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Reduction of reverse-bias leakage current in Schottky diodes on GaN grown by molecular-beam epitaxy using surface modification with an atomic force microscope

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The characteristics of dislocation-related leakage current paths in an AlGaN/GaN heterostructure grown by molecular-beam epitaxy and their mitigation by local surface modification have been investigated using conductive atomic force microscopy. When a voltage is applied between the tip in an atomic force microscope (AFM) and the sample, a thin insulating layer is formed in the vicinity of the leakage paths where current is observed. As the insulating layer reaches a thickness of 2–3 nm, the leakage current is blocked and subsequent growth of the layer is prevented. Although conductive screw or mixed dislocations are observed, dislocations with a screw component that do not conduct current are also apparent. The reverse-bias leakage current is reduced by a factor of two in a large-area diode fabricated on an area modified in this manner with an AFM compared to typical diodes fabricated on unmodified areas with comparable series resistances, confirming that dislocation-related leakage current paths are a major component of the reverse-bias leakage current in Schottky diodes fabricated on nitride material. *© 2002 American Institute of Physics.* [DOI: 10.1063/1.1478793]

I. INTRODUCTION

Reverse-bias leakage current in GaN-based electronic devices remains an obstacle to their use in low-noise and low-power circuit applications.[1] Studies of the gate leakage current mechanisms in AlGaN/GaN heterostructure field-effect transistors have shown that tunneling from the Schottky gate contact into the barrier layer cannot account for the high level of leakage current in the device, suggesting that additional leakage mechanisms such as defect-related conduction[2] must be present. For material grown by metal-organic chemical-vapor deposition (MOCVD), a comparison of p-n junction diodes fabricated on low threading dislocation (TD) density, lateral epitaxial overgrowth GaN to diodes fabricated on GaN with a high-TD density, typical of standard epitaxially grown nitride material,[3] has shown that reverse-bias leakage current in these devices is strongly influenced by the TD density of the GaN.[4] Recent work has also shown that conduction along threading dislocations is the primary mechanism responsible for the leakage current in GaN grown by molecular-beam epitaxy (MBE).[5] This understanding of the importance of TDs to reverse-bias leakage current in GaN devices motivates investigation of ways to minimize the contribution of dislocations to leakage current in Schottky contacts.

Conductive atomic force microscope (AFM) is an attractive method for studying dislocation-related leakage current due to its ability to detect localized current paths in the material while simultaneously recording topographic information.[6] The use of an AFM to modify semiconductor surfaces by applying a voltage between the tip and sample and growing a thin insulating layer is well established,[7–10] and in this article is shown to lead to the blockage of current paths caused by dislocations. The present article focuses on the demonstration and characterization of this method to decrease the leakage current in an AlGaN/GaN heterostructure, in which the current that flows through dislocations is blocked by an insulating layer formed where current from the tip to the sample is observed. The current-voltage characteristics of large-area diodes fabricated on areas modified in this manner by AFM and on unmodified areas are further studied to show that the reverse leakage current in conventionally fabricated, large-area Schottky diodes can be significantly reduced by modification of the surface with an AFM. This observation then suggests that other surface treatments based on a similar physical process could have a comparable or greater effectiveness in reducing leakage currents in MBE-grown nitride material.

II. EXPERIMENT

The heterostructure used in this article was grown by MBE at 750 °C in the Ga-droplet regime[11] on a 2 μm GaN template grown by MOCVD on a sapphire substrate with a high-temperature AlN nucleation layer. The layer structure is shown in Fig. 1. Ohmic contacts to the sample were fabricated using Ti/Al annealed for 60 s at 650 °C, and Schottky contacts were fabricated using Ni metallization. In order to perform conductive AFM, a voltage was applied between a

