Demonstration and analysis of reduced reverse-bias leakage current via design of nitride semiconductor heterostructures grown by molecular-beam epitaxy

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An approach for reducing reverse-bias leakage currents in Schottky contacts formed to nitride semiconductor heterostructures grown by molecular-beam epitaxy is described, demonstrated, and analyzed. By incorporation of a GaN cap layer atop a conventional $Al_xGa_{1-x}N/GaN$ heterostructure field-effect transistor epitaxial layer structure, the direction of the electric field at the metal-semiconductor interface of a Schottky contact is reversed, resulting in a suppression of electron flow into conductive screw dislocations that are known to dominate reverse-bias leakage currents in nitride semiconductors grown by molecular-beam epitaxy. Analysis of temperature-dependent current-voltage characteristics indicates that, in structures incorporating a GaN cap layer, reverse-bias leakage currents are reduced by one to three orders of magnitude, with the mechanism for leakage current flow differing from that established previously for the more conventional structure due to the alteration in the electric field at the metal-semiconductor interface. Scanned probe measurements of local, nanoscale current distributions confirm directly that current flow via conductive dislocations is suppressed in structures incorporating the GaN cap layer. © *2006 American Institute of Physics*. [DOI: 10.1063/1.2150591]

I. INTRODUCTION

High levels of reverse-bias leakage current in Schottky contacts formed to *n*-type nitride semiconductor material grown by molecular-beam epitaxy (MBE) are a major concern in efforts to develop high-performance $Al_xGa_{1-x}N/GaN$ heterostructure field-effect transistor (HFET) structures based on MBE-grown material.[1,2] A number of studies have helped to elucidate the nature of these leakage currents, which have been shown to arise due to the presence of highly conductive screw dislocations,[3–6] and guide the development of strategies for their mitigation based on selective suppression of current flow associated with these dislocations via local surface oxidation.[7,8]

More recently, studies of temperature-dependent current-voltage characteristics for Schottky diodes fabricated from MBE-grown *n*-type GaN and $Al_xGa_{1-x}N/GaN$ HFET structures have revealed that, at temperatures of ~250 K and above, Frenkel-Poole emission of electrons from near-surface traps in the nitride semiconductor material into conductive dislocation states is the key process governing reverse-bias leakage current flow.[9] The Frenkel-Poole emission process is a strong function of the electric field at the metal-semiconductor interface, suggesting that design of a nitride heterostructure in which the electric field at that interface is appropriately engineered could serve as a highly effective approach for suppressing leakage current flow via conductive dislocations.

In the present study, we have shown that incorporation of a thin GaN layer capping the conventional AlGaN/GaN HFET epitaxial layer structure, by reversing the direction of the electric field at the metal-semiconductor interface compared to that present in the conventional HFET structure, serves to reduce the reverse-bias leakage current in Schottky contacts by suppressing carrier transport into conductive dislocation states. At low to moderate reverse-bias voltages, the presence of the GaN cap layer causes the electric field at the metal-semiconductor interface to oppose the flow of electrons into conductive dislocation states, thereby eliminating the primary source of reverse-bias leakage current. At large reverse-bias voltages, leakage current conduction via dislocations does occur, but is significantly suppressed due to the reduced magnitude of the electric field compared to that in a conventional HFET structure.

It should be noted that this mechanism for reverse-bias leakage current suppression in structures containing such a GaN capping layer is different from that reported in earlier studies of similar structures grown by metal organic vapor phase epitaxy (MOVPE).[10] In these earlier studies, the principal mechanism for reduction of Schottky contact leakage current was the increase in effective barrier height induced by the presence of negative polarization charge at the upper GaN/AlGaN interface, as highly conductive screw dislocations are not found to be present in nitride semiconductor material grown by techniques other than MBE.[11,12] The suppression of leakage current flow in MBE-grown nitride material described here is associated specifically with the nature of the electric field at the metal-semiconductor interface and the suppression of the Frenkel-Poole emission process, and is not dependent on the barrier height itself.

