Direct measurement of the polarization charge in AlGaN/GaN heterostructures using capacitance–voltage carrier profiling

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The polarization charge at $Al_xGa_{1-x}N$/GaN heterostructure interfaces arising from differences in spontaneous polarization between $Al_xGa_{1-x}N$ and GaN and the presence of piezoelectric polarization in strained layers has been directly measured using capacitance–voltage carrier profiling in GaN/$Al_xGa_{1-x}N$/GaN heterostructures with varying Al composition grown by molecular-beam epitaxy. The measured polarization charge densities ($2.36\pm0.30\times10^{12}$ e/cm^2, $6.79\pm0.48\times10^{12}$ e/cm^2, and $6.92\pm0.74\times10^{12}$ e/cm^2 for 5%, 12%, and 16% $Al_xGa_{1-x}N$/GaN interfaces, respectively) reveal substantial bowing in the polarization charge as a function of Al composition, and are in reasonable agreement with those calculated using a model that accounts for the nonlinearity of the spontaneous and piezoelectric polarizations as functions of Al composition. Our results yield an explicit expression for polarization charge as a function of Al composition at an $Al_xGa_{1-x}N$/GaN interface. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1477275]

The large polarization charge present at heterostructure interfaces in group III-nitride alloys provides a powerful means by which to control the distribution of electric fields and charges in nitride-based electronic and optical devices.[1–4] To design heterostructure devices that take advantage of this property, an accurate determination of the polarization charge that will be present at each interface in a nitride heterostructure is essential. Furthermore, accurate knowledge of the polarization charge is required for characterization and analysis of nitride devices to separate the effects of polarization charge from other factors that influence device characteristics.

Values for the polarization charge have been calculated using theoretical predictions[5,6] for the spontaneous polarization, piezoelectric coefficients, and elastic constants of nitride alloys; however, direct, precise measurements of polarization charge in nitride heterostructures are still lacking. Estimates of the polarization charge have been made based on measurements of nitride device properties, such as the sheet carrier concentration in $Al_xGa_{1-x}N$/GaN heterostructure field-effect transistors (HFETs)[1,4,7,8] and the electric field present in quantum-well optoelectronic devices,[9,10] but these may not provide an unambiguous determination of polarization charge due to the possible presence of other factors that influence the measured device characteristics.

In previous studies, capacitance–voltage ($C-V$) profiling has been used to determine the amount of fixed charge located at semiconductor heterojunction interfaces in structures where one can measure the dopant concentration in the material on both sides of the interface.[11] Although the carrier profile obtained from $C-V$ profiling is distorted due to the intrinsic Debye length limitation and, therefore, yields only an apparent carrier concentration, $\hat{n}(x)$, the number of charges depleted in profiling through a heterojunction interface is accurately reflected in the integrated apparent carrier concentration, and can be written as[12]

$$\int_a^b \hat{n}(x)\,dx = \sigma_i + \int_a^b N_D(x)\,dx, \quad (1)$$

where σ_i is the fixed charge at the interface, $N_D(x)$ is the ionized dopant concentration, and the integrals are from point a on one side of the interface to point b on the other. In this article, we describe the application of this technique to the measurement of the polarization charge in GaN/$Al_xGa_{1-x}N$/GaN heterostructures using Schottky diode device structures.

Because the polarization charge present at $Al_xGa_{1-x}N$/GaN heterojunction interfaces is exceptionally large—on the order of $10^{12}-10^{13}$ e/cm^2 for the structures under investigation[5]—the fixed charge at the interface is expected to be dominated by these polarization charges. Other charges at the interface are likely to be small compared to the polarization charge and will, therefore, not be considered further in this study. With this simplification Eq. (1) directly yields the polarization charge σ_{pol} at the AlGaN/GaN interface:

$$\sigma_{pol} = \int_a^b [\hat{n}(x) - N_D(x)]\,dx. \quad (2)$$

The $Al_xGa_{1-x}N$/GaN heterostructures used in these studies were designed specifically to allow an accurate, robust determination of σ_{pol}. To simplify the analysis of the carrier profile, it is convenient to utilize heterostructures with similar or, ideally, equal dopant concentrations in the materials on both sides of the interface. This approach minimizes errors in the extraction of the polarization charge from the

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20nm GaN - 1×10^{17} cm^{-3}
100nm GaN - 1×10^{18} cm^{-3}
100nm $Al_xGa_{1-x}N$ - 1×10^{18} cm^{-3}
50nm GaN - 1×10^{18} cm^{-3}
300nm GaN - 4×10^{18} cm^{-3}
2 μm GaN - uid
high-temp. AlN buffer layer
sapphire substrate

FIG. 1. Schematic diagram of the epitaxial layer structure used in these studies, indicating the dopant concentration in the MBE-grown films and the unintentional doping (uid) in the MOCVD-grown GaN template layer.