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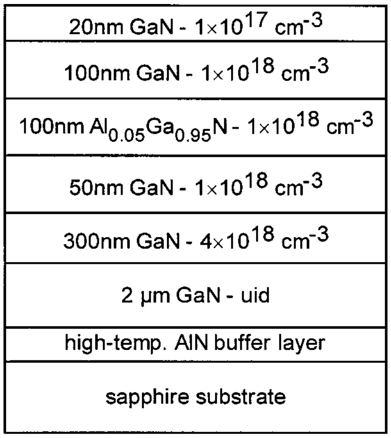

FIG. 1. Schematic of epitaxial layer structure indicating the dopant concentration in the MBE-grown films and the unintentional doping (uid) in the MOCVD-grown GaN template layer.

conducting probe tip and the sample in a standard AFM, and the current was detected using an external preamplifier. Metal-coated, conductive tips were used in contact mode operation, and were found to show little deterioration in tip shape after several hours of scanning despite the applied force required to maintain contact between the tip and sample and prevent repulsion due to the voltage being applied between the sample and tip. Experiments were performed at room temperature with an ambient humidity of 45%–55%. By measuring the current through a leakage path and the thickness of the insulating layer formed due to the current flow, it was possible to analyze the mechanisms responsible for the measured current.

An AFM was also used to modify a large area $(150\times150\ \mu\mathrm{m})$ of the sample surface, and the current-voltage characteristics of conventionally fabricated Schottky contacts on AFM-modified and unmodified areas were compared. Modeling the leakage paths covered by each of the Schottky diodes as a network of parallel resistors allows the resistance of the insulating layer to be related to the original resistance of the dislocation. Finally, the time spent on each dislocation during modification is calculated to determine the time needed to completely block a leakage path via AFM-induced formation of an insulating layer.

III. RESULTS AND DISCUSSION

Before applying a bias between the tip and sample, a high-quality AFM topographic image was obtained; growth steps were clearly visible in these images, as shown in Fig. 2(a). When a bias of 8 V was applied to the sample, current was observed at discrete points, as shown in Fig. 2(b), and a small island was formed in the region within which current flow occurred, as evinced by the topographic image obtained immediately after the current image, shown in Fig. 2(c). The measured current was initially on the order of 100 pA and each isolated, conducting region had a diameter of approximately 40–100 nm, whereas the islands that were formed were approximately 60–120 nm in diameter with heights of 2–3 nm. After scanning the surface 3–4 times with the tip-

