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M. S. Shur

A. D. Bykhovski

R. Gaska

J. W. Yang

Grigory Simin

University of South Carolina - Columbia, simin@enr.sc.edu

See next page for additional authors

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Author(s)

M. S. Shur, A. D. Bykhovski, R. Gaska, J. W. Yang, Grigory Simin, and M. A. Khan

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Accumulation hole layer in *p*-GaN/AlGaN heterostructures

M. S. Shur, A. D. Bykhovski, and R. Gaska^{a)}

Center for Integrated Electronics and Electronic Manufacturing and Department of Electrical, Computer, and Systems Engineering, Rensselaer Polytechnic Institute, Troy, New York 12180

J. W. Yang, G. Simin, and M. A. Khan

Department of Electrical and Computer Engineering, University of South Carolina, Columbia, South Carolina 29208

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We present the results on piezoelectric and pyroelectric doping in AlGa_N-on-GaN and GaN-on-AlGa_N heterostructures and demonstrate *p*-GaN/AlGa_N structures with accumulation hole layer. Our results indicate that polarization charge can induce up to $5 \times 10^{13} \text{ cm}^{-2}$ holes at the AlGa_N/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 AlGa_N/GaN-based heterostructure bipolar transistors. © 2000 American Institute of Physics. [S0003-6951(00)00421-6]

Recent proposals of inducing two-dimensional (2D) hole gas by piezoelectric effects in AlGa_N/GaN heterostructures¹ stimulated interest in exploring these heterostructures for a drastic reduction of the base spreading resistance in GaN-based 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 AlGa_N/GaN HBT, a sheet resistance of 75 kΩ 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 kΩ per square.

In this letter, we demonstrate an experimental evidence of the accumulation of holes in *p*-GaN/AlGa_N heterostructures. Also, we present the calculated band diagrams and sheet hole density in AlGa_N/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 $2 \times 10^{17} \text{ cm}^{-3}$ 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*-AlGa_N layer. The measured sheet density in our sample at room temperature was $4.5 \times 10^{12} \text{ cm}^{-2}$, 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 cm²/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 cm²/V s, the estimated transition from three-dimensional 3D to 2D holes corresponds to $7.5 \times 10^{12} \text{ cm}^{-2}$ (see Fig. 2). Since measured sheet hole density was smaller than $7.5 \times 10^{12} \text{ cm}^{-2}$, 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 $p_s > 10^{13} \text{ cm}^{-2}$ (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

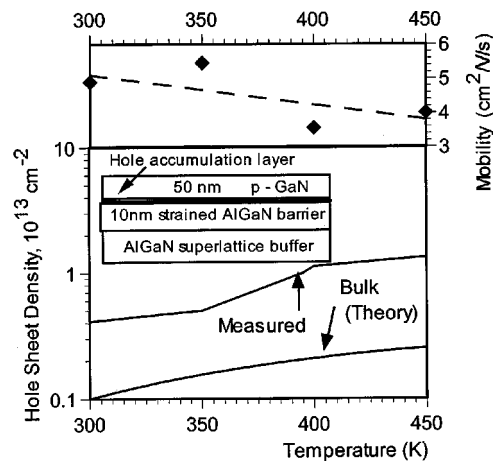


FIG. 1. Measured temperature dependence of hole mobility in the hole accumulation layer (top). Temperature dependence of the measured sheet hole density and the bulk contribution (theory) in the hole accumulation layer (bottom). Inset shows epilayer design of the structure.

^{a)}Author to whom correspondence should be addressed; electronic mail: gaskar@rpi.edu

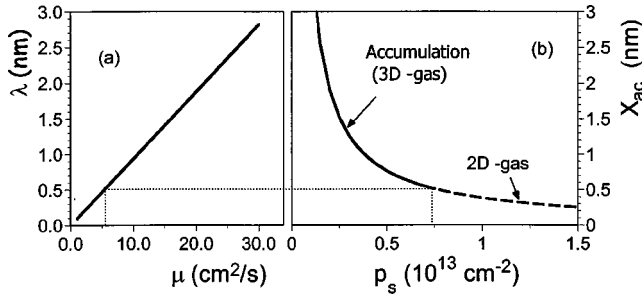


FIG. 2. Estimated mean free path, λ , vs hole mobility (a) and hole gas accumulation layer width, X_{ac} , vs sheet hole density (b). For the measured hole mobility of $6 \text{ cm}^2/\text{V s}$, the estimated transition from hole accumulation layer (3D holes) to 2D-hole gas occurs at hole sheet density $7.5 \times 10^{12} \text{ cm}^{-2}$. 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 $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ interface accounted for the piezoelectric effect and spontaneous polarization