$C-V$ measurement as it reduces or completely eliminates the need to determine the interface position. In addition, the heterostructures were designed so that an undepleted region was present on both sides of each heterojunction interface. This allows the dopant concentration in each material to be extracted directly from the $C-V$ measurement, and ensures that the full effect of the interfacial charge is observed in the $C-V$ profile and that the measurement of $\sigma_{\rm pol}$ is not influenced by the polarization induced charges located at other interfaces in the heterostructure or by surface charges. This objective can be met by having sufficiently large dopant concentrations and layer thicknesses for the materials on both sides of each interface. Another essential requirement was to maintain the $Al_xGa_{1-x}N$ thickness below the critical thickness for strain relaxation. This constraint insures the presence of the full piezoelectric polarization, which would be diminished if the $Al_xGa_{1-x}N$ layer were partially relaxed.[4] Finally, the use of a buried $Al_xGa_{1-x}N$ layer yields two $Al_xGa_{1-x}N$/GaN interfaces in each sample, in principle enabling measurement of the polarization charge at each interface to provide a self-consistent check of the results; however, profiling through both interfaces proved difficult in practice as discussed below. Based on these and a number of other, secondary factors, optimal structures were designed using detailed one-dimensional electrostatic simulations,[13] and the resulting sample structure is shown in Fig. 1.

Samples were grown by molecular-beam epitaxy (MBE) on a $\sim$2-μm-thick metalorganic chemical vapor deposition (MOCVD) GaN/sapphire template, which included a high-temperature AlN nucleation layer shown to produce Ga-polar films.[14] The MBE growth was performed at 750 °C under Ga-rich growth conditions (Ga-droplet regime)[15] with Al concentrations of 5%, 12%, and 16% in the $Al_xGa_{1-x}N$ layer as determined by triple-axis x-ray diffraction analysis. These measurements also showed that in the omega scan, the widths of the peaks corresponding to the GaN and $Al_xGa_{1-x}N$ layers were the same, confirming that the $Al_xGa_{1-x}N$ layers were coherently strained. Evidence of step-flow growth was apparent in atomic force microscope images of the sample surface.

Schottky diode structures were fabricated consisting of ring-shaped Ti/Al Ohmic contacts annealed at 650 °C for 60 s with circular Ni Schottky contacts in the middle of each Ohmic contact. A SiO_2 layer, 30 to 180 nm in thickness, was deposited before the Ni Schottky contact metallization to decrease reverse-bias leakage current to an acceptable level. A surface treatment consisting of organic solvent cleaning, NH_4OH dip, and N_2 plasma treatment[16] was performed prior to the oxide deposition to reduce the interface trap density at the oxide-semiconductor interface and prevent Fermi-level pinning of the surface, which was found to be problematic when attempting to deplete any significant distance into the heterostructure without the surface treatment.

$C-V$ measurements were performed using an HP 4285A Precision LCR Meter with an ac bias frequency in the range of 100 kHz to 1 MHz at room temperature under ambient lighting conditions. The measurement circuit configuration for the LCR meter was a capacitance and conductance in parallel: C_p and G_p, respectively. The first step in extracting the semiconductor capacitance from this circuit was to correct for the series resistance present between the Schottky gate and Ohmic contact.[17] The semiconductor capacitance could then be found from analysis of the simple series circuit, which includes both the semiconductor and oxide capacitances. The apparent carrier profile was then determined using a standard expression,[17] and a typical profile is shown in Fig. 2(a) with the dopant concentration indicated in the figure. Due to increased noise and leakage current at large reverse-bias voltages, this technique was only applied to the first $Al_xGa_{1-x}N$/GaN interface, which has a negative polarization charge resulting in a decreased carrier concentration near the interface. The polarization charge was obtained using Eq. (2), and Fig. 2(b) shows the polarization charge densities measured using the $C-V$ profiling method as a function of Al concentration.

Our experimental values for polarization charge can be compared directly to those predicted on the basis of theoretical calculations or experimentally estimated polarization charge densities. Values for the polarization charge have been calculated by summing the contributions from the spontaneous polarization P_s and piezoelectric polarization P_{pz} for the appropriate $Al_xGa_{1-x}N$ and GaN layers, and determining the change in polarization between the two layers. The nonlinearity of the spontaneous polarization, which has recently been predicted for nitride alloys,[18] has been included in the calculation of the total plarization charge for the $Al_xGa_{1-x}N$ layer using the procedure outlined by Ambacher *et al.*[19] for an $Al_xGa_{1-x}N$ layer coherently strained to a GaN substrate. This procedure also takes into account the nonlinearity of the piezoelectric polarization that results from the dependence of the elastic constants and piezoelectric coefficients on Al composition, and the nonlinear dependence of P_{pz} on strain for the binary compounds AlN and GaN. The lattice constants for GaN and AlN used in the calculation were 3.189 and 3.112 Å, respectively.[20] Figure 2(b) shows the values of the polarization charge calculated using the approach outlined above, as well as the values that one would obtain using a simple linear interpolation of the polarization fields and charge densities for AlN and GaN.

