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POLARIZATION INDUCED EFFECTS IN AlGaN/GaN HETEROSTRUCTURES

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Two-dimensional hole and electron gases in wurtzite GaN/$Al_xGa_{1-x}N$/GaN heterostructures areinduced by strong polarization induced effects. The sheet carrier concentration and the confinement of the two-dimensional carrier gases located close to one of the AlGaN/GaN interfaces are sensitive to a high number of different physical properties such as polarity, alloy composition, strain, thickness, and doping. We have investigated the structural quality, the carrier concentration profiles, and electrical transport properties by a combination of high resolution X-ray diffraction, Hall effect, and $C-V$ profiling measurements. The investigated heterostructures with N- and Ga-face polarity were grown by metalorganic vapor phase or plasma induced molecular beam epitaxy covering a broad range of alloy compositions and barrier thickness. By comparison of theoretical and experimental results we demonstrate that the formation of two-dimensional hole and electron gases in GaN/AlGaN/GaN heterostructures both rely on the difference of the polarization between the AlGaN and the GaN layer. In addition the role of polarity on the carrier accumulation at different interfaces in n- and p-doped heterostructures will be discussed in detail.

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1. Introduction

AlGaN/GaN polarization induced high electron mobility transistors (PI-HEMTs) have been a subject of intense recent investigations and have emerged as attractive candidates for high voltage, high power operation at microwave frequencies [1–3]. Recent investigations of these heterostructures have shown that two-dimensional electron gases forming the device channel are generated by positive polarization induced interface charges [4].

Kozodoy et al. [5] observed an enhancement of hole concentration by over five orders of magnitude in Mg-doped AlGaN/GaN superlattices compared to Mg:GaN films. The high sheet hole concentration of the superlattices demonstrated the pivotal role of polarization in determining the band structure of the heterostructure and the accumulation of holes with high sheet carrier concentration in the GaN

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wells [5]. In this paper we will focus on the formation of two-dimensional electron (2DEGs) and hole gases (2DHGs) in n-type and p-type doped GaN/AlGaN/GaN heterostructures. Conduction and valence band profiles are calculated in order to determine the carrier distribution and the formation of two-dimensional carrier gases at interfaces of heterostructures with N- and Ga-face polarity. The theoretical predictions for $Al_xGa_{1-x}N$/GaN based structures with different alloy composition of the barriers are compared to experimental results achieved by a combination of high resolution X-ray diffraction, Hall effect, and $C-V$ profiling measurements.

2. Spontaneous and piezoelectric polarization

Bernardini et al. predicted that spontaneous polarization P_{SP}, is present in wurtzite group III nitride crystals [6]. The calculated values of spontaneous polarization are large and increase from GaN to AlN. The sign of the spontaneous polarization is found to be negative assuming that the orientation of the negative polarization is defined by the direction from the nitrogen (anion) to the nearest neighbor metal atom (cation) along the c-axis.

The piezoelectric constants also increase from GaN to AlN, leading to a larger piezoelectric polarization, P_{PE}, of AlN compared to GaN for the same amount of strain. To discuss the carrier confinement in group III nitride based heterostructures, we will focus on GaN/AlGaN heterostructures grown pseudomorphically on the top of thick relaxed GaN buffer layers. In this special case $Al_xGa_{1-x}N$ barrier layers are under tensile strain and the piezoelectric and the spontaneous polarization are pointing in the same direction. Since the value of the negative spontaneous polarization and the tensile strain of the barrier become larger with increasing Al concentration, an increase in total polarization, P, has to be expected. To calculate the spontaneous and piezoelectric polarization of alloys we are using a linear interpolation between the spontaneous polarization, piezoelectric and elastic constants of the binary compounds discussed in more detail in Refs. [4, 7]. As a consequence of the higher value of polarization of AlGaN compared to GaN, at an abrupt AlGaN/GaN interface the gradient in polarization is causing a fixed polarization interface charge (Fig. 1) defined by

$$\begin{aligned}\sigma(\mathrm{AlGaN/GaN}) &= P(\mathrm{GaN}) - P(\mathrm{AlGaN}) \\ &= P_{SP}(\mathrm{GaN}) - [P_{SP}(\mathrm{AlGaN}) + P_{PE}(\mathrm{AlGaN})] = -\sigma(\mathrm{GaN/AlGaN}). \qquad (1)\end{aligned}$$

The value of the polarization induced sheet charge σ/e, versus Al-concentration of the barrier, x, can be approximated by

$$\frac{\sigma}{e}(x) = (6.41 \times 10^{13}\ \mathrm{cm}^{-2})x - (1.17 \times 10^{13}\ \mathrm{cm}^{-2})x(1-x). \qquad (2)$$

The sign of the bound interface charge in AlGaN/GaN heterostructures is determined by the polarity.

