Influence of surface processing and passivation on carrier concentrations and transport properties in AlGaN/GaN heterostructures

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The influence of surface chemical treatments and of deposition of a SiO₂ surface passivation layer on carrier distributions and mobility in AlₓGa₁₋ₓN/GaN heterostructure field-effect-transistor epitaxial layer structures is investigated. Surface chemical treatments are found to exert little influence on carrier distribution and mobility. Deposition of a SiO₂ surface passivation layer is found to induce an increase in electron concentration in the transistor channel and a decrease in mobility. These changes are largely reversed upon removal of the SiO₂ layer by wet etching. These observations are quantitatively consistent with a shift in Fermi level at the AlₓGa₁₋ₓN surface of approximately 1 eV upon deposition of SiO₂, indicating that the AlₓGa₁₋ₓN/SiO₂ interface has a different, and possibly much lower, density of electronic states compared to the AlₓGa₁₋ₓN free surface. © 2001 American Institute of Physics. [DOI: 10.1063/1.1383014]

I. INTRODUCTION

AlₓGa₁₋ₓN/GaN heterostructure field-effect transistors (HFETs) are currently of outstanding interest for application in high-power microwave-frequency electronic systems. Although very impressive device performance has been achieved by a number of groups,1–5 pronounced current slump effects,5–8 variations in device response under pulsed and variable-frequency bias conditions,9–12 and microwave power degradation1,9 are often observed. A variety of phenomena, including surface, interface, and bulk trap states6–8,12 and dielectric response,11 have been invoked to explain these effects. Surface passivation using silicon nitride has recently been found to mitigate current slump and microwave power degradation,13 but a much improved understanding of these phenomena and their physical origins will be required to design, fabricate, and optimize the performance of nitride HFET structures for microwave power applications.

In this article, we describe characterization of carrier distributions and charge transport in AlₓGa₁₋ₓN/GaN HFET epitaxial layer structures subjected to various surface treatments and passivated by deposition of SiO₂. Our results indicate that deposition of SiO₂ on an AlₓGa₁₋ₓN/GaN HFET epitaxial layer structure induces substantial, reversible changes in carrier distribution consistent with a large shift in the position of the Fermi level at the AlₓGa₁₋ₓN/SiO₂ interface compared to that at the AlₓGa₁₋ₓN surface; our observations indicate that a substantial change, possibly a large reduction, in the electronic density of states at the AlₓGa₁₋ₓN/SiO₂ interface occurs compared to that at a free AlₓGa₁₋ₓN surface. These results are of relevance for approaches to mitigation of current slump effects based on dielectric passivation layers, surface passivation for other nitride-based device structures,14 and metal–insulator–nitride semiconductor HFET structures in which a dielectric layer such as SiO₂ is incorporated within the transistor gate structure to reduce gate leakage current.15–17

II. EXPERIMENT

The AlₓGa₁₋ₓN/GaN HFET epitaxial layer structures used in these studies were grown by metalorganic chemical vapor deposition on sapphire substrates. Structures with either intentionally doped or nominally undoped AlₓGa₁₋ₓN barrier layers were employed. The doped-barrier sample, shown schematically in Fig. 1(a), consisted of a 3 μm nominally undoped GaN buffer layer followed by a 20 Å Al₀.₂₅Ga₀.₇₅N spacer layer, 150 Å Al₀.₂₅Ga₀.₇₅N doped with Si at a concentration of 8 × 10¹⁸ cm⁻³, and finally, 30 Å undoped Al₀.₂₅Ga₀.₇₅N. The undoped-barrier sample, shown schematically in Fig. 1(b), consisted of a 3 μm nominally undoped GaN buffer layer followed by a 200 Å nominally undoped Al₀.₃₅Ga₀.₆₅N barrier layer. Van der Pauw patterns were fabricated on these samples using Al/Ti to form ohmic contacts. Contacts on the undoped-barrier sample were annealed in N₂ at 830 °C; no annealing was required to form low-resistance ohmic contacts to the doped-barrier sample. Both types of samples were then subjected to a variety of surface treatments, after each of which Hall measurements were performed at room temperature to assess the effect of these treatments on sheet carrier concentration and mobility in the two-dimensional electron gas (2DEG) channel of the AlₓGa₁₋ₓN/GaN HFET structures. Specifically, samples were subjected sequentially to rapid thermal annealing at 600 °C in N₂, a 10–15 s etch in HCl:HF:H₂O (1:1:2), a 10 s etch in 14% HF buffered oxide etch (BOE), deposition of a ~1300 Å SiO₂ passivation layer, and subsequent removal of...
the passivation layer by etching in 14% HF BOE. The SiO$_2$ passivation layer was deposited using plasma-enhanced chemical vapor deposition (PECVD) at a substrate temperature of 300 °C and rf power level of 30 W. After each etch step described above, the sample was rinsed in deionized water and blown dry prior to measurement.

