbO_3$/AlGaN/GaN structure. The first category is more interesting from the point of view of junction transport while the second category is more interesting for very high sheet conductivity channels. For the purposes of this work, the term *forward sweep* refers to the lowering of the metal Fermi level with respect to the substrate Fermi level.

(1) *Diode like structures*: The structure is 15 Å AlN layer and 65 Å $LiNbO_3$ on a GaN substrate. The charge control results are shown in Fig. 1(a). The charge induced in the GaN layer shows interesting trends. In the *forward sweep*, the charge induced in GaN layer is insignificant, while in the *reverse sweep*, the charge is high and shows a variation of six orders of magnitude over the voltage range.

The current voltage results are shown in Fig. 1(b). The result here indicates a "reverse" sweep diode-like behaviour in the forward bias region of a diode with a relatively small turn on voltage ($\simeq$0.2 V). However, in the "forward" sweep, the current is severely suppressed owing to change in the band structure arising from effects of hysteresis. The ratio in the magnitudes of the currents is as high as 10^{30}. This kind of structure is ideal for switching devices that need to operating in only one direction, such as high power rectifiers. In a real structure, defect related transport would probably affect the low current regions and we would not expect to see such large ON/OFF ratios.

(2) *Undoped high sheet charge channels*: The structure selected is 50 Å AlN and 150 Å $LiNbO_3$ on a GaN substrate. The charge control results, shown in Fig. 2(a), indicate that the charge induced in the channel GaN region is nearly constant at $\simeq 5\times10^{13}$ cm^{-2} in the "reverse sweep", while in the opposite sweep, this charge falls to negligible levels. This indicates a device that can be switched off nearly completely in one direction of operation, while providing a high, nearly constant conductivity in the other direction.

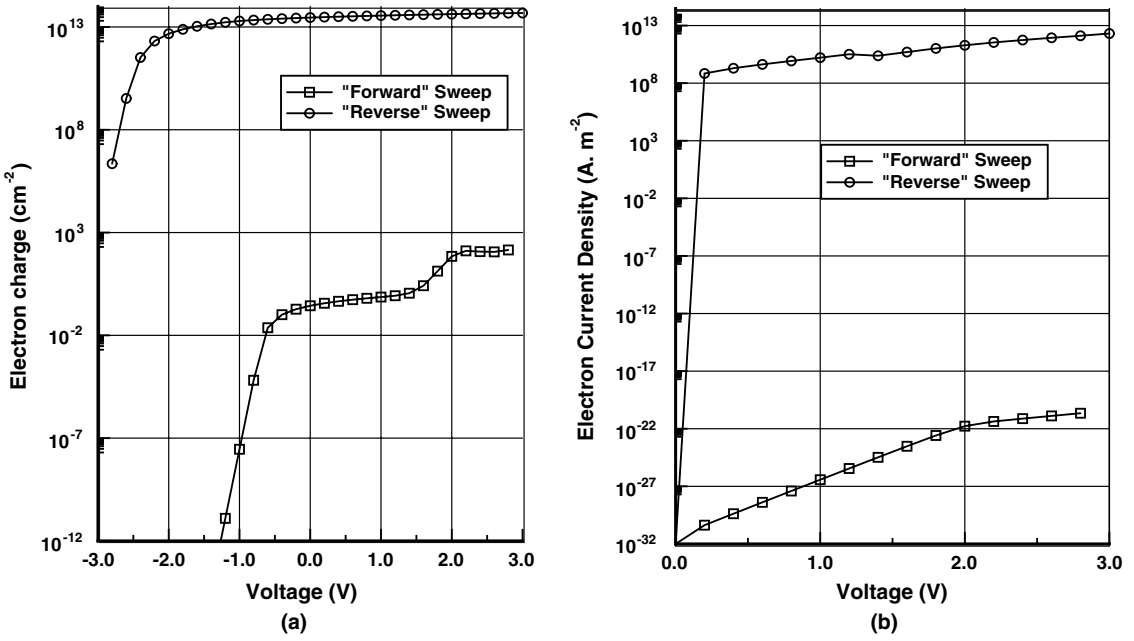

Fig. 1. (a) Charge control results for the diode structure. The charge shown is the electron charge in the GaN channel region of the device. In the "reverse" sweep, the charge induced is orders of magnitude higher than it is under the "forward" sweep. (b) Forward bias characteristics for the diode structure. The current almost completely shuts off in the "forward" sweep. In the "reverse" sweep, this current shows nearly classic diode behaviour.