For crystals with Ga(Al)-face polarity one bilayer consists of a metal layer above the nitrogen layer (Fig. 1). As a consequence, the total polarization of AlGaN and GaN is pointing from the surface towards the sapphire substrate, the gradient in polarization at the interface becomes negative and the bound charge density — positive. If the polarity is flipped to N-face one bilayer consists of a nitrogen monolayer which is located above a metal monolayer. Therefore the orientation

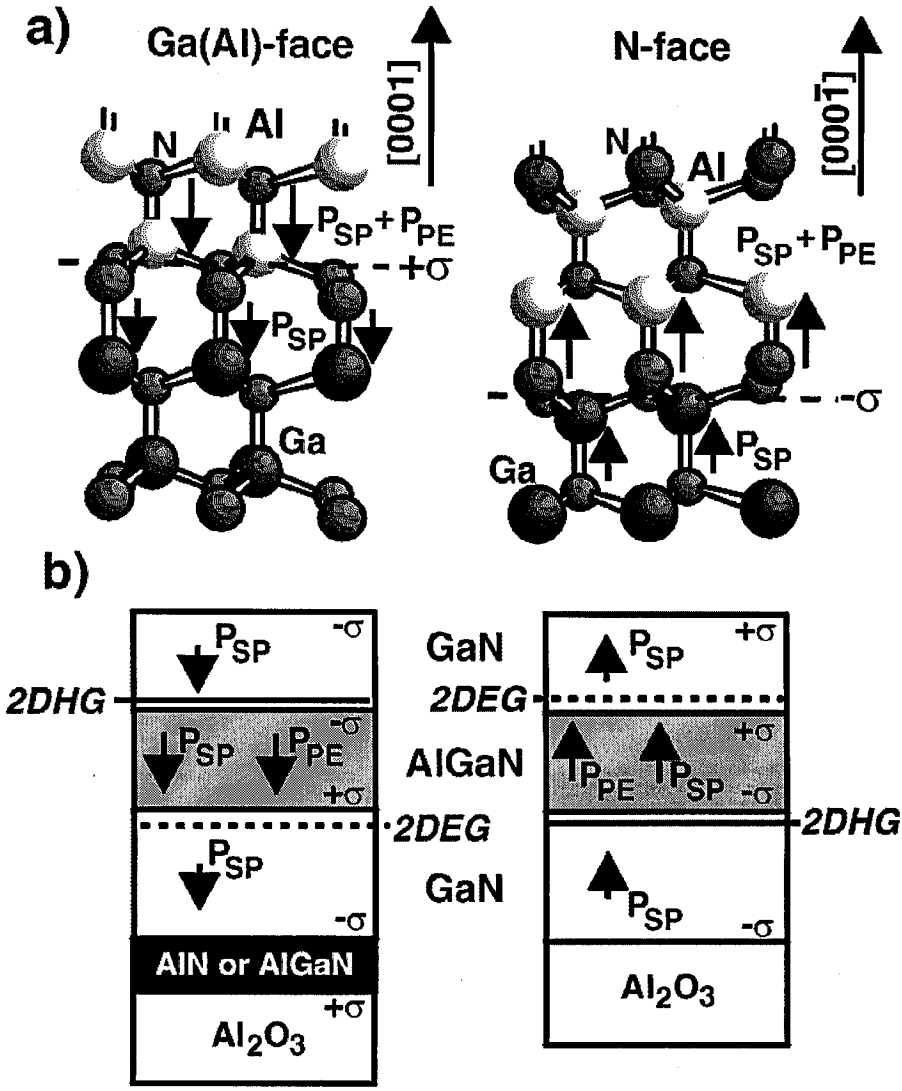

Fig. 1. (a) Spontaneous, piezoelectric polarization and polarization induced interface charges in Ga- and N-face AlGaN/GaN heterostructures. (b) Confinement of polarization induced 2DEGs (dashed lines) and 2DHGs (solid lines) in GaN/AlGaN/GaN heterostructures with Ga- or N-face polarity.