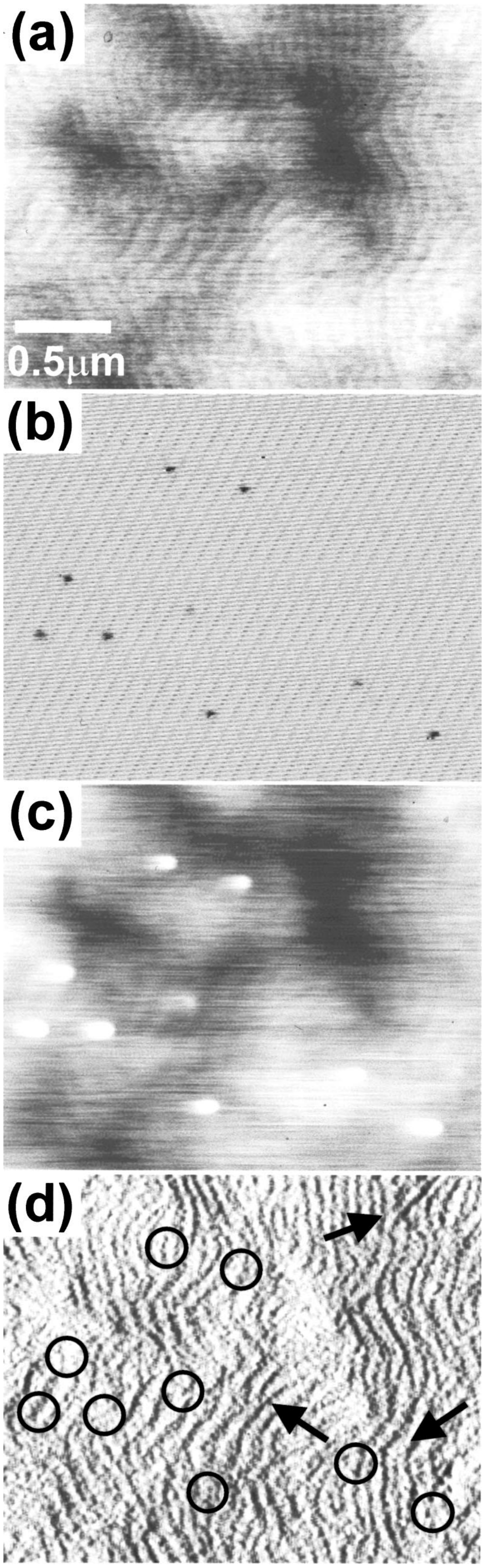

FIG. 2. AFM images of (a) topography obtained before application of a tip-sample voltage, (b) current through the tip to sample with 8 V applied to the sample, (c) topography obtained after scanning the surface with a tip-sample bias applied showing the growth of islands where current flow was observed, and (d) tip deflection obtained before surface modification with the locations of current flow indicated with circles and nonconducting dislocations with a screw component labeled with arrows. The vertical scale for the topography images (a) and (c) was 10 nm and the dark spots in the current image (b) correspond to approximately 100 pA.

sample voltage applied, current was no longer observed within the ~0.2 pA detection limit of the preamplifier.

To correlate the leakage paths with surface features which may be indicative of certain dislocation types, we show in Fig. 2(d) the deflection image of the surface prior to scanning with an applied tip-sample voltage, upon which is superimposed a map of the points where current was observed with a bias between the tip and sample. A recent study reported that in similarly grown material a majority of the current leakage paths are located on spiral hillocks, suggesting that screw or mixed dislocations are responsible for the leakage current.[5] Although leakage paths located near screw or mixed dislocations were observed in this article, Fig. 2(d) shows evidence of dislocations with a screw component, identifiable by the termination of two step edges and indicated by arrows in Fig. 2(d), that do not conduct current. Thus, it can be concluded that not all dislocations with a screw component contribute equally to the reverse-bias leakage current observed in Schottky diodes. Other recent work has shown that the presence of dislocations under microscopic Schottky contacts fabricated on MOCVD-grown GaN does not influence the current-voltage characteristics of the diode when compared to contacts on dislocation-free material.[12] In addition, conductive AFM studies of MOCVD-grown GaN[13] and of GaN grown by MBE under a variety of growth conditions[14] suggest that growth technique and conditions can strongly influence the conduction behavior of dislocations.

The reverse bias at which the leakage paths begin to conduct current was determined by performing a series of measurements in which successive scans of the surface were taken with an increasing sample voltage. Between each scan, a topographic image was recorded with no bias applied between the tip and sample. This enabled a topographic image to be obtained that was high in resolution compared to topographic images obtained with a nonzero tip-sample bias, due to the tip-sample interaction distorting the topographic image acquired when scanning with a sample bias applied. Current on the order of 1 pA was observed along the leakage paths beginning at approximately +4 V sample bias, which corresponds to a reverse-bias voltage on the Schottky diode formed by the tip and sample. This is the same reverse-bias voltage at which the onset of significant leakage current in macroscopic Schottky diodes was detected. At this voltage, growth of the islands on top of the leakage paths was also observed. Upon increasing the sample bias, current was again observed, but the insulating island limited the amount of current that flowed between the tip and sample, thus partially blocking the leakage path. Figure 3 shows the dependence of the thickness of the insulating layer and the measured current on the voltage that was applied to the sample for four representative leakage paths. For each sample voltage shown in Fig. 3, the measured current values were obtained from the initial scan of the surface during which the voltage on the *x* axis was applied between the sample and tip. The thickness of the insulating layer was then extracted from a subsequent scan of the surface without an applied tip-sample bias. At approximately 8 V sample bias, the layer thickness and current through the leakage path reached values such that further increases in sample bias had little effect on either the thickness or current until an irreversible reverse-bias breakdown occurred at approximately 14–16 V sample bias.