The measured values for the polarization charge agree fairly well with those calculated using the nonlinear model, but differ significantly from those obtained by simple linear interpolation. Use of polarization charge values obtained from the experimentally verified nonlinear model is essential to understanding device characteristics that are influenced by

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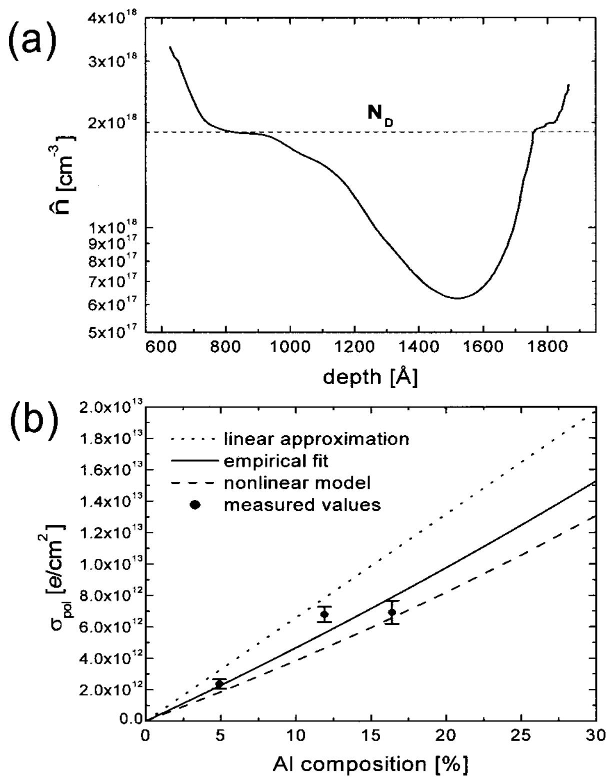

FIG. 2. (a) Apparent carrier concentration profile (solid line) obtained from the $GaN/Al_{0.12}Ga_{0.88}N/GaN$ sample, with the dopant concentration, N_D (dashed line), indicated. (b) Measured (symbols) and calculated values (dotted and dashed lines) and experimental fit of Eq. 3 (solid line) for the polarization charge. The polarization charge calcualted using a linear interpolation between the total polarization charges of GaN and AIN (dotted line) is significantly greater than the correctly calculated values (dashed line) and the measured values.

the polarization charge. It is, therefore, useful to develop an expression to estimate the polarization charge at the interface between a GaN layer and a $Al_xGa_{1-x}N$ layer of any Al composition coherently strained to a GaN substrate of the form

$$\sigma_{pol}(x_{Al}) = a x_{Al} + b x_{Al}^2, \quad (3)$$

where a and b are constants, which takes into account the nonlinearity of the polarization charge as a function of Al composition. Assuming no polarization charge will be present for $x_{Al}=0$ and using the calculated value of σ_{pol} for AlN coherently strained to GaN and the three data points for σ_{pol} obtained from this investigation, we fit a curve in the form of Eq. (3) to these 5 points and find a and b to be 4.45×10^{13} and 2.13×10^{13} e/cm^2, respectively. The empirical fit to the measured data and the calculated values of the polarization charge at an $Al_xGa_{1-x}N/GaN$ interface are shown in Fig. 2(b). Considering the limited data, this expression should be used only as an estimate of the polarization charge, but it does provide a significantly better approximation to the experimentally measured values and to the values calculated using the complete, nonlinear model than a linear interpolation approach. This expression also yields a useful estimate of the bowing in the polarization charge versus the Al composition curve. It is essential to understand, however, that Eq. (3) yields the amount of fixed polarization charge at an $Al_xGa_{1-x}N/GaN$ interface and not necessarily the sheet concentration of electrons that would be present in a two-dimensional electron gas located at an interface with positive polarization charge.

In summary, $C-V$ carrier profiling has been used to directly measure the polarization charge in $Al_xGa_{1-x}N/GaN$ heterostructures. We have found that the values agree well with the polarization charge calculated using theoretical predictions for the spontaneous polarization, piezoelectric coefficients, and elastic constants of the materials, provided that the nonlinearity of the spontaneous and piezoelectric polarization charges is taken into account. Our measurements yield an explicit expression for the polarization charge as a function of Al composition at an $Al_xGa_{1-x}N/GaN$ interface.

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