III. RESULTS AND DISCUSSION

Figure 2 shows sheet carrier concentration $n_s$ and Hall mobility $\mu$ measured after each processing step described above for the doped-barrier sample. As shown in the figure, the sheet carrier concentration is essentially unaffected by annealing at 600 °C and by etching in HCl:HF:H$_2$O. However, the mobility decreases slightly following each of these steps. Subsequent etching in BOE affects neither the mobility nor the sheet carrier concentration. The most noteworthy observations from Fig. 2 are that PECVD deposition of a SiO$_2$ layer on the Al$_{0.25}$Ga$_{0.75}$N surface results in a significant change in both sheet carrier concentration and mobility, and that these changes are essentially reversed upon removal of the SiO$_2$ layer by wet etching for 150 s. Similar behavior is evident in the undoped-barrier sample, as shown in Fig. 3. The observed changes in 2DEG properties upon deposition of the SiO$_2$ layer are consistent with prior suggestions that Al$_{x}$Ga$_{1-x}$N surface properties are closely coupled to 2DEG properties via polarization effects, and the observation that removal of the SiO$_2$ layer largely reverses these changes confirms that Al$_{x}$Ga$_{1-x}$N surface properties, rather than plasma-induced damage incurred during PECVD deposition of the SiO$_2$ layer, are the relevant factor leading to the observed changes in sheet carrier concentration and mobility. Stress within the Al$_{0.25}$Ga$_{0.75}$N/GaN heterojunction induced by the presence of the SiO$_2$ layer is unlikely to be a significant factor, as any change in the piezoelectric sheet charge at the Al$_{0.25}$Ga$_{0.75}$N/GaN interface due to the Al$_{x}$Ga$_{1-x}$N piezoelectric polarization field will be compensated by a corresponding change, approximately equal in magnitude and opposite in sign, in the piezoelectric sheet charge arising from stress in the GaN channel layer.

The influence of the Al$_{x}$Ga$_{1-x}$N surface on the 2DEG sheet carrier concentration can be seen most easily from a simple electrostatic analysis. Figure 4 shows the conduction-band-edge profile and electrostatic charge distribution for an Al$_{0.25}$Ga$_{0.75}$N/GaN HFET epitaxial layer structure with a SiO$_2$ passivation layer. Spontaneous and piezoelectric polarization effects lead to the existence of polarization-induced sheet charges at the Al$_{x}$Ga$_{1-x}$N/GaN heterojunction interface, $\sigma_{\text{pol,hj}}$, and at the Al$_{x}$Ga$_{1-x}$N/SiO$_2$ interface, $\sigma_{\text{pol,surf}}$. The former is due to the discontinuities in strain and spontaneous polarization at the Al$_{x}$Ga$_{1-x}$N/GaN heterojunction interface,
and the latter to the piezoelectric and spontaneous polarization within the Al$_{1-x}$Ga$_x$N layer. In addition to these polarization-induced charge densities are those arising from donors in the Al$_{1-x}$Ga$_x$N layer ($eN_d$), charge within the SiO$_2$ layer ($\sigma_{ox}$), electrons in the 2DEG ($\sigma_{2DEG}=en_s$), and electronic states at the Al$_{1-x}$Ga$_x$N/SiO$_2$ interface ($\sigma_{surf}$). In the absence of the SiO$_2$ passivation layer, states at the Al$_{1-x}$Ga$_x$N surface would lead to the existence of a surface charge $\sigma_{surf}$.

