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Accumulation hole layer in p-GaNÕAlGaN heterostructures

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We present the results on piezoelectric and pyroelectric doping in AlGaN-on-GaN and GaN-on-AlGaN heterostructures and demonstrate *p*-GaN/AlGaN structures with accumulation hole layer. Our results indicate that polarization charge can induce up to 5×10^{13} cm⁻² holes at the $AIGaN/GaN$ heterointerfaces. We show that the transition from three-dimensional $(3D)$ to two-dimensional (2D) hole gas can be only achieved for hole sheet densities on the order of 10^{13} cm⁻² or higher. At lower densities, only 3D-hole accumulation layer may exist. These results suggest that a piezoelectrically induced 2D-hole gas can be used for the reduction of the base spreading resistance in AlGaN/GaN-based heterostructure bipolar transistors. © *2000 American Institute of Physics.* $[$0003-6951(00)00421-6]$

Recent proposals of inducing two-dimensional (2D) hole gas by piezoelectric effects in AlGaN/GaN heterostructures¹ stimulated interest in exploring these heterostructures for a drastic reduction of the base spreading resistance in GaNbased heterostructure bipolar transistors (HBTs). One of the most challenging problems in realizing these devices is to achieve a reasonable base spreading resistance. A small base-spreading resistance is the most important feature of GaAs- or InP-based HBTs. In a grown AlGaN/GaN HBT, a sheet resistance of 75 k Ω per square was estimated.² We expect that, using a piezoelectric effect, a 2D-hole density induced into the base of a GaN-based HBT can result in the considerable reduction of the base-spreading resistance, and, possibly, reduction of the contact resistance as well. Since the holes in the 2D gas might have a higher mobility (for example, around 100 cm²/V s), we speculate that the sheet resistance can be reduced to approximately 1 k Ω per square.

In this letter, we demonstrate an experimental evidence of the accumulation of holes in *p*-GaN/AlGaN heterostructures. Also, we present the calculated band diagrams and sheet hole density in AlGaN/GaN heterostructures where spontaneous and piezoelectric polarizations, as well as strain relaxation effects, are taken into account.

Figure 1 shows the sample structure we used for our measurements. The top 50 nm *p*-GaN layer was Mg doped to yield the bulk hole concentration of 2×10^{17} cm⁻³ for the total estimated sheet density of 10^{12} cm⁻². This layer was grown on top of the superlattice structure with the top 10 nm strained *p*-AlGaN layer. The measured sheet density in our sample at room temperature was 4.5×10^{12} cm⁻², well above the estimated contribution from the top *p*-GaN layer. This value is consistent with the calculations based on the theory of elasticity. The measured hole mobility was 5–6 cm^2 /V s. As shown in Fig. 1, with an increase in temperature up to 450 K, the sheet hole density, p_s , increased to 10^{13} cm⁻², but the hole mobility further decreased to approximately 4 cm²/V s. We estimated mean free path, λ , versus hole mobility and hole gas accumulation layer width, X_{ac} , versus sheet hole density (see Fig. 2). For a given hole mobility, an accumulation layer exists if $\lambda < X_{ac}$, and 2D gas corresponds to $\lambda > X_{ac}$. For the measured hole mobility of 6 cm^2 /V s, the estimated transition from three-dimensional 3D to 2D holes corresponds to 7.5×10^{12} cm⁻² (see Fig. 2). Since measured sheet hole density was smaller than 7.5 $\times 10^{12}$ cm⁻², we conclude that we must have 3D and not 2D holes in the measured sample at room temperature. We estimate that the holes become two dimensional for p_s $>10^{13}$ cm⁻² (at 450 K in our sample).

We calculate typical densities of the 2D-hole gas for a model heterostructure with a Schottky gate contact shown in Fig. 3. Our calculations use an analytical self-consistent solution of the Poisson and Schrödinger equations for inverted

FIG. 1. Measured temperature dependence of hole mobility in the hole accumulation layer (top). Temperature dependence of the measured sheet hole density and the bulk contribution (theory) in the hole accumulation layer (bottom). Inset shows epilayer design of the structure.

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FIG. 2. Estimated mean free path, λ , vs hole mobility (a) and hole gas accumulation layer width, X_{ac} , vs sheet hole density (b). For the measured hole mobility of 6 cm²/V s, the estimated transition from hole accumulation layer (3D holes) to 2D-hole gas occurs at hole sheet density 7.5 $\times 10^{12}$ cm⁻². Dashed line in (b) corresponds to 2D-hole gas, solid line shows 3D-hole accumulation.

heterostructures with an accumulation layer at the heterointerface. For noninverted heterostructures, we used a solution of Poisson's equation to describe the depletion near the interface. The boundary condition for the $Al_xGa_{1-x}N/GaN$ interface accounted for the piezoelectric effect and spontaneous polarization

FIG. 3. Calculated 2D charge density distribution including piezoelectric and spontaneous polarization charges, metal surface charge, accumulation hole charge (top N) [Fig. 3(a)] and depletion charge (top Ga) [Fig. 3(b)] for AlGaN. In GaN, $N_a = 10^{17}$ cm⁻³.