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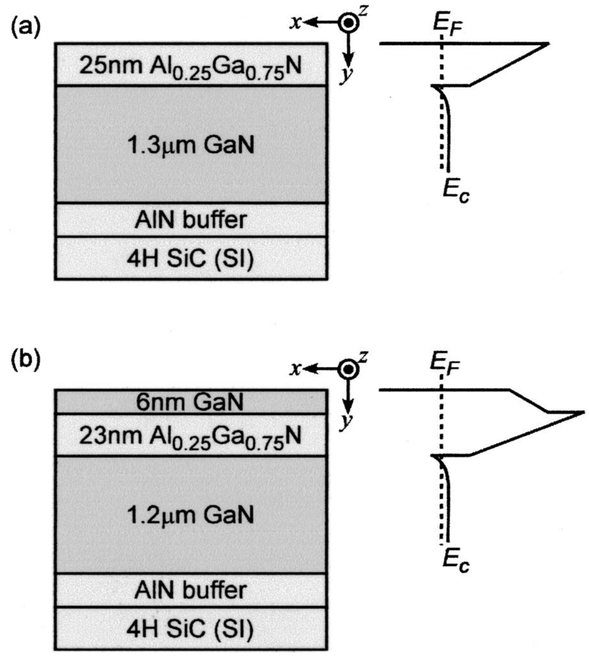

FIG. 1. Epitaxial layer structure and schematic energy-band-edge diagram for (a) conventional $Al_{0.25}Ga_{0.75}N/GaN$ HFET structure, and (b) $GaN/Al_{0.25}Ga_{0.75}N/GaN$ HFET structure incorporating a GaN cap layer.

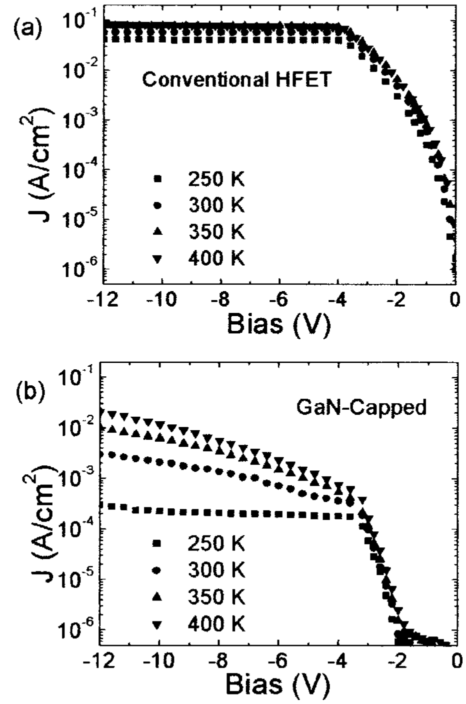

FIG. 2. Reverse-bias current-voltage characteristics at temperatures ranging from 250 to 400 K for (a) conventional $Al_{0.25}Ga_{0.75}N/GaN$ HFET structure, and (b) $GaN/Al_{0.25}Ga_{0.75}N/GaN$ HFET structure incorporating a GaN cap layer.

II. EXPERIMENT

The samples used in these studies were grown by MBE, with the epitaxial layer structures and schematic energy-band-edge diagrams shown in Fig. 1. The conventional HFET structure, shown in Fig. 1(a), consisted of a 25 nm $Al_{0.25}Ga_{0.75}N$ barrier layer atop a 1.3 μm GaN channel layer. Both layers are nominally undoped, and the structure was grown on an AlN nucleation layer deposited at 720 °C on a 4H semi-insulating SiC substrate. The GaN-capped HFET structure, shown in Fig. 1(b), consisted of a 6 nm GaN cap layer grown on a 23 nm $Al_{0.25}Ga_{0.75}N$ layer atop a 1.2 μm GaN channel layer. As in the first structure, all layers are nominally undoped and were grown on an AlN nucleation layer deposited on a 4H semi-insulating SiC substrate. Ohmic contact rings were formed using Ti/Al/Ti/Au metallization deposited by electron-beam evaporation and annealed at 800 °C for 1 min (GaN-capped HFET structure) or 3 min (conventional HFET structure). Schottky contacts consisting of 125-μm-diam dots were then formed within the Ohmic contact rings using Ni metallization and a conventional liftoff process. Current-voltage characteristics were measured for all Schottky diodes fabricated in this manner at temperatures ranging from 250 to 400 K.