of polarization, the sign of the polarization gradient and of the interface charge are inverted. The positive polarization induced interface charge can be compensated by electrons leading to the formation of 2DEGs. In *n*-type Ga-face (N-face) GaN/AlGaN/GaN heterostructures the 2DEG is located at the lower (upper) AlGaN/GaN (GaN/AlGaN) interface. In analogy 2DHGs in *p*-type Ga-face (N-face)

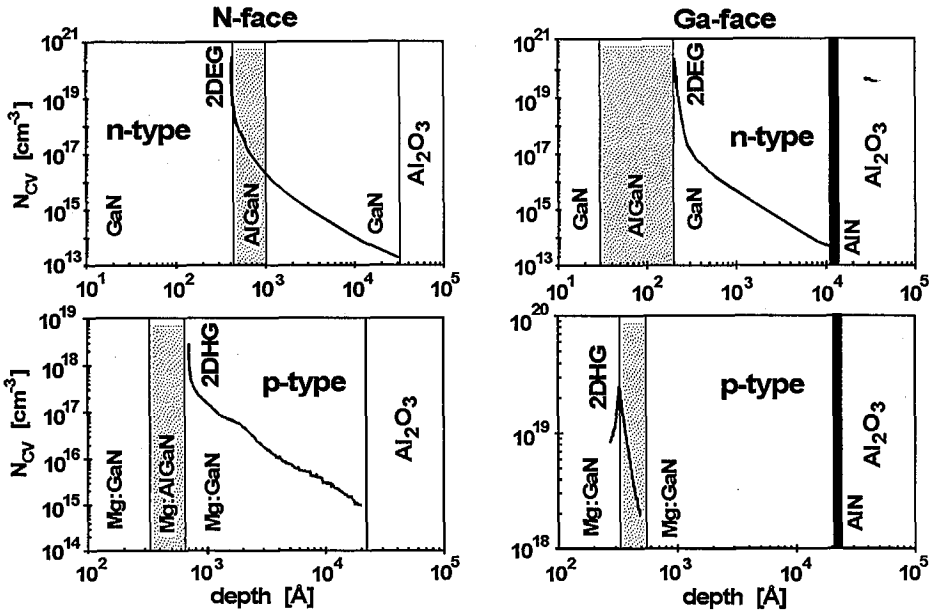

Fig. 2. Carrier concentration versus depth determined by $C-V$ profiling in n-type and p-type GaN/AlGaN/GaN heterostructures with N- or Ga-face polarity.

GaN/AlGaN/GaN heterostructures are located at the upper (lower) GaN/AlGaN (AlGaN/GaN) interface. To provide experimental evidence for these theoretical predictions we have deposited n- and p-type doped GaN/AlGaN/GaN heterostructures by plasma induced molecular beam epitaxy (PIMBE) [8]. Heterostructures with N-face and Ga(Al)-face polarity were realized by depositing on O-terminated and AlN covered sapphire substrates, respectively [9]. By a combination of Hall effect and $C-V$ profiling measurements, the interface at which the carriers are accumulated and the sign of the carriers were identified (Fig. 2). For n-type heterostructures with 30 nm thick $Al_{0.33}Ga_{0.67}N$ barriers as determined by X-ray diffraction, electron accumulation with sheet carrier concentrations of 1.1×10^{13} cm^{-2} was detected at the lower (upper) interface for Ga- (N-) face GaN/AlGaN/GaN heterostructues, respectively. The two-dimensional confinement of the confined electrons was determined by Shubnikov–de Haas measurements [8]. To provide holes for the formation of 2DHGs, p-type heterostructures were grown with Mg concentrations of 10^{16} and 5×10^{19} cm^{-3} incorporated into the GaN and AlGaN layer, respectively. Hole accumulation located at the lower (upper) interface of Ga- (N-)face heterostructures with sheet carrier concentrations of 0.4×10^{13} cm^{-2} (2.0×10^{13} cm^{-2}) was observed in agreement with our predictions (Fig. 2).

3. Sheet carrier concentrations of 2DEGs and 2DHGs

Based on a theoretical understanding of the polarization induced charge we now wish to attempt the sheet carrier concentration of two-dimensional carrier gases and its dependence on alloy composition for pseudomorphic AlGaN/GaN heterostructures.

