III-V nitride heterostructure field-effect transistors (HFETs) have been a subject of intense recent investigation, and have emerged as attractive candidates for high-voltage, high-power operation at microwave frequencies. Contributions to the outstanding performance of nitride-based HFETs is the ability to achieve sheet carrier concentrations of ~1 × 10^{13} cm^{-3} or higher in the channel region of the transistor—well in excess of those achievable in other III-V material systems. It has been shown previously that piezoelectric affects can exert a substantial influence on charge density and electric field distributions in zincblende semiconductors grown in the (111) orientation, and more recently in III-V nitride heterostructures with the wurtzite crystal structure grown in the (0001) orientation.

In this letter we describe experimental measurements and analysis of carrier density distributions in GaN/Al_{1-x}N HFET structures grown by both molecular-beam epitaxy (MBE) and metalorganic vapor phase epitaxy (MOVPE). Carrier distributions measured in these structures are interpreted as consequences of piezoelectrically induced electric polarization charges at the GaN/Al_{1-x}N heterojunction interfaces. These studies demonstrate the influence of piezoelectric affects on carrier distributions in HFET structures, and the importance of proper inclusion of these effects in the design and analysis of high-performance nitride-based HFET structures.

The epitaxial structures used in these experiments were grown on c-plane (0001) sapphire substrates. Details of the growth procedures and epitaxial layer characteristics for samples grown by MBE and low-pressure MOVPE have been provided elsewhere. Schottky diodes were fabricated using evaporated Ti/Al annealed at 950 °C to form large-area Ohmic contacts to the HFET layers, and Ni to form Schottky contacts consisting typically of 320 μm diam dots.

Initial studies were performed using a nominally undoped 300 Å Al_{0.15}Ga_{0.85}N/GaN heterostructure, shown schematically in Fig. 1. Despite the absence of intentional doping in this structure, a high sheet carrier concentration is observed at the GaN/Al_{0.15}Ga_{0.85}N interface, which can be explained as a consequence of the presence of piezoelectrically induced polarization charge at the GaN/Al_{0.15}Ga_{0.85}N interface. The piezoelectrically induced charges shown schematically in Fig. 1(c) arise from the lattice mismatch between the Al_{1}Ga_{1-x}N barrier layer and the underlying GaN epilayer. For growth in the (0001) orientation of III-V nitrides with the wurtzite crystal structure, there will be present...
in a strained layer a polarization field $P_z$ aligned along the [0001] direction, given by

$$P_z = 2d_{31}(c_{11} + c_{12} - 2c_{13}^2/c_{33})\varepsilon_{xx},$$

(1)

where $d_{31}$ is the relevant piezoelectric constant, $c_{ij}$ are the elastic constants, and $\varepsilon_{xx} = a_{GaN}/a_{AlGaN}^{-1}$; $a_{GaN}$ and $a_{AlGaN}$ are the lattice constants of GaN and Al$_x$Ga$_{1-x}$N, respectively.

For AlN, a value of $-2 \times 10^{10}$ cm/V has been reported for $d_{31},^{12}$ and negative values of slightly smaller magnitude are expected for GaN and Al$_x$Ga$_{1-x}$N alloys. For Al$_x$Ga$_{1-x}$N, which when grown pseudomorphically on a strain-relaxed GaN layer is under tensile strain, the polarization field will point in the [0001] direction, i.e., from the A (cation-terminated) face to the B (N-terminated) face in the crystal. This direction is opposite to that found in III-V zincblende semiconductors grown in the (111) orientation, but is the same as that observed in CdS, which forms in the wurtzite crystal structure and has piezoelectric coefficient $d_{31} < 0.11$. That the polarization field is in the opposite direction for nitride compounds compared to other III-V semiconductors is not unexpected given the greater ionicity of the nitrides compared to other III-V materials.\textsuperscript{13}

Associated with the polarization field given by Eq. (1) is a piezoelectrically induced charge density $\rho_{pc}$ given by $\nabla \cdot P = \rho_{pc}$. In the Al$_x$Ga$_{1-x}$N/GaN heterostructure shown in Fig. 1, a positive piezoelectric sheet charge density $\rho_{pc}$ will be present at the GaN/Al$_x$Ga$_{1-x}$N interface, and a corresponding negative sheet charge $-\rho_{pc}$ at the top of the Al$_x$Ga$_{1-x}$N layer. We see immediately that any strain component common to both the GaN and Al$_x$Ga$_{1-x}$N layers, or slowly varying in comparison to the strain induced by pseudomorphic growth, will not contribute significantly to $\rho_{pc}$—the lattice-mismatch-induced component of strain will exert the dominant influence. Variations in composition or strain distribution near an interface will alter the local distribution of piezoelectrically induced charge; however, the total piezoelectric sheet charge density associated with the interface will be very nearly equal to that present at an abrupt interface between materials with the same compositions as those found away from the immediate vicinity of the interface. And finally, local process-induced variations in strain arising from, for example, etching for mesa isolation or recessing for Ohmic or Schottky contacts in FET structures will produce corresponding local variations in $\rho_{pc}$ and, consequently, free-carrier concentrations.

Using values reported in the literature for the piezoelectric coefficient\textsuperscript{11} and elastic constants,\textsuperscript{14} we estimate that $\rho_{pc}$ in Fig. 1 is $-4 \times 10^{12}$ cm$^{-2}$ V$^{-1}$. The electric field in the Al$_{0.15}$Ga$_{0.85}$N layer implied by this value is far too large to be consistent with reasonable values for the Schottky barrier height $e\phi_b$ for Al$_{0.15}$Ga$_{0.85}$N and the conduction-band offset $\Delta E_c$ at the GaN/Al$_{0.15}$Ga$_{0.85}$N interface. Thus, a two-dimensional electron gas (2DEG) is formed at the GaN/Al$_{0.15}$Ga$_{0.85}$N interface, the negative charges from which act to cancel partially the electric field arising from the piezoelectrically induced charges. At the top of the Al$_{0.15}$Ga$_{0.85}$N layer, the piezoelectric charge density will induce the formation in a Schottky barrier structure of a positive sheet charge in the metal at the metal-nitride interface, or at a free surface of a positive sheet charge that most likely arises from charging of surface states.