Local conductivity measurements were carried out by conductive atomic force microscopy (AFM) in a modified Digital Instruments Nanoscope® IIIa MultiMode™ microscope under ambient atmospheric conditions (~20 °C with 50% relative humidity). The conductive AFM technique has been described previously.[13] Briefly, a highly doped diamond-coated tip is held in contact with the sample surface and acts as a Schottky contact to the sample. While scanning in contact mode, forward (reverse) bias conditions are established through the application of a negative (positive) bias to an Ohmic contact on the *n*-type sample surface and the current through the tip is measured with a current amplifier; in this manner, correlated topographic and current images are obtained.

Numerical modeling was used to determine the energy-band-edge profiles and electric field distributions in these structures as functions of bias voltage applied to the Schottky contact. Specifically, two-dimensional simulations of potential, carrier, and electric field distributions were performed using Silvaco simulation software. Two-dimensional simulations were required to enable us to model accurately the vertical electric field near the metal-semiconductor Schottky interface at bias voltages below the threshold voltage for accumulation of electrons in the two-dimensional electron gas (2DEG) formed at the lower $GaN/Al_{0.25}Ga_{0.75}N$ interface.

III. RESULTS AND DISCUSSION

Figure 2 shows reverse-bias current-voltage characteristics for Schottky diodes fabricated from the conventional and GaN-capped HFET structures at temperatures ranging from 250 to 400 K. At 300 K, the reverse-bias leakage currents are reduced by approximately one to three orders of magnitude, depending on the bias voltage, in the GaN-capped HFET structure compared to those in the conventional HFET; the reduction is most pronounced at bias voltages of 0 to −4 V.

To elucidate the origin of the reduction in leakage current in the GaN-capped structure, we have used two-dimensional numerical simulations to determine the energy-band-edge profiles, carrier distributions, and electric fields in both structures shown in Fig. 1. In the simulation, the

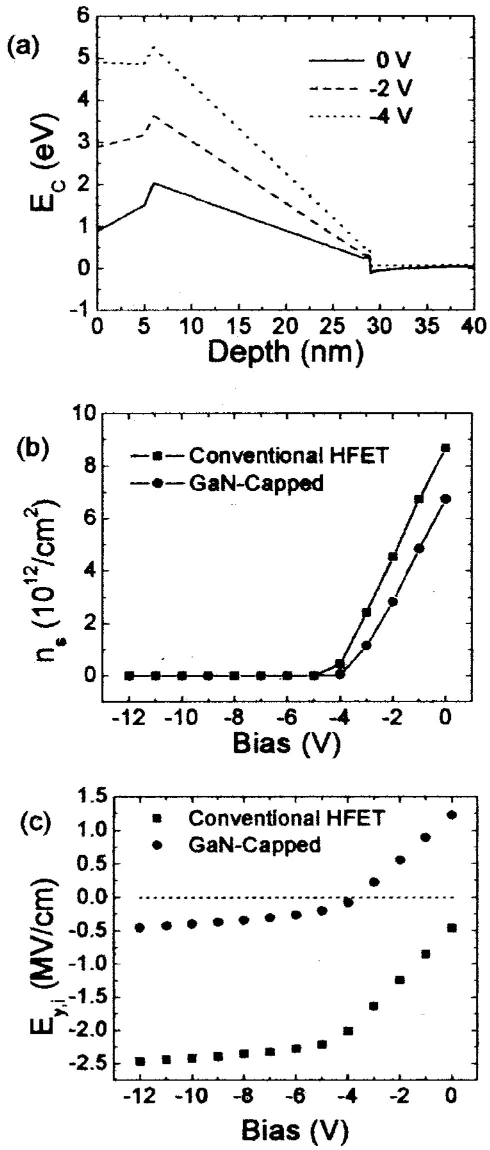

FIG. 3. (a) Conduction-band-edge energy profile for the GaN-capped HFET structure at bias voltages of 0 V, −2 V, and −4 V. (b) Electron sheet concentration in the channel of the conventional and GaN-capped HFET structures, as functions of bias voltage. (c) Vertical electric field at the metal-semiconductor Schottky interface of the conventional and GaN-capped HFET structures, as functions of bias voltage.

