Analysis of leakage current mechanisms in Schottky contacts to GaN and $Al_{0.25}Ga_{0.75}N/GaN$ grown by molecular-beam epitaxy

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Temperature-dependent current-voltage measurements combined with conductive atomic force microscopy and analytical modeling have been used to assess possible mechanisms of reverse-bias leakage current flow in Schottky diodes fabricated from GaN and $Al_{0.25}Ga_{0.75}N/GaN$ structures grown by molecular-beam epitaxy. Below 150 K, leakage current is nearly independent of temperature, indicating that conduction is dominated by tunneling transport. At higher temperatures, leakage current in both GaN and $Al_{0.25}Ga_{0.75}N/GaN$ diode structures is well described by a Frenkel-Poole emission model. Based on the inferred emission barrier heights and the observation that room-temperature leakage current is dominated by the presence of highly conductive dislocations, it is suggested that the key carrier transport process is emission of electrons from a trap state near the metal-semiconductor interface into a continuum of states associated with each conductive dislocation. In this model for leakage current flow, the emission barrier heights measured for the GaN and $Al_{0.25}Ga_{0.75}N/GaN$ diode structures indicate that the conductive dislocation states are aligned in energy between GaN and $Al_{0.25}Ga_{0.75}N$. © *2006 American Institute of Physics*. [DOI: 10.1063/1.2159547]

I. INTRODUCTION

Excessive reverse-bias leakage current in *n*-type Schottky contacts remains an outstanding challenge in the development of electronic devices, most notably $Al_xGa_{1-x}N/GaN$ heterostructure field-effect transistor (HFET) structures, based on nitride semiconductor material grown by molecular-beam epitaxy (MBE).[1] Conduction associated with threading screw dislocations, which are generally present in high concentrations in epitaxially grown nitride semiconductor material, has been shown to be the dominant source of high leakage currents at room temperature.[2–4] A variety of methods has been developed to suppress the influence of conductive dislocations on reverse-bias leakage currents in Schottky contacts to *n*-type GaN grown by MBE.[5,6] However, more detailed characterization and a more complete understanding of the relevant mechanisms of current transport are desirable both on fundamental scientific grounds and to inform the development of simpler and more effective methods for minimizing Schottky contact leakage current in devices.

In previous work,[7] analysis of temperature-dependent current-voltage characteristics of Schottky diodes formed on *n*-type GaN grown by MBE was used to elucidate possible mechanisms of carrier transport associated with reverse-bias leakage currents. While tunneling transport appeared to be dominant at low temperatures, it was not possible to pinpoint a single mechanism responsible for leakage current transport at room temperature, although trap-assisted tunneling and one-dimensional variable-range hopping emerged as prominent possibilities. In the present study, we have extended this analysis to include studies of temperature-dependent current-voltage characteristics in Schottky diodes formed on $Al_xGa_{1-x}N/GaN$ HFET structures as well as *n*-type GaN. By confirming the role of conductive dislocations in leakage currents for both GaN and $Al_xGa_{1-x}N/GaN$ structures, and therefore requiring a single model to describe reverse-bias leakage current flow in both structures, it is possible at any given temperature between 110 and 400 K to identify a single conduction mechanism—tunneling at low temperature and Frenkel-Poole emission at higher temperatures—that correctly describes current transport in both structures.

II. EXPERIMENT

All samples used in these studies were grown by MBE. The GaN sample consisted of 350 nm GaN deposited at 660 °C near the upper crossover point in the Ga droplet regime[8] on a 2 μm GaN template layer grown by metal-organic chemical-vapor deposition (MOCVD) on a sapphire substrate. The MBE-grown GaN layer was *n* type with a dopant concentration in the mid-10^{16} cm^{-3} range. The $Al_xGa_{1-x}N/GaN$ HFET structure consisted of 25 nm $Al_{0.25}Ga_{0.75}N$ grown on a 1.3 μm GaN layer; both layers were nominally undoped and were deposited on a 4H semi-insulating SiC substrate at 720 °C. Ti/Al metallization annealed either at 750 °C for 30 s (on GaN) or at 800 °C for 3 min (on $Al_{0.25}Ga_{0.75}N/GaN$) was employed to form Ohmic contact rings, within which 125-μm-diam Ni dots were used to form Schottky contacts. Current-voltage characteristics were measured for all Schottky diodes fabricated in this manner at temperatures ranging from 110 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