Following the analysis of Refs. 18 and 20, the charge density in the 2DEG is given by

$$\sigma_{2DEG} = e\left(\phi_b - \frac{\Delta E_c - E_f}{e}\right) - \frac{1}{2} eN_d d - \sigma_{pol,hj},$$

where $e$ is the electron charge, $N_d$ and $d$ are the dopant concentration within and thickness of the Al$_{1-x}$Ga$_x$N barrier layer, respectively, $\phi_b$ is the dielectric constant of the Al$_{1-x}$Ga$_x$N layer, $\Delta E_c$ is the Al$_{1-x}$Ga$_x$N/GaN conduction-band offset, $E_f$ is the Fermi energy at the Al$_{1-x}$Ga$_x$N/GaN interface, and $e\phi_b$ is the energy difference between the Fermi level and Al$_{1-x}$Ga$_x$N/GaN conduction-band edge at the Al$_{1-x}$Ga$_x$N/SiO$_2$ interface (or at the free Al$_{1-x}$Ga$_x$N surface in the absence of the SiO$_2$ passivation layer). From Eq. (1), we see that the only quantity upon which $\sigma_{2DEG}$ depends that will be influenced by the presence of the SiO$_2$ passivation layer is $\phi_b$; thus, any change in $n_s$ induced by the presence of the SiO$_2$ layer should reflect a corresponding change in $\phi_b$ for the Al$_{1-x}$Ga$_x$N/SiO$_2$ interface relative to that for the free Al$_{1-x}$Ga$_x$N surface.

These basic trends have been confirmed in detailed numerical simulations using a self-consistent one-dimensional Poisson solver. In these simulations, the Al$_{1-x}$Ga$_x$N barrier thickness was assumed to be 245 Å (as determined from capacitance–voltage profiling for the undoped-barrier sample), and the background donor concentration in nominally undoped Al$_{1-x}$Ga$_x$N regions was assumed to be $2 \times 10^{18}$ cm$^{-3}$. Polarization charge densities at the Al$_{1-x}$Ga$_x$N/GaN interface of 1.06 $\times 10^{13}$ e/cm$^2$ and 1.36 $\times 10^{13}$ e/cm$^2$ were assumed for Al concentrations of 25% and 30%, respectively. The background donor concentrations and polarization charge densities were chosen to yield a value of $\phi_b$ at the free Al$_{1-x}$Ga$_x$N surface consistent with measured sheet carrier concentrations and the experimental value of the Al$_{1-x}$Ga$_x$N free-surface barrier height reported by Ibbetson et al.\(^{19}\)

Figures 5 and 6 show sheet carrier concentrations derived from these simulations as functions of $\phi_b$ for samples with doped and undoped Al$_{1-x}$Ga$_x$N barriers, respectively. Sheet carrier concentrations in the 2DEG and in the Al$_{1-x}$Ga$_x$N barrier, together with their sum, are plotted. The carrier concentrations obtained from the Hall measurements reported here are sums of the carrier concentrations in the 2DEG and Al$_{1-x}$Ga$_x$N barrier, and are also indicated in the figures for samples with and without SiO$_2$ passivation layers. As shown in the figures, the change in sheet carrier concentration induced by the presence of the SiO$_2$ passivation layer corresponds to a reduction in $\phi_b$, upon deposition of the SiO$_2$ passivation layer, of approximately 1.0 V for the doped
Al0.25Ga0.75N barrier, and of approximately 1.1 V for the undoped Al0.30Ga0.70N barrier. From these observations we may conclude that the electronic density of states at the Al1-xGa1-xN/SiO2 interface differs considerably from that of the free Al1-xGa1-xN surface; the Fermi level at the Al1-xGa1-xN/SiO2 interface is considerably closer to that expected for an unpinned surface, consistent with what one might expect on the basis of studies of GaN/SiO2 interfaces that suggest the presence of relatively low densities of interface states. 22–25

Our simulation results may also be used to assess the origins of the reduction in mobility induced by the presence of the SiO2 passivation layer. Denoting the sheet carrier concentration and mobility in the 2DEG by \( n_s \) and \( \mu_{2\text{DEG}} \), respectively, and those in the Al1-xGa1-xN barrier by \( n_b \) and \( \mu_b \), we estimate the measured mobility \( \mu \) to be given by

\[
\mu = \left( n_s \mu_{2\text{DEG}} + n_b \mu_b \right) / \left( n_s + n_b \right)
\]