Schottky contact dot was approximated by a 125 μm wide metal strip with a work function of 5.0 eV. The concentric Ohmic contact ring was represented by two parallel metal strips 120 μm in width located on each side of the Schottky contact, separated from the Schottky contact by 17.5 μm as in the actual fabricated Schottky diodes. The epitaxial layer structures were as shown in Fig. 1, with a donor concentration of 5×10^{16} cm^{-3}, representing unintentional background doping, in each layer. A polarization charge density of 1.15 $\times 10^{13}$ cm^{-2} was assumed to be present at the GaN/$Al_{0.25}Ga_{0.75}N$ interfaces.[14,15] These simulations enabled us to determine accurately the vertical electric field $E_{y,i}$ at the metal-semiconductor Schottky interface over the entire range of bias voltages studied experimentally.

Figure 3(a) shows the conduction-band-edge energy profile for the GaN-capped structure at bias voltages of 0 V, −2 V, and −4 V. At 0 V and −2 V, the electric field $E_{y,i}$ at the metal-semiconductor interface is positive, i.e., directed away from the interface into the semiconductor, whereas in the conventional HFET structure $E_{y,i}$ would point in the opposite direction. At −4 V, however, $E_{y,i}$ at the interface is nearly zero, while at more negative bias voltages $E_{y,i}$ is in the same direction as in the conventional HFET structure. Figure 3(b) shows the electron concentration in the 2DEG, n_s, as a function of bias voltage for the conventional and GaN-capped HFET structures. The threshold voltages for both structures are at approximately −4 V, although the carrier concentrations in the GaN-capped structure are systematically lower than in the conventional HFET structure due to partial depletion of electrons by the negative polarization charge at the upper GaN/$Al_{0.25}Ga_{0.75}N$ interface in the former.[10] Figure 3(c) shows the vertical electric field, $E_{y,i}$, at the metal-semiconductor interface as a function of bias voltage. A comparison of Fig. 3(b) and Fig. 3(c) shows that the "kinks" in $E_{y,i}$ as a function of bias voltage near −4 V coincide with the threshold voltages for electron accumulation in the 2DEG in each structure; these "kinks" occur because at voltages below the threshold voltage, the field penetrates below the 2DEG channel and there is a substantial lateral component to the electric field between the Schottky and Ohmic contacts, reducing the dependence of $E_{y,i}$ on applied bias. For the conventional HFET structure, we see that $E_{y,i}$ is negative, i.e., the electric field is directed out of the semiconductor, at all bias voltages shown. For the GaN-capped structure, $E_{y,i}$ is negative only for bias voltages below approximately −4 V, and in this range of voltages $E_{y,i}$ is much smaller in magnitude than in the conventional HFET structure.

The size and direction of $E_{y,i}$ at the metal-semiconductor interface is significant because of the nature of the Frenkel-Poole emission process that dominates reverse-bias leakage current flow in these structures at the temperatures shown here.[9] Specifically, the current density in the Frenkel-Poole emission model is given by

$$J = CE_{y,i} \exp\left(-\frac{q(\phi_t - \sqrt{-qE_{y,i}/\pi\varepsilon_0\varepsilon_s})}{kT}\right), \quad (1)$$

where C is a constant, q is the electron charge magnitude, ϕ_t is the electron emission barrier height, ε_s is the high frequency dielectric permittivity, ε_0 is the permittivity of free space, k is Boltzmann's constant, and T is the temperature. Our earlier studies established values for ϕ_t of 0.33 ± 0.01 V and 0.30 ± 0.03 V for GaN and $Al_{0.25}Ga_{0.75}N$, respectively, and for ε_s of 5.4 ± 0.1 and 5.1 ± 1.0 for GaN and $Al_{0.25}Ga_{0.75}N$, respectively.[9] Because of the dependence of J on $E_{y,i}$ in the exponential function in Eq. (1), it is anticipated that reversal of the sign of $E_{y,i}$, as occurs in the GaN-capped structure for bias voltages above −4 V, will dramatically suppress the Frenkel-Poole emission process and consequently leakage current flow via conductive dislocations; the reduction in magnitude of $E_{y,i}$ in the GaN-capped structure at more negative bias voltages should, while not eliminating dislocation-related leakage current, substantially reduce its magnitude.