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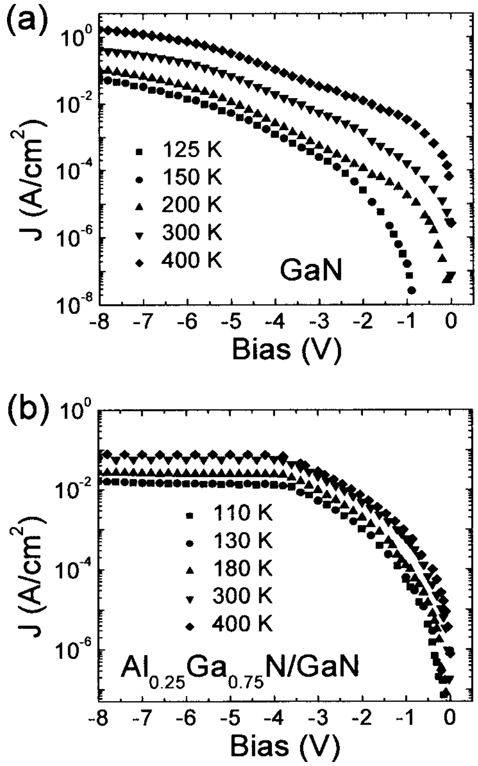

FIG. 1. Current density vs bias voltage for Schottky diodes fabricated on (a) GaN and (b) $Al_{0.25}Ga_{0.75}N$/GaN HFET epitaxial layer structures, for temperatures ranging from 110 to 400 K.

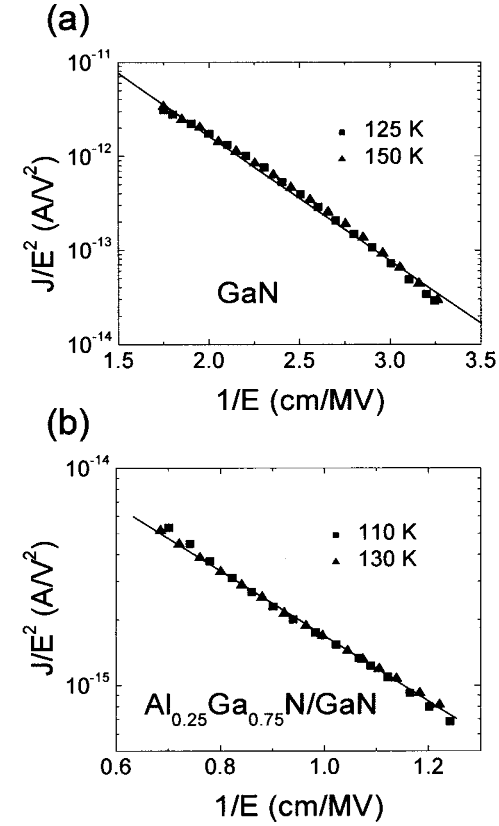

FIG. 2. Measured current density divided by the square of the electric field vs inverse electric field for Schottky diodes fabricated on (a) GaN and (b) $Al_{0.25}Ga_{0.75}N$/GaN HFET epitaxial layer structures, for temperatures ranging from 110 to 150 K.

50% relative humidity). The conductive AFM technique has been described previously.[5] 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.

III. RESULTS AND DISCUSSION

Given the large *n*-type barrier heights typical for Schottky contacts to GaN and $Al_xGa_{1-x}N$, we assume that thermionic emission over the Schottky barrier makes only a negligible contribution to reverse-bias current flow. Figure 1 shows the current density as a function of bias voltage for the GaN and $Al_{0.25}Ga_{0.75}N$/GaN Schottky diodes. At temperatures below approximately 150 K, the reverse-bias leakage current is nearly independent of temperature, suggesting that tunneling is the dominant source of current flow. Because the electric-field profile within the $Al_{0.25}Ga_{0.75}N$/GaN HFET structure differs from that in a conventional Schottky contact to an *n*-type semiconductor, we describe the current density as a function of the electric field in the barrier, which is then calculated as a function of bias voltage in each structure. In this approach, the current density is given by the Fowler-Nordheim tunneling expression,[9,10]

$$J = AE_b^2 \exp\left(-\frac{B}{E_b}\right), \tag{1a}$$

$$A = \frac{q^2(m_e/m_n^*)}{8\pi h\phi_b} = 1.54 \times 10^{-6}\frac{(m_e/m_n^*)}{\phi_b} \quad \left(\frac{A}{V^2}\right), \tag{1b}$$