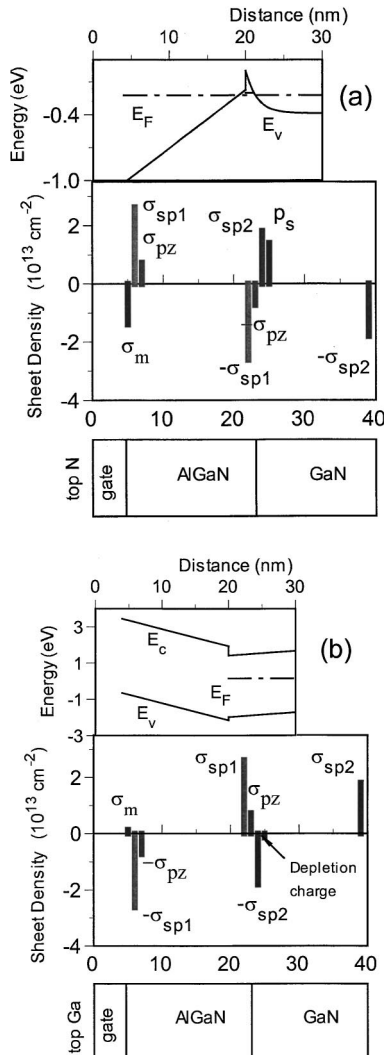


FIG. 3. Calculated 2D charge density distribution including piezoelectric and spontaneous polarization charges, metal surface charge, accumulation hole charge (top N) [Fig. 3(a)] and depletion charge (top Ga) [Fig. 3(b)] for metal/AlGaIn/GaN heterostructure. Al molar fraction is 0.25. No donors in AlGaIn. In GaN, $N_a = 10^{17} \text{ cm}^{-3}$.

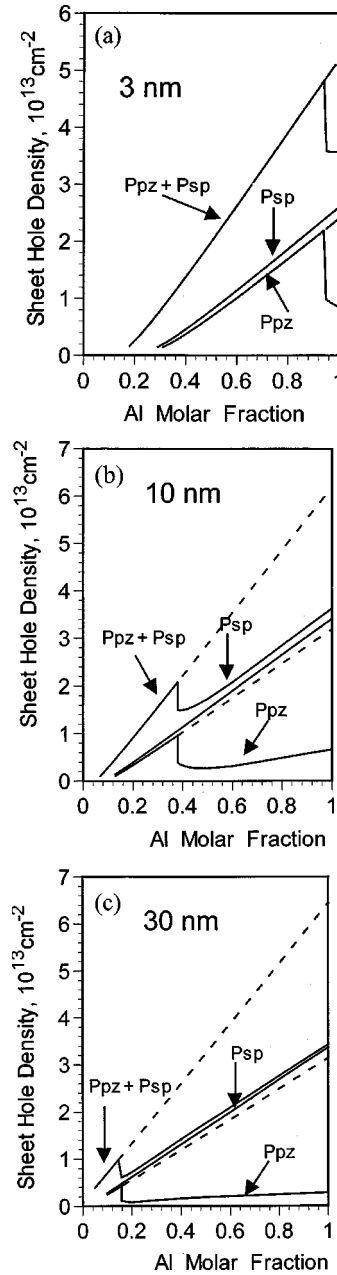


FIG. 4. Sheet hole density at zero bias voltage as a function of Al molar fraction calculated taking into account strain relaxation (solid lines). Dashed lines are for fully strained heterostructures. Barrier thicknesses are 3 nm (a), 10 nm (b), and 30 nm (c). The Schottky barrier is 0.8 eV. $N_a(\text{GaN}) = 10^{17} \text{ cm}^{-3}$. Separate curves show the effect of spontaneous polarization, the effect of the piezoelectric polarization, and combined effect.

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

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 AlGaIn and GaN, respectively. For the (0001) growth direction, the piezoelectric polarizations are

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

Here c_{31} , c_{33} and e_{31} , e_{33} are the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ or GaN elastic constants and piezoelectric constants, respectively, and u_{xx} is the strain component in the interface plane. The piezoelectric

constants of GaN were extracted from GaN electromechanical coupling coefficients (see Ref. 3). The spontaneous polarizations were taken from Ref. 4

$$P_{s1} - P_{s2} = \pm 0.052x. \quad (3)$$

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 Al_{*x*}Ga_{1-*x*}N/*p*-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 $5 \times 10^{13} \text{ cm}^{-2}$ 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 $3 \times 10^{13} \text{ cm}^{-2}$ 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 $5 \times 10^{13} \text{ cm}^{-2}$. 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 important (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 $5 \times 10^{13} \text{ cm}^{-2}$ 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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