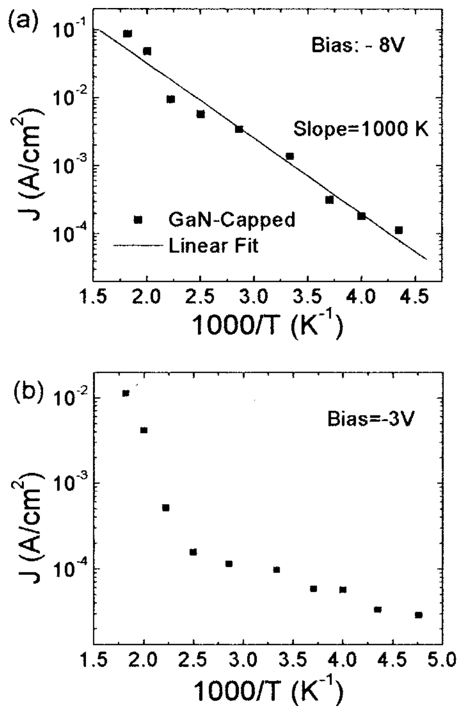

FIG. 4. Current density as a function of inverse temperature for the GaN-capped HFET structure at bias voltages of (a) −8 V and (b) −3 V.

Our previous studies[9] have established that, at moderate negative bias voltages, reverse-bias leakage current flow in the conventional HFET structure within the temperature range studied here is well described by the Frenkel-Poole emission model. For large negative bias voltages the Frenkel-Poole emission model is no longer physical, as the large magnitude of $E_{y,i}$ yields a negative emission barrier, for which the current should saturate rather than continue to increase exponentially. We believe this explains the very weak dependence of leakage current density on bias voltage, and correspondingly on electric field, for bias voltages below approximately −4 V in the conventional HFET structure, which is in contrast to the significant dependence of leakage current density on bias voltage in this same voltage range for the GaN-capped structure, in which the magnitude of $E_{y,i}$ is much smaller.

To determine the applicability of the Frenkel-Poole emission model, and hence the influence of leakage current flow via conductive dislocations, in the GaN-capped structure, we consider the measured current density as a function of temperature for this structure, as shown in Fig. 4. Figure 4(a) shows current density as a function of inverse temperature at −8 V bias; as predicted by Eq. (1), $\log J$ varies linearly with $1/T$, with a slope determined by least-squares fitting to be 1000 ± 70 K. From this value for the slope, combined with an electric field determined from Fig. 3(c) of -3.4×10^5 V/cm at −8 V and $\varepsilon_s = 5.4$ for GaN, we derive a barrier height $\phi_t = 0.38 \pm 0.03$ V. Repeating this analysis for bias voltages ranging from −4 V to −12 V, we obtain an average value for ϕ_t of 0.37 ± 0.1 V, which is in good agreement with the value 0.33 ± 0.01 V determined independently in our earlier studies. This analysis confirms that in this range of bias voltages, the reverse-bias leakage current in the GaN-capped structure is, as expected, dominated by the Frenkel-Poole emission process and carrier transport along conductive dislocations. However, due to the reduced magnitude of the electric field $E_{y,i}$ compared to that in a conventional AlGaN/GaN HFET structure at the same bias voltage, the reverse-bias leakage current is substantially reduced.

Figure 4(b) shows current density as a function of inverse temperature for the GaN-capped structure at −3 V bias. From Fig. 3(c), we see that at this bias voltage, the direction of the electric field is opposite to that at more negative bias voltages; consequently, the Frenkel-Poole emission process and current flow along conductive dislocation states are suppressed, and the linear dependence of $\log J$ on $1/T$ is not observed. At this bias voltage, and in general for bias voltages at which the electric field $E_{y,i}$ is directed towards the semiconductor, the dominant source of reverse-bias leakage current in conventional AlGaN/GaN HFET structures grown by MBE is therefore suppressed, leading to a large reduction in leakage current.