FIG. 4. Sheet hole density at zero bias voltage as a function of Al molar fraction calculated taking into account strain relaxation (solid lines). Dashed lines are for fully strained heterostructures. Barrier thicknesses are 3 nm (a), 10 nm (b), and 30 nm (c). The Schottky barrier is 0.8 eV. N_a (GaN)=10¹⁷ cm⁻³. Separate curves show the effect of spontaneous polarization, the effect of the piezoelectric polarization, and combined effect.

$$
\epsilon_1 F_1 + P_1 + P_{s1} = \epsilon_2 F_2 + P_2 + P_{s2}, \tag{1}
$$

where ϵ_1 and ϵ_2 are the dielectric permittivities, F_1 , F_2 are the interface electric fields, and P_1 , P_{s1} , and P_2 , P_{s2} are the piezoelectric and spontaneous polarizations in AlGaN and GaN, respectively. For the (0001) growth direction, the piezoelectric polarizations are

$$
P_1 = \pm 2(e_{31} - e_{33}c_{31}/c_{33})u_{xx}.
$$
 (2)

Here c_{31} , c_{33} and e_{31} , e_{33} are the $Al_xGa_{1-x}N$ or GaN elastic constants and piezoelectric constants, respectively, and u_{xx} is the strain component in the interface plane. The piezoelectric 129.252.69.176 On: Fri, 23 Jan 2015 22:33:10This ametal/AlGaN/GaN beterostructure. Al molar fraction is 0.25. No donors in subject to the terms at http://solguon.ap.prg/termsconditions. Downloaded to IP: constants of GaN were extracted from GaN electromechanical coupling coefficients (see Ref. 3). The spontaneous polarizations were taken from Ref. 4

$$
P_{s1} - P_{s2} = \pm 0.052x. \tag{3}
$$

The sign in Eqs. (2) – (3) depends on the face orientation at the surface and at the heterointerfaces. A hole concentration enhancement corresponds to a nitrogen-terminated top surface, whereas electron concentration enhancement corresponds to a gallium-terminated top surface (see Fig. 3).³

Figure 3 shows the calculated band diagrams, 2D charge density, and schematics for AlGaN/*p*-GaN heterostructures. The hole density strongly depends on the piezo- and pyroelectric polarizations, and AlGaN barrier thickness. Figure 4 shows the calculation results for the sheet hole density, p_s , generated by the piezoelectric doping in $\text{Al}_x\text{Ga}_{1-x}\text{N}/p\text{-}\text{GaN}$ heterostructure field effect transistors (HFETs) as a function of the Al molar fraction. The sheet electron density was calculated at zero bias voltage taking into account the spontaneous polarization and strain relaxation in AlGaN. A sheet hole density from 1 to 5×10^{13} cm⁻² can be generated at zero bias voltage (see Fig. 4). Strain in AlGaN was analyzed using a misfit dislocation relaxation mechanism.

Our calculations show that, as in *n* type, larger sheet concentration can be generated by the total polarization in HFETs with thinner barrier layers and higher Al concentrations. For example, at $x=0.9$, almost two times larger p_s can be generated using 3 nm AlGaN than using 30 nm AlGaN (see Fig. 4). Even in partially relaxed structures, the maximum p_s is over 3×10^{13} cm⁻² for high Al molar fractions. As can be seen from the figure, the maximum sheet hole concentration in unrelaxed heterostructures at zero bias voltage is estimated to be approximately 5×10^{13} cm⁻². For comparison, in Fig. 4 we plotted separately the contributions into sheet hole density from the spontaneous polarization and the piezoelectric effect. In unrelaxed heterostructures, these contributions are almost equal, and, therefore, equally impor $tant$ (see Fig. 4). This is despite the fact that spontaneous polarization charge is substantially larger than the piezoelectric charge in AlGaN (see Fig. 3). The reason for that is the partial compensation of the spontaneous polarization charge of AlGaN by an opposite spontaneous polarization charge of GaN at the heterointerface (see Fig. 3).

In conclusion, our calculations show that a sheet hole density as high as 5×10^{13} cm⁻² can be obtained due to the piezoelectric and spontaneous polarization effects. We expect that a similar 2D-hole density can be induced into the base of a GaN-based HBT resulting in the considerable reduction of the base spreading resistance, and, possibly, reducing the contact resistance as well. The results suggest that a reasonable base spreading resistance in GaN-based HBTs might be realized by piezoelectric doping if the hole mobility is enhanced.

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