$$B = \frac{8\pi\sqrt{2m_n^*(q\phi_b)^3}}{3qh} = 6.83 \times 10^7 \sqrt{(m_n^*/m_e)(q\phi_b)^3} \quad \left(\frac{V}{\text{cm}}\right), \tag{1c}$$

where E_b is the electric field in the semiconductor barrier, q is the fundamental electronic charge, m_e is the free-electron mass, m_n^* is the conduction-band effective mass in the semiconductor, h is Planck's constant, and ϕ_b is the effective barrier height at the Schottky contact, taking into account image-force lowering of the barrier. For the GaN Schottky diode, m_n^* is taken to be that of GaN, while the electric field in Eq. (1a) is assumed to be that at the metal-GaN interface. For the $Al_{0.25}Ga_{0.75}N$/GaN HFET structure, m_n^* is taken to be that of $Al_{0.25}Ga_{0.75}N$ and the electric field is calculated assuming that the field is constant within the $Al_{0.25}Ga_{0.75}N$ barrier layer.

Figure 2 shows a log-scale plot of J/E_0^2 as a function of $1/E_b$ for both the GaN and $Al_{0.25}Ga_{0.75}N$/GaN HFET Schottky diodes, at temperatures between 110 and 150 K. The two curves shown for each diode structure are nearly

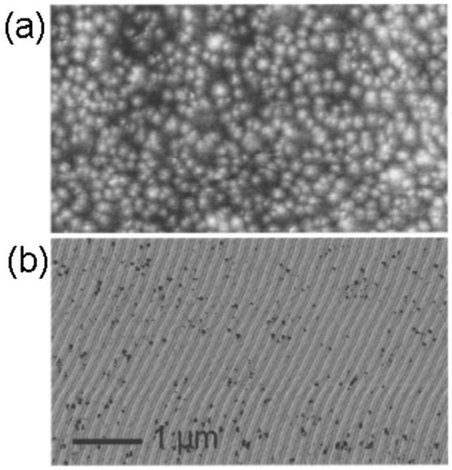

FIG. 3. (a) Topographic and (b) current images of the $Al_{0.25}Ga_{0.75}N/GaN$ HFET structure, obtained by conductive AFM.

identical, confirming the very weak temperature dependence of the current in this range of temperatures. From Eqs. (1) we see that, according to the Fowler-Nordheim tunneling model, the slope of $\log(J/E_0^2)$ vs $1/E_b$ should be independent of temperature—in good agreement with the data shown in Fig. 2—and proportional to $\sqrt{m_n^* \phi_b^3}$. Assuming effective barrier heights of 0.84 eV for GaN and 1.17 eV for $Al_{0.25}Ga_{0.75}N$,[11] we derive effective masses from the data in Fig. 2 of $(3.4\pm0.3)\times10^{-3}m_e$ and $(1.8\pm0.2)\times10^{-3}m_e$ for GaN and $Al_{0.25}Ga_{0.75}N$, respectively. While these effective-mass values are much smaller than typically measured or estimated values of $0.22m_e$ for GaN and $\sim0.4m_e$ for $Al_{0.25}Ga_{0.75}N$,[12,13] they are consistent with those obtained in other similar analyses of tunneling transport in Schottky contacts to n-type nitride semiconductors. The small effective-mass values inferred from these and other transport measurements are most likely indicative of the presence of additional mechanisms of current transport such as defect-assisted tunneling, which would tend to decrease the apparent value of the effective mass in an analysis of transport by tunneling. The smaller value of effective mass inferred for $Al_{0.25}Ga_{0.75}N$ compared to GaN suggests that these defect-related tunneling transport mechanisms are more prevalent in $Al_{0.25}Ga_{0.75}N$ than in GaN, as might be expected. However, the observed dependence of the current densities on electric field and their very weak dependence on temperature indicate that tunneling is, in fact, the dominant mechanism of current transport at temperatures below approximately 150 K.

At room temperature, reverse-bias leakage currents in Schottky contacts to n-type nitride semiconductor material grown by MBE are typically associated with the presence of conductive screw dislocations.[2,3,5,6] Figure 3 shows AFM topograph and conductive AFM image of corresponding areas for $Al_{0.25}Ga_{0.75}N/GaN$ epitaxial layer structures. The conductive AFM images were obtained under reverse-bias conditions, with a voltage of +12 V applied to the sample. Localized regions of high current flow associated with conductive dislocations are clearly visible, with density of approximately 1×10^9 cm^{-2}. The conductive AFM measurement on the GaN sample has been performed by Miller *et al.*,[14] with density of about 3×10^7 cm^{-2}. The observation of these conductive dislocations confirms their role, at room temperature, in reverse-bias leakage current flow in both structures.