The applicability of the Frenkel-Poole emission model in describing, quantitatively, reverse-bias current flow over a wide range of bias voltages provides very clear evidence that the influence of the GaN cap layer on current flow is predominantly via suppression of Frenkel-Poole emission from near-surface trap states into dislocations, rather than through other possible effects such as a reduction in threading dislocation density, or some other improvement in structural quality, at the metal-semiconductor interface. However, to confirm further the effect of the GaN capping layer in suppressing current flow into and along conductive dislocations, we examine AFM topographs and conductive AFM current images of both the conventional and GaN-capped HFET structures. Figures 5(a) and 5(b) show topographic and current images of the conventional HFET structure obtained at bias voltages of −8 V and −12 V, respectively, applied to the conducting probe tip. In both current images, highly conductive regions corresponding to screw dislocations are clearly visible as dark spots (negative current) in the images, with visible conductive dislocation densities of 3.6×10^8 cm^{-2} at −8 V and 1.0×10^9 cm^{-2} at −12 V. Figures 5(c) and 5(d) show topographic and current images of the GaN-capped HFET structure, also obtained at bias voltages of −8 V and −12 V, respectively. No conductive dislocations are visible in the image obtained at −8 V, while at −12 V a conductive dislocation density of approximately 1.5×10^8 cm^{-2} is evident.

We interpret the results shown in Fig. 5 as follows. In the conventional HFET sample, the localized current paths imaged at negative bias voltage confirm the prominence of conductive screw dislocations in giving rise to the leakage currents observed, as shown in Fig. 2(a), in macroscopic Schottky diodes fabricated from those structures. The observable leakage path density increases substantially between −8 V and −12 V, despite only a minimal change in macroscopic Schottky diode leakage current between these voltages. We attribute this to two factors. First, at −8 V the current observed at each point near a conductive dislocation is near the threshold of detection in our system (approximately 0.1 pA); as the bias voltage becomes more negative, proba-

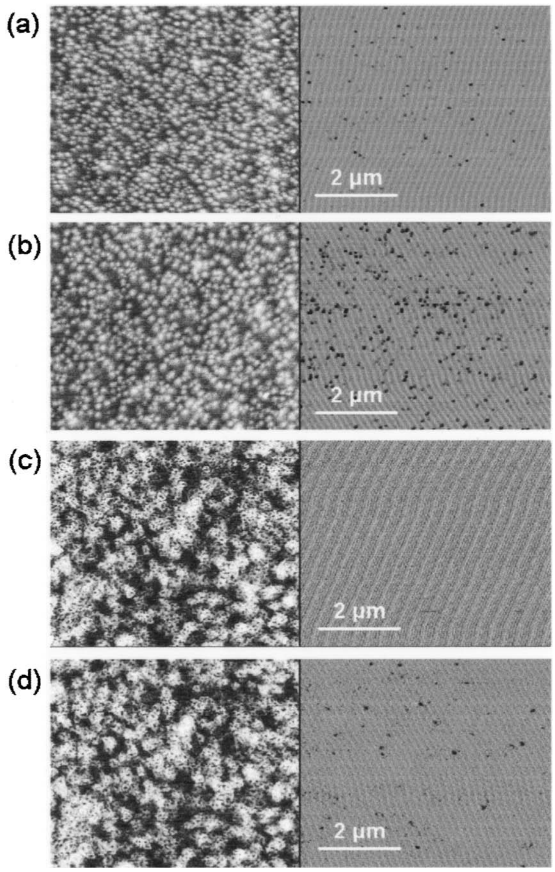

FIG. 5. Topographic (left) and current (right) images of conventional and GaN-capped HFET structures obtained via conductive atomic force microscopy. (a) Conventional HFET structure at −8 V bias. (b) Conventional HFET structure at −12 V bias. (c) GaN-capped HFET structure at −8 V bias. (d) GaN-capped HFET structure at −12 V bias.