To enable the determination of the sheet carrier concentration and carrier distribution profile in modulation doped AlGaN/GaN structures including spon-

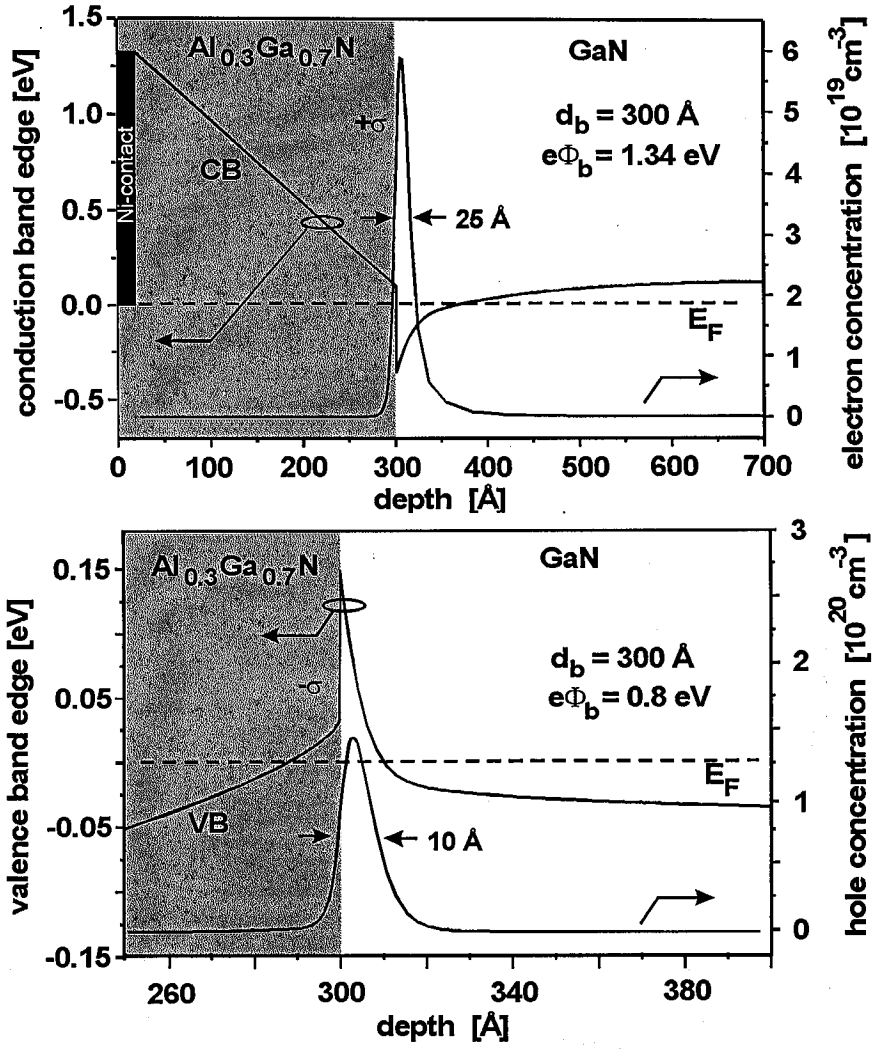

Fig. 3. Carrier concentration profiles and band edges for n-type Ga- and p-type N-face $Ni/Al_{0.3}Ga_{0.7}N/GaN$ (30/30/2000 nm) heterostructures. A 2DEG and a 2DHG with sheet carrier concentrations above 10^{13} cm^{-3} are predicted for Ga- and N-face heterostructures, respectively.

taneous and piezoelectric polarization induced bound sheet charges as well as the splitting of the valence band maximum due to crystal field and spin–orbit coupling, we have used a modified one-dimensional Schrödinger–Poisson solver [10]. To specify the boundary conditions at the surface and substrate interfaces we have assumed a Ni-Schottky contact with a known barrier at the sample surface. At the interface towards the substrate, the Fermi level was fixed in the middle of the GaN band gap. In agreement with the measured electron concentrations, the background free carrier concentration in our calculation was assumed to be 10^{14} cm^{-3} in the GaN buffer layer. We used linear interpolations between the relevant physical constants of the binary compounds GaN and AlN to describe the physical properties of $Al_xGa_{1-x}N$ in our calculations [4, 7]. For p-type samples, in addition the activation energy of the Mg acceptor, E_{Mg}, and the Ni-Schottky barrier on p-type GaN, $e\Phi_b$, as a function of Al-concentration x was approximated by

$$E_{Mg}(x) = (0.7\text{ eV})x + 0.17\text{ eV} \quad \text{and} \quad e\Phi_b(x) = (1.3\text{ eV})x + 0.55\text{ eV}. \qquad (3)$$