The piezoelectric effect therefore leads to the formation of a 2DEG with a high sheet charge density even in Al$_x$Ga$_{1-x}$N/GaN HFET structures without intentional doping. The sheet carrier densities in nominally undoped nitride HFET structures can in fact be comparable to those achievable in doped-channel structures, but without the degradation in mobility resulting from the presence of ionized impurities in the channel. A simple electrostatic analysis shows that the sheet carrier concentration $n_s$ in the 2DEG at the Al$_x$Ga$_{1-x}$N/GaN interface for a nominally undoped HFET structure should be given by

$$n_s = \frac{\sigma_p}{e} - \left( \frac{\epsilon_{AlGaN}}{D} \right) \left( e\phi_b + E_F - \Delta E_c \right),$$

$$\sigma_p/e = 2d_{31}(c_{11} + c_{12} - 2c_{13}^2/c_{33})(a_{GaN}/a_{AlN}^{-1})x_{AI},$$

(2)

where $\epsilon_{AlGaN}$ is the dielectric constant of Al$_x$Ga$_{1-x}$N, $d$ is the width of the Al$_x$Ga$_{1-x}$N barrier, $E_F$ is the Fermi level with respect to the GaN conduction-band-edge energy at the GaN/Al$_x$Ga$_{1-x}$N interface, and $x_{AI}$ is the AI concentration. An analysis of carrier concentrations measured in several nominally undoped Al$_x$Ga$_{1-x}$N/GaN HFET structures grown by both MBE and MOVPE has provided quantitative confirmation of this behavior.\textsuperscript{8}

Figure 2 shows the carrier concentration profile versus depth measured in the HFET structure shown in Fig. 1. The barriers are located primarily at the GaN/Al$_{0.15}$Ga$_{0.85}$N interface, and we obtain a sheet carrier concentration $n_s$ of $3.8 \times 10^{12}$ cm$^{-2}$ at zero bias. Furthermore, we do not see significant evidence of electron transfer into the Al$_{0.15}$Ga$_{0.85}$N layer, as would be expected if a high level of unintentional doping were present in that barrier layer. The absence of electron transfer into the Al$_{0.15}$Ga$_{0.85}$N layer can be shown to imply that any uniformly distributed space charge in the Al$_{0.15}$Ga$_{0.85}$N layer must be confined to within a distance $d_0$ of the Al$_{0.15}$Ga$_{0.85}$N/GaN interface, where

$$d_0 \leq \left( \frac{2\epsilon_{AlGaN}}{e^*n_s} \right) (\Delta E_c - E_F).$$

(3)

For the structure shown in Fig. 1, an estimate using $n_s = 3.8 \times 10^{12}$ cm$^{-2}$ as determined from our capacitance volt-
The presence of piezoelectrically induced charges must be properly accounted for in nitride heterostructure device design. Figure 3 shows a schematic diagram, the calculated energy band structure, and the distribution of piezoelectric and free-carrier charges expected for an Al$_{0.15}$Ga$_{0.85}$N/GaN HFET structure incorporating a buried Al$_{0.15}$Ga$_{0.85}$N isolation layer below the GaN channel. Figure 4 shows the carrier concentration profile versus depth measured for such a structure grown by MOVPE. The 2DEG carrier concentration at the upper GaN/Al$_{0.15}$Ga$_{0.85}$N interface is considerably reduced compared to that in the structure without the buried Al$_{0.15}$Ga$_{0.85}$N layer. We attribute this reduction to the presence of a negative piezoelectrically induced sheet charge at the top of the buried Al$_{0.15}$Ga$_{0.85}$N layer, which as shown in Fig. 3 acts to deplete carriers from the 2DEG. In the absence of the piezoelectric effect the lower Al$_{0.15}$Ga$_{0.85}$N layer should have little influence on this carrier density. Furthermore, there is evidence in the carrier concentration profile shown in Fig. 4 for the formation of a second 2DEG below the lower Al$_{0.15}$Ga$_{0.85}$N layer, arising from the presence of positive piezoelectrically induced charge at the bottom of that layer, as indicated in Fig. 3(c). These results provide a clear demonstration of the influence of piezoelectric effects on III-V nitride device characteristics, and the importance of incorporating these effects in nitride device design.

In summary, we have performed measurements of carrier concentration profiles in two Al$_{1-x}$Ga$_x$/GaN HFET structures. Analysis of a nominally undoped Al$_{0.15}$Ga$_{0.85}$N/GaN HFET structure revealed the presence of a high sheet carrier density in the HFET channel, which we interpret as a consequence of piezoelectrically induced polarization charges present at the GaN/Al$_{0.15}$Ga$_{0.85}$N interface. C–V profiling of an Al$_{0.15}$Ga$_{0.85}$N/GaN HFET structure with an Al$_{0.15}$Ga$_{0.85}$N isolation layer located beneath a 500 Å GaN channel demonstrated that piezoelectrically induced polarization charges in the Al$_{0.15}$Ga$_{0.85}$N isolation layer act to reduce the sheet carrier density in the HFET channel and to induce the accumulation of electrons at the GaN/Al$_{0.15}$Ga$_{0.85}$N interface at the bottom of the isolation layer. These results confirm the importance of including piezoelectric phenomena in the design and analysis of III-V nitride heterostructure devices.

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