bilistically a greater number of conductive dislocations exceed the threshold for detection, causing the observable leakage path density to increase despite a minimal change in macroscopic leakage current. Second, the pixel spacing for the images shown in Fig. 5 is approximately 40 nm, which combined with a typical tip radius of 10–20 nm means that the probe tip often may not sample the location directly above the dislocation core. The maximum electric field above the dislocation core will vary depending on the distance between the tip and the dislocation, but will increase in magnitude with increasing bias voltage magnitude. Thus, at more negative bias voltages the likelihood of the electric field above a dislocation core exceeding the value required for the current to exceed our detection threshold will increase, leading to a corresponding increase in observable leakage current density. However, the detection probability increases very rapidly with electric field $E_{y,i}$, and therefore fairly rapidly with bias voltage, eventually saturating at unity—at which point any further increase of the reverse bias voltage would not increase the concentration of detected leakage paths.

In the GaN-capped HFET sample, these same considerations apply, but due to the reduced magnitude of the electric field above the dislocation core at a given bias voltage, compared to that present for the conventional HFET structure, a substantially larger magnitude bias voltage is required to attain current levels in each leakage path that exceed our detection threshold. Thus, the conductive dislocations become visible in conductive AFM current images only at bias voltages of −12 V and below in the GaN-capped HFET structure, corresponding to a vertical electric field $E_{y,i}$ of -5×10^5 V/cm; this is consistent with our earlier studies of local current flow in *n*-type GaN epitaxial layers, in which the minimum electric field at which conductive dislocations were visible was similar in magnitude.[16] Thus we observe directly by conductive AFM that incorporation of the GaN capping layer in the HFET structure reduces the current flow associated with an individual conductive dislocation very substantially at a given bias voltage compared to that for a conventional HFET structure, thereby confirming the role of the GaN capping layer in suppressing reverse-bias leakage currents associated with conductive dislocations in MBE-grown nitride material. More generally, these results indicate that the direction and magnitude of the electric field at a metal-semiconductor interface can be engineered in the design of MBE-grown nitride semiconductor heterostructures to suppress reverse-bias Schottky leakage currents arising from the presence of conductive dislocations.

IV. CONCLUSIONS

In summary, we have demonstrated a strategy for reduction of leakage currents in Schottky contacts to MBE-grown nitride-based HFET structures based on engineering of the electric field near the metal-semiconductor Schottky interface to reduce Frenkel-Poole emission into conductive dislocations. Building upon prior studies in our group that elucidated basic mechanisms of leakage current in MBE-grown nitride semiconductor material, we have compared temperature-dependent current-voltage characteristics and scanned probe imaging of a conventional HFET structure and an HFET structure incorporating a GaN capping layer. The reverse-bias leakage current is found to be reduced by approximately one to three orders of magnitude in the structure incorporating the GaN capping layer, with the reduction being most pronounced at small reverse bias voltages. Two-dimensional numerical simulations of these device structures are used to determine the electric field at the metal-semiconductor interface as a function of bias voltage, and the current-voltage characteristics of the GaN-capped HFET structure are analyzed in terms of the Frenkel-Poole emission mechanism shown in prior work to be the key process in leakage current flow via conductive dislocations. At large negative bias voltages, for which the electric field is directed towards the semiconductor, the leakage current in the GaN-capped structure is well described by the Frenkel-Poole emission model, indicating that current flow via conductive dislocations dominates; however, the magnitude of current observed is much lower than in the conventional HFET structure, as predicted by the Frenkel-Poole emission model based on the reduced magnitude of the electric field in the GaN-capped structure. At smaller negative bias voltages, for which the electric field is directed away from the semiconductor, the leakage current in the GaN-capped structure is dramatically reduced compared to that in the conventional

HFET, and the observed temperature dependence of the current is not consistent with Frenkel-Poole emission—indicating that a different physical mechanism is contributing to the current flow. AFM topographic images and conductive AFM current images confirm that current flow via dislocations dominates reverse-bias leakage in the conventional HFET structure and, at sufficiently large negative bias voltages, in the GaN-capped structure, while at smaller reverse-bias voltages the contribution of conductive dislocations to leakage currents in the GaN-capped structure is suppressed. These results also suggest an obvious, more general strategy that can be employed to reduce reverse-bias Schottky leakage currents in MBE-grown nitride semiconductor material.

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