As shown in Figs. 5 and 6, the increases in carrier concentration induced by the presence of the SiO2 passivation layer correspond partly to increased carrier concentrations in the Al1-xGa1-xN barrier relative to those in the 2DEG. Since the mobility in the Al1-xGa1-xN barrier is expected to be considerably lower than that in the 2DEG, a reduction in overall mobility upon deposition of the SiO2 passivation layer is to be expected. From the data shown in Figs. 2(b) and 3(b) immediately prior to and following deposition of the SiO2 passivation layer, we derive values of 1090 and 280 cm2/V s for \( \mu_{2\text{DEG}} \) and \( \mu_b \), respectively, for the sample containing a doped Al0.25Ga0.75N barrier, and values of 950 and 100 cm2/V s for \( \mu_{2\text{DEG}} \) and \( \mu_b \), respectively, for the sample containing an undoped Al0.30Ga0.70N barrier. The values derived for \( \mu_{2\text{DEG}} \) are within expectations for Al1-xGa1-xN/GaN HFET samples, and the values for \( \mu_b \) are consistent with those deduced from analysis of current-voltage characteristics in Al1-xGa1-xN/GaN HFETs. 26

The observed increase in carrier concentration following deposition of the SiO2 passivation layer should lead to reductions in source and drain series resistance in an Al1-xGa1-xN/GaN HFET device, resulting in an increase in transistor currents. 27 These expectations are consistent with studies in which an increase in saturated current density was reported following silicon nitride passivation of an Al1-xGa1-xN/GaN HFET. 13 The reduction in \( \phi_b \) deduced from our measurements indicates that the Al1-xGa1-xN/SiO2 interface contains a significantly different electronic density of states compared to that present at the free Al1-xGa1-xN surface, and studies of GaN/SiO2 interfaces suggest the presence of a relatively low density of states at the nitride–SiO2 interface. 22–25

Studies of Al1-xGa1-xN/GaN HFET structures have also been invoked to suggest that donor-like states at the Al1-xGa1-xN surface with a density of \( 1.1 \times 10^{13} \text{ cm}^{-2} \) or higher are present and become positively charged, thereby compensating much of the negative polarization charge at the Al1-xGa1-xN surface and providing carriers to the 2DEG at the Al1-xGa1-xN/GaN interface. 19 Should the presence of SiO2 silicon nitride, or other dielectric passivation layers lead to a reduction in surface-state density, the mechanisms by which the polarization charge at the AlGaN surface is compensated and by which carriers are provided to the 2DEG would remain to be elucidated. Charges in the passivation layer, as indicated schematically in Fig. 4, are one possibility.

IV. CONCLUSIONS

We have performed detailed studies of the influence of a variety of annealing procedures, surface processing treatments, and surface passivation layers on carrier concentrations and transport properties in Al1-xGa1-xN/GaN HFET epitaxial layer structures. In previous studies, silicon nitride passivation layers have been found to lead to increased dc current density and improved rf power output in Al1-xGa1-xN/GaN HFET’s. 13 and SiO2 surface passivation was found to reduce leakage current in III–V nitride Schottky diodes. 14 In addition, there is growing interest in the use of SiO2 as a gate insulator in III–V nitride HFETs. 15, 28 The current studies were motivated by a desire to assess the influence of surface processing and of surface passivation layers on the electronic properties of the Al1-xGa1-xN surface and, by extension, the properties of the 2DEG in an Al1-xGa1-xN/GaN HFET structure. Our studies have shown that surface chemical treatments have little effect on 2DEG carrier concentration and produce at most a slight degradation in mobility. However, deposition of a SiO2 layer by PECVD induces a significant increase in carrier concentration and decrease in mobility that is largely reversed upon removal of the SiO2 layer by wet etching. The observed increases in carrier concentration and reductions in mobility are quantitatively consistent with a shift in the Fermi level at the Al1-xGa1-xN surface of approximately 1 eV towards the conduction-band edge in the presence of the SiO2 layer compared to its position for the free Al1-xGa1-xN surface for Al concentrations of 25%–30%. These results indicate that the electronic density of states at the Al1-xGa1-xN surface is altered significantly, and possibly reduced, in the presence of the SiO2 passivation layer. In the latter case, alternate mechanisms for compensation of polarization charge at the AlGaN surface and for providing carriers to the 2DEG might need to be invoked.

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