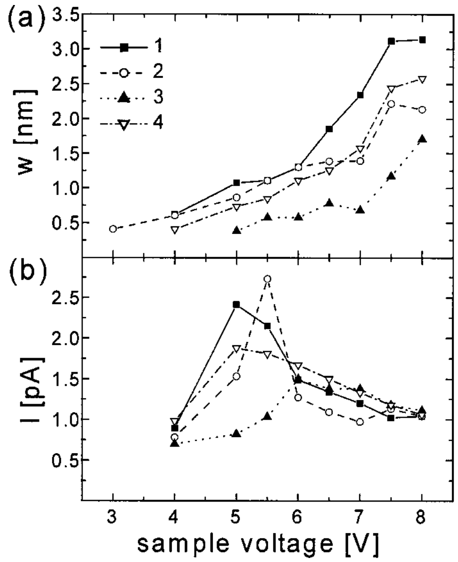

FIG. 3. (a) Insulating layer thickness and (b) measured leakage current for four representative leakage paths as a function of sample bias, illustrating the growth of the islands and the blocking of the leakage paths.

Growth of the insulating layer occurred only where and when current was flowing. This suggests that the growth kinetics were strongly related to the transport of ionic species, such as O^- or OH^-, across the insulating layer, as has been reported for similar experiments,[8–10,15] including the plasma anodization of Si.[16] For such experiments, growth is limited by the field-induced drift of the oxidizing species across the layer and leads to an ion current density j_i which obeys[16]

$$j_i \propto w^{n-1}, \tag{1}$$

where w is the thickness of the insulating layer and n is an adjustable model parameter expected to be in the range 0.3–0.7. Figure 4 shows the measured currents versus the measured thicknesses on a log-log scale for two representative leakage paths. Each current-thickness value was obtained

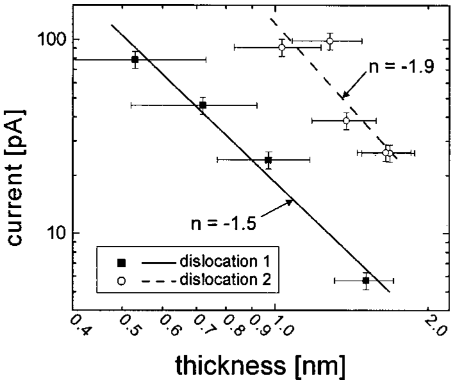

FIG. 4. Measured current (symbols) and linear fits (lines) for two representative leakage paths a function of thickness of the insulating layer. The slopes of the linear fits are used to determine *n*, a parameter associated with the power-law relationship predicted by the ionic transport model.

from two subsequent scans of the surface. First, a current map of the surface was taken with a high scan rate and a bias of 10 V applied to the sample, and the currents through a number of discrete locations on the sample surface were extracted from the current map. A high-quality topographic scan was then obtained without an applied tip-sample bias, and the thicknesses of the insulating layers that had formed over the same, discrete locations on the sample surface were extracted. This procedure was repeated until no current flow was observed. Fits to the plotted data yield values for n of -1.5 and -1.9, in contrast to the values expected based on the model of Li and Peeters,[16] suggesting that ionic current flow alone cannot account for the observed current. This is unsurprising given that other current transport mechanisms such as electron tunneling, which would yield a stronger dependence of current on insulating layer thickness than that given in Eq. (1), are also likely to be present.