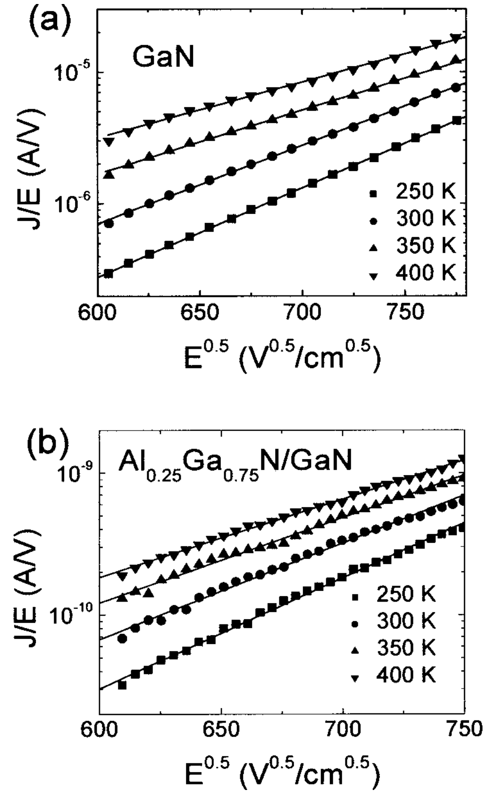

FIG. 4. Measured current density divided by the electric field vs square root of electric field, for Schottky diodes fabricated on (a) GaN and (b) $Al_{0.25}Ga_{0.75}N/GaN$ HFET epitaxial layer structures, for temperatures ranging from 250 to 400 K.

For temperatures above 250 K, the measured macroscopic current densities in both GaN and $Al_{0.25}Ga_{0.75}N/GaN$ Schottky diodes are observed to be dependent on both electric field and temperature. Specifically, as shown in Fig. 4, we observe for both diode structures a linear dependence of $\log(J/E_b)$ on $\sqrt{E_b}$, where J is the current density and E_b the electric field at the semiconductor surface; J is also observed to increase rapidly with increasing temperature. Given the dominance of dislocation-related conductivity in the leakage current at room temperature for both the GaN and the $Al_{0.25}Ga_{0.75}N/GaN$ Schottky diodes, we require in our analysis that a single transport mechanism accurately describes current flow in both (although the physical parameters may differ for each, corresponding in one case to GaN and the other to $Al_{0.25}Ga_{0.75}N$). Of numerous possibilities evaluated, only a transport model based on Frenkel-Poole emission satisfied this criterion while yielding realistic values for the necessary physical parameters.

Frenkel-Poole emission refers to electric-field-enhanced thermal emission from a trap state into a continuum of electronic states—usually, but not necessarily, the conduction band in an insulator. The current density associated with Frenkel-Poole emission is given by[15–17]

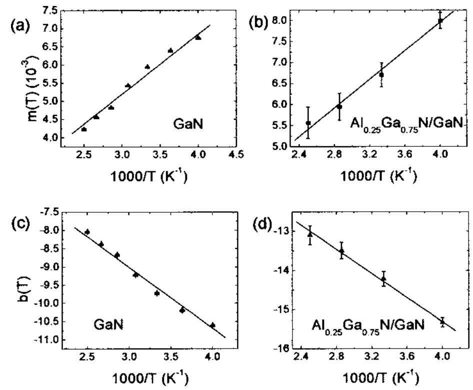

FIG. 5. Slopes $m(T)$ of the curves shown in (a) for GaN and (b) for $Al_{0.25}Ga_{0.75}N/GaN$. Intercepts $b(T)$ of the curves shown in (c) for GaN and (d) for $Al_{0.25}Ga_{0.75}N/GaN$. Data from curves not shown in Fig. 4 are also included.

$$J = CE_b \exp\left[-\frac{q(\phi_t - \sqrt{qE_b/\pi\varepsilon_0\varepsilon_s})}{kT}\right], \tag{2}$$

where E_b is the electric field in the semiconductor barrier at the metal-semiconductor interface, ϕ_t is the barrier height for electron emission from the trap state, ε_s is the relative dielectric permittivity at high frequency, T is temperature, ε_0 is the permittivity of free space, and k is Boltzmann's constant. Because the electrons emitted from the trap states do not polarize the surrounding atoms, the relevant dielectric constant is that at high frequency, rather than the static dielectric constant.[16]