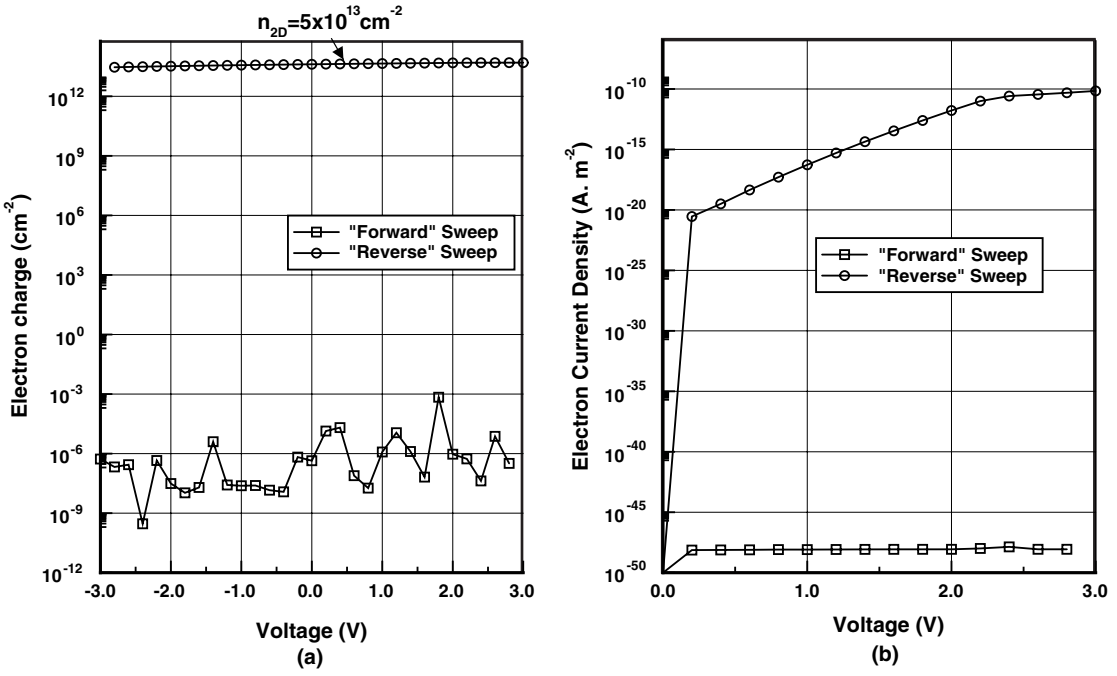

Fig. 2. (a) Charge control results for the undoped high sheet charge structure. The charge shown is the electron charge in the GaN region as before. The difference in the charge induced in the two sweeps is even greater than it is in Fig. 1. (b) Forward bias characteristics for the structure. In both sweeps, the vertical tunneling current is extremely low.

The current voltage results are shown in Fig. 2(b). In the "reverse" sweep, the charge in the $LiNbO_3$ is also substantial ($\simeq 2\times10^{13}$ cm^{-2}). However, this charge is not mobile. The result indicates a severe suppression of the vertical tunneling current under both conditions of operation due to the very low tunneling probability with large thicknesses.

In addition, we have also considered structures in which $LiNbO_3$ and GaN layers are separated by an AlGaN high barrier region. In particular, we find that for a structure consisting of metal–$Al_{0.3}Ga_{0.7}N$ (60 Å)/$LiNbO_3$ (120 Å)/$Al_{0.3}Ga_{0.7}N$ (20 Å)/GaN, we get two-dimensional charge densities of 1.3×10^{14}, 5.47×10^{13} and 1.36×10^{13} cm^2 in the $LiNbO_3$, AlGaN and GaN regions, respectively. Even if we assume that the charge in $LiNbO_3$ does not contribute to transport in the channel, such a channel would have an areal conductivity ($\sum n_i e\mu_i$) of 8×10^{-3} Ω^{-1}. This would be about a factor of 20 larger than what is possible in AlGaAs/GaAs system and a factor of $\simeq$2 higher that what is possible in the AlGaN/GaN system.

4. Discussion

From the results in Section 3, it is evident that some rather interesting structures can be designed by incorporating a ferroelectric material into a semiconductor heterostructure. These include junctions with tailorable I–V characteristics and very high conductivity channels.

It is important to note that there are a number of unknowns in our study. An important concern is the defect density in the ferroelectric region. The areal density of the defects can be estimated as, $n_{\text{defect}} \times d_{\text{ferroelectric}}$, where n_{defect} is the volume defect density and $d_{\text{ferroelectric}}$ is the layer thickness for the ferroelectric. We find that interesting effects occur when $d_{\text{ferroelectric}}$ is $\simeq$20–100 Å. This implies that n_{defect} should be lower than $\simeq10^{20}$ cm^{-3}, otherwise the mobile charge density may be overwhelmed by defect trapping.

Acknowledgements

Work at the University of Michigan has been supported by grants F001681 (the POLARIS program) and F000629 from the US Office of Naval Research.

References

[1] Singh M, Zhang Y, Singh J, Mishra U. Examination of tunnel junctions in the AlGaN/GaN system: consequences of polarization charge. Appl Phys Lett 2000;77(12):1867–9.
[2] Ambacher O, Smart J, Shealy JR, Weimann NG, Chu K, Murphy M, et al. Two-dimensional electron gases induced by spontaneous and piezoelectric polarization charges in

N- and Ga-face AlGaN/GaN heterostructures. J Appl Phys 1999;85:3222–33.

[3] Bernardini F, Fiorentini V, Vanderbilt D. Spontaneous polarization and piezoelectric constants of III–V nitrides. Phy Rev B 1997;56(16):10024–6.

[4] Zembilgotov AG, Pertsev NA, Kohlstedt H, Waser R. Ultrathin epitaxial ferroelectric films grown on compressive substrates: competition between the surface and strain effects. J Appl Phys 2002;91(4):2247–54.

[5] Zhang Y, Singh J. Charge control and mobility studies for an AlGaN/GaN high electron mobility transistor. J Appl Phys 1999;85(1):587–94.

[6] Kim S, Gopalan V, Gruverman A. Coercive fields in ferroelectrics: a case study in lithium niobate and lithium tantalate. Appl Phys Lett 2002;80(15):2740–2.

[7] Singh M, Singh J, Mishra U. Current–voltage characteristics of polar heterostructure junctions. J Appl Phys 2002; 91(5):2989–93.