The decreased growth rate of an AFM-induced insulating layer for larger layer thicknesses has been attributed to a number of different physical mechanisms besides the first-order effect of the decrease in the electric field across the insulating layer, which is due to the tip-sample voltage being dropped over a larger distance. Avouris *et al.*[8] suggest that the stress induced by the growth of an insulating layer on a semiconductor surface during oxidation with an AFM can contribute an additional energetic barrier to oxide growth as the thickness of the insulating layer increases. Li and Peeters[16] attribute the decreased growth rate for thicker layers to a larger spatial barrier across which ions must diffuse without losing their charge. Dubois and Bubendorff[15] have proposed that the buildup of fixed charges generated by the oxide growth at the oxide/semiconductor interface distorts the electric field needed to transport ionic species across the oxide layer and thereby impedes the growth of the layer. Our measurements do not enable us to distinguish definitely among these mechanisms for the decrease in growth rate. Considering, however, the relatively thin insulating layer thicknesses at which we observe a decreased growth rate (2–3 nm), it is possible that the mechanisms proposed by Avouris *et al.* or by Dubois and Bubendorff relating to the decrease in growth rate as a function of insulating layer thickness are more applicable to our measurements.

There are two possible explanations for the insulator growth occurring near dislocations. First, the formation of the insulating layer could be caused by chemical differences in the material in the vicinity of the dislocation compared to that away from the dislocation. A recently proposed model suggests that the core of screw dislocations is filled with Ga as opposed to being hollow.[17] It is possible, and in fact quite likely, that metallic Ga reacts more easily with O^- or OH^- ions than do Ga atoms that are present in the chemically stable bulk GaN to form an insulating Ga_xO_y compound, although experiments to confirm the chemical composition of the insulating layer were not performed in the current investigation. The second explanation is that the formation of the insulating layer is due to the electronic properties of the dislocation. As described above, an electric field across the oxide layer is required to transport ionic species to the oxide/semiconductor interface for the AFM-tip-induced oxidation reaction to occur. In GaN, the resistance of screw dislocations could be significantly less than that of surrounding dislocation-free material due to the presence of electronic states in the energy band gap.[17] This decreased resistance, which was observed experimentally, would lead to a larger fraction of the applied tip-sample bias being dropped across the air/oxide gap between the tip and sample, rather than being dropped in the sample itself. The larger voltage drop across the air/oxide gap in the vicinity of the dislocation might effect growth of an oxide layer through the presence of a larger electric field available to transport ions to the oxide/semiconductor interface. Considering our experimental observations, either explanation is feasible, and it is possible that both factors contribute to the growth of the insulating layer.

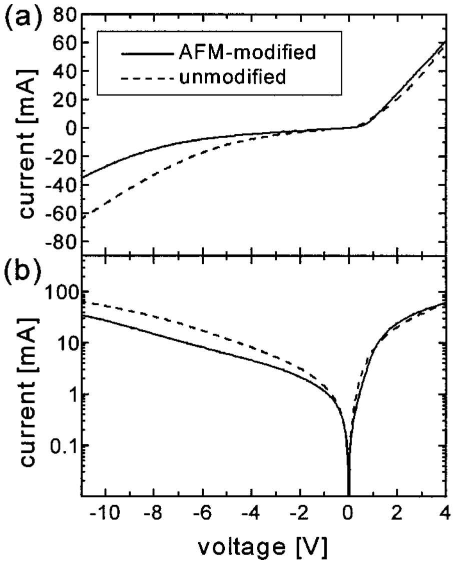

FIG. 5. Measured current-voltage characteristics for macroscopic Schottky diodes fabricated on AFM-modified and unmodified areas, demonstrating the ability to reduce the reverse-bias leakage current by blocking the observed leakage paths with a thin insulating layer.

To assess the relevance of these ideas to current flow in conventionally fabricated Schottky diodes, large-area surface modification was performed with the AFM, and Schottky diodes were fabricated on both AFM-modified and unmodified areas. While surface modification by AFM is unlikely to be viable for routine fabrication of devices, it provides a useful method for investigation of the basic mechanisms responsible for current leakage, and of possible methods for their amelioration. To accomplish the desired surface modification, the AFM tip was scanned ten times over a 150×150 μm area at 0.1 Hz with 8 V applied to the sample. Circular Schottky contacts 125 μm in diameter were then fabricated on the scanned area and the current-voltage characteristics were compared to those of diodes fabricated without the AFM surface modification process.