In Fig. 3 the band edge profiles and carrier distribution profiles are shown for Ga-face and N-face $Ni/Al_{0.3}Ga_{0.7}N/GaN$ (50/30/2000 nm) heterostructure. The barrier of the Ga-face structure was doped with Si ([Si] = 5×10^{19} cm^{-3}) over a depth of 20 nm. A 2DEG is obtained close to the interface with a sheet carrier concentration of 1.4×10^{13} cm^{-2} in good agreement with the experimental observations. To enable hole confinement close to the AlGaN/GaN interface the

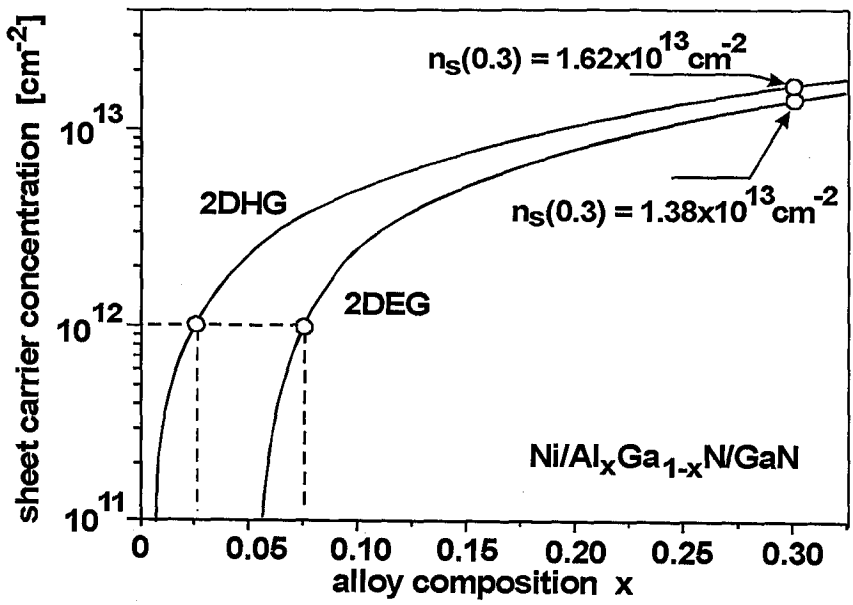

Fig. 4. Sheet carrier concentration versus Al-concentration of n-type Ga- and p-type N-face $Ni/Al_{0.3}Ga_{0.7}N/GaN$ (30/30/2000 nm) heterostructures.

polarity of sample has to be N-face. Using a p-doped barrier ([Mg] = 5×10^{19} cm^{-3}) a 2DHG with a sheet carrier concentration of 1.6×10^{13} cm^{-2} should result.

The formation of hole and electron gases with high sheet carrier concentrations is dominated by the polarization induced interface charge of $\sigma/e(0.3) = 1.68 \times 10^{13}$ cm^{-2}. In Fig. 4 the calculated sheet carrier concentrations of 2DEGs and 2DHGs are shown versus the Al-concentration of the barrier. The sheet carrier concentrations increase with increasing Al-concentration because of increasing spontaneous and piezoelectric polarization of the barrier. The carrier density of the 2DHGs is slightly higher than those of the 2DEGs mainly because of the higher Schottky barrier of Ni on n-type in comparison to p-type AlGaN.

4. Summary

In conclusion, we have calculated the polarization induced sheet charges in GaN/AlGaN/GaN heterostructures of different polarity, using linear interpolations between the physical properties of GaN and AlN. A formation of 2DEGs with a high sheet carrier concentration is predicted for n-type Ga-face (N-face) heterostructures close to the lower (upper) AlGaN/GaN (GaN/AlGaN) interface. In analogy, polarization induced 2DHGs can be obtained close to the upper (lower) AlGaN/GaN interface in p-type heterostructures of Ga-face (N-face) polarity. Experimental evidence for the predicted important role of polarization induced interface charges and the polarity on the formation of two-dimensional carrier gases comes from a combination of high-resolution X-ray diffraction, Hall effect, and $C-V$ profiling measurements.

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