From Eq. (2) we see that, for current transport by Frenkel-Poole emission, $\log(J/E_b)$ should be a linear function of $\sqrt{E_b}$, i.e.,

$$\log(J/E_b) = \frac{q}{kT}\sqrt{\frac{qE_b}{\pi\varepsilon_0\varepsilon_s}} - \frac{q\phi_t}{kT} + \log C \equiv m(T)\sqrt{E_b} + b(T), \tag{3a}$$

$$m(T) \equiv \frac{q}{kT}\sqrt{\frac{q}{\pi\varepsilon_0\varepsilon_s}}, \tag{3b}$$

$$b(T) \equiv -\frac{q\phi_t}{kT} + \log C. \tag{3c}$$

As shown in Fig. 4, the current densities in both the GaN and the $Al_{0.25}Ga_{0.75}N/GaN$ diode structures are well described by the electric-field dependence of Eqs. (2) and (3). Figure 5 shows the functions $m(T)$ and $b(T)$, as defined in Eqs. (3b) and (3c), respectively, plotted as functions of $1/T$ for both diode structures. We see from these plots that the measured current densities exhibit both the electric field and the temperature dependence expected in Frenkel-Poole emission. Furthermore, it is possible to extract from these data values for the high-frequency relative dielectric constant ε_s and the emission barrier height ϕ_t for both the GaN and the $Al_{0.25}Ga_{0.75}N/GaN$ diodes. From the slopes of $m(T)$ vs $1/T$, plotted in Figs. 5(a) and 5(b), we obtain $\varepsilon_s^{GaN}=5.4\pm0.1$ and $\varepsilon_s^{AlGaN}=5.1\pm1.0$, and from the slopes of $b(T)$ vs $1/T$, plotted in Figs. 5(c) and 5(d), we obtain $\phi_t^{GaN}=0.33\pm0.01$ V and $\phi_t^{AlGaN}=0.30\pm0.03$ V.

The values obtained for ε_s^{GaN} and ε_s^{AlGaN} are in good agreement with the reported values[18,19] of 5.35 for GaN and 4.77 for AlN, further supporting the validity of the Frenkel-Poole emission model in describing current transport in these structures. The interpretation of the emission barrier height is less straightforward. However, given the established prominence of conductivity associated with dislocations in producing leakage currents in this range of temperatures, it is reasonable to postulate that emission either into or from dislocation-related trap states, or conduction along dislocation lines, should be the dominant factor determining the electric field and temperature dependence of the leakage current density.

Given the emission barrier height of ~0.3 V measured for both diode structures, it is unlikely that the process governing the leakage current density is emission of carriers from a dislocation-related trap state into the semiconductor conduction band. Such a scenario would require the relevant trap state to be located ~0.3 eV below the conduction-band edge of GaN and $Al_{0.25}Ga_{0.75}N$ in the GaN and $Al_{0.25}Ga_{0.75}N/GaN$ diode structures, respectively, which would be unexpected based on the manner in which the emission energies of specific deep-level traps typically vary among different semiconductor materials.[20] Furthermore, at the metal-semiconductor interface the trap level would be located 0.5–0.6 eV above the metal Fermi level in the GaN diodes and 0.8–0.9 eV above the metal Fermi level in the $Al_{0.25}Ga_{0.75}N/GaN$ diodes, in which case thermal emission of carriers from the metal into the dislocation-related trap state would most likely be the key process governing leakage current flow. It is also unlikely that conduction along the dislocation line governs leakage current flow in these devices. While our prior work indicated that the temperature dependence of the leakage current density could be adequately described using an expression for conductivity corresponding to a one-dimensional variable-range hopping model,[7] the characteristic temperature resulting from such an analysis is field dependent and differs significantly for GaN compared to $Al_{0.25}Ga_{0.75}N$. In contrast, the Frenkel-Poole emission model yields a very accurate description of current density using clearly justifiable and realistic physical parameters.