Current-voltage characteristics for both types of Schottky diodes are shown in Fig. 5. Due to the time-intensive nature of the surface modification process, only two modified-surface diodes were fabricated; the unmodified diodes chosen for this comparison had series resistances, which were estimated from the forward bias characteristics, very close to those for the modified diode shown in Fig. 5. Diodes fabricated on the AFM-modified area exhibited significantly reduced reverse-bias leakage current, and by examining the resistance of the diodes, it was estimated that the lumped resistance of the leakage paths was increased by more than 50% compared to diodes with similar series resistance values fabricated on unmodified surfaces. This change is significantly greater than the maximum variation of ~10% observed among approximately 20 diodes fabricated on the unmodified surface with comparable series resistances. The ideality factors for diodes on both AFM-modified and unmodified areas were relatively high (between two and three for all measured diodes), but there was no significant difference in the ideality factor for diodes fabricated on surfaces after modification with an AFM compared to diodes fabricated on unmodified surfaces. These results show clearly that blockage of the current leakage paths via surface modification in an AFM substantially reduces the leakage current in macroscopic devices, consistent with other work suggesting that these leakage paths are the primary mechanism for leakage in Schottky diodes fabricated on GaN grown by MBE under Ga-rich conditions.[5,14]

The increase in resistance of the leakage paths can be used to assess the degree to which each leakage path was blocked by the AFM-induced surface modification, and thereby to evaluate the effectiveness of the treatment and the potential for improvement. By modeling the leakage paths as a network of parallel resistors in series with another bulk resistance R_S, as shown in Figs. 6(a) and 6(b) for the system with and without surface modification, the measured resistances of the diodes fabricated on AFM-modified and unmodified surfaces can be used to determine the number of dislocations that were blocked N_b according to

$$\frac{N_b}{N_{\mathrm{tot}}} = \frac{\left(1-\frac{R_2}{R_1}\right)\left(1+\frac{R_{\mathrm{ins}}}{R_{\mathrm{lp}}}\right)}{-\frac{R_{\mathrm{ins}}}{R_{\mathrm{lp}}}\frac{R_2}{R_1}}, \tag{2}$$

where N_{tot} is the total number of leakage paths, R_1 and R_2 are the lumped resistances of the network of leakage paths before and after AFM modification, respectively, R_{ins} is the resistance of the insulating layer grown on each dislocation, and R_{lp} is the original resistance of the leakage path. The resistances R_1 and R_2, which have values of 38 and 61 Ω respectively, are found by subtracting the series resistance from the total resistance values measured for large reverse-bias voltages, where the leakage paths in each diode have begun to conduct current. Figure 6(c) shows the percentage of blocked leakage paths as a function of the ratio of insulating-layer resistance to leakage-path resistance $(R_{\mathrm{ins}}/R_{\mathrm{lp}})$. It is apparent from this figure that either only ~40% of the leakage paths were blocked completely, or a higher percentage were partially blocked, i.e., the insulating layer was insufficient to completely block current flow. In either case, it should be possible by further surface modification to decrease the reverse leakage current to a greater extent than demonstrated here.