Thus, we suggest that the process that governs leakage current flow is Frenkel-Poole emission from a state within the semiconductor—most likely a trap state near the metal-semiconductor interface—into a continuum of states associated with a conductive dislocation. Because the dependence of the current density on electric field and temperature is that of Frenkel-Poole emission rather than Schottky emission, carrier transport from the metal contact into the conductive dislocation must occur via a trap state rather than by direct thermionic emission from the metal. Furthermore, the trap-state energy must be close to the metal Fermi level: if the trap level were significantly lower in energy, emission of carriers from the metal directly into conductive dislocation states would most likely dominate, while if the trap level

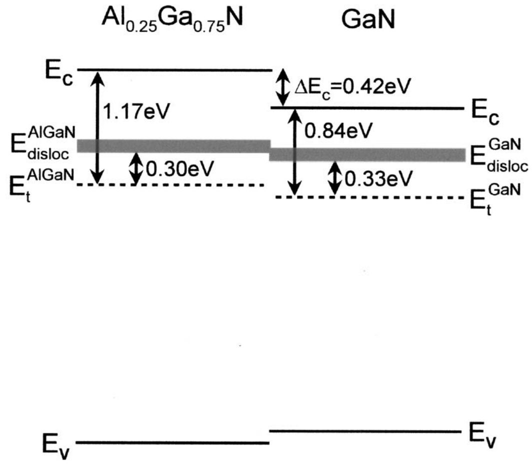

FIG. 6. Energy-band diagram showing conduction- and valence-band-edge energies and postulated trap-state and dislocation-state energies for GaN and $Al_{0.25}Ga_{0.75}N$ based on measured emission barrier heights and reported Schottky barrier heights and band offsets.

were significantly higher in energy, emission of carriers from the metal into the trap state would also be a significant factor. Finally, the similarity of the emission barrier heights measured for GaN and $Al_{0.25}Ga_{0.75}N$ implies that the continua of states associated with conductive dislocations are approximately aligned in energy in GaN and $Al_{0.25}Ga_{0.75}N$—as would be expected for states exhibiting deep-level behavior,[20] and required for conduction along dislocation lines across heterojunction interfaces.

If we assume for the sake of definiteness that the postulated trap state is at an energy equal to the metal Fermi level, the band-edge energies of GaN and $Al_{0.25}Ga_{0.75}N$ and the energies of the postulated trap and conducting dislocation states would be as shown in Fig. 6. As in our modeling of current flow, we have assumed Schottky barrier heights of 0.84 and 1.17 eV for GaN and $Al_{0.25}Ga_{0.75}N$, respectively, and a conduction-band offset between GaN and $Al_{0.25}Ga_{0.75}N$ of 0.42 eV based on the reported experimental results of 0.37 and 0.47 eV.[21,22] As shown in the figure, based on these values the conducting dislocation states in GaN and AlGaN are aligned to within ~60 meV or better, well within the experimental uncertainties of the energies used to derive the positions of the conducting dislocation states in each material. It should be noted that the alignment of these conducting dislocation states in GaN and $Al_{0.25}Ga_{0.75}N$ does not depend on the assumption that the postulated trap state is aligned with the metal Fermi level; it is necessary only for the trap-state energies in GaN and $Al_{0.25}Ga_{0.75}N$ to be similarly positioned relative to the metal Fermi level for Schottky contacts to each material, which is a very likely situation given the typical behavior of deep-level traps.

IV. CONCLUSIONS

In summary, we have used measurements and analysis of temperature-dependent current-voltage characteristics for Schottky diodes fabricated from *n*-type GaN and $Al_{0.25}Ga_{0.75}N/GaN$ HFET epitaxial layer structures grown by MBE to assess possible mechanisms of reverse-bias leakage current flow. At temperatures below approximately 150 K, we find that tunneling is the dominant carrier transport mechanism, consistent with previously reported measurements performed on Schottky contacts to *n*-type GaN grown by MBE. At higher temperatures, reverse-bias leakage current flow is dominated by Frenkel-Poole emission in Schottky diodes fabricated from both GaN and $Al_{0.25}Ga_{0.75}N/GaN$ epitaxial layer structures. Conductive AFM measurements performed on both epitaxial layer structures confirm that, at room temperature, carrier transport via conductive dislocations is the dominant source of reverse-bias leakage current, as expected for epitaxial material grown by MBE. A detailed analysis of the current-voltage behavior in both structures suggests that the key process in leakage current flow is emission of electrons from a trap state near the metal-semiconductor interface into a continuum of states associated with each conductive dislocation. In this model for leakage current flow, the emission barrier heights measured for the GaN and $Al_{0.25}Ga_{0.75}N/GaN$ Schottky diode structures indicate that the conductive dislocation states are aligned in energy between GaN and $Al_{0.25}Ga_{0.75}N$. This observation combined with the very accurate description of leakage current flow by Frenkel-Poole emission using realistic values for all physical parameters lends credence to the proposed model for leakage current flow in Schottky contacts formed to *n*-type nitride semiconductor material grown by MBE.

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