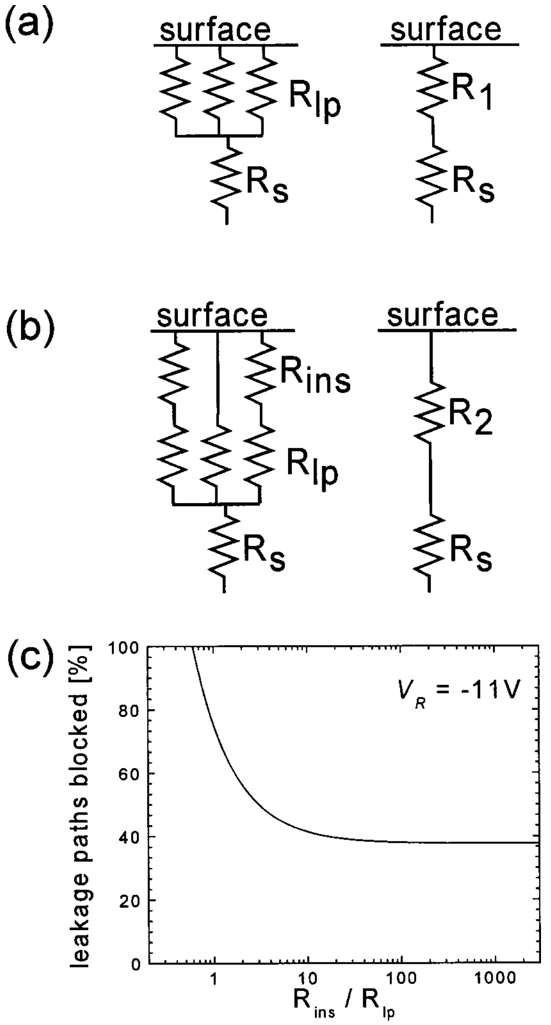

FIG. 6. Complete and simplified circuit models of (a) the unmodified and (b) AFM-modified surfaces used to extract the resistance of the insulating layer, and (c) the calculated percentage of leakage paths that were blocked with the AFM vs the resistance of the insulating layer relative to the original leakage path resistance, showing that incomplete passivation of the surface occurred and that a further reduction in the reverse-bias leakage current should be possible.

A detailed analysis of the surface modification process suggests in fact that this incomplete blocking of the current leakage paths is most likely a result of an insufficient amount of time spent by the AFM tip over the leakage paths with a tip-sample bias applied and, hence, an insulating layer that was not sufficiently thick to block current flow completely. During the large-area surface modification with the AFM, two factors accounted for the decreased time spent on each dislocation compared to our earlier, small-scale surface modification experiments: (i) the tip velocity was much greater due to the minimum scan rate of 0.1 Hz of the AFM and (ii) successive scan lines were separated by a much greater distance as a result of the maximum scan resolution of 512 lines/scan and, thus, each leakage path was scanned fewer times. For the large-area modification, the tip velocity and line spacing were 30 μm/s and 293 nm, respectively, compared to 8 μm/s and 8 nm for the small-scale modification scans. From these parameters, it is possible to calculate the amount of time spent on each leakage path for a certain tip radius and distribution of leakage path radii for both the large- and small-scale modification experiments.

Performing the calculation for a tip radius of 15 nm and a Gaussian distribution of leakage path radii centered at 20 nm with a 10 nm standard deviation, it was found that the average time spent on each leakage path in the large-area surface modification experiment was approximately 40% of the total time needed to completely block the leakage paths as determined by the small-scale surface modification experiments. This accounts for the partially conductive insulating layer found in the macroscopic diode fabricated on the AFM-modified surface and suggests that the reverse-bias leakage current could have been reduced further by increasing the amount of time spent on each leakage path with an applied tip-sample bias.

IV. SUMMARY

An investigation of the reverse-bias leakage current paths and their mitigation in an AlGaN/GaN heterostructure has been performed using conductive AFM in conjunction with current-voltage studies of macroscopic Schottky diodes fabricated on AFM-modified and unmodified areas. Leakage paths associated with screw and mixed dislocations were apparent based on observations of the surface morphology; however, nonconducting dislocations with a screw component were also identifiable. Reverse-bias leakage current was observed at discrete locations on the sample surface, and the leakage paths were blocked by the voltage-induced formation of an insulating layer that reaches up to 2–3 nm in thickness given a sufficient amount of time spent over the leakage path with a tip-sample voltage applied. Current through the insulating layer could not be described by a model based on the field-induced drift of ionic species across the insulating layer, suggesting that other current mechanisms must have been present to account for the observed tip-sample current flow.

A macroscopic Schottky diode fabricated on an area of the surface that had been modified by AFM-induced current flow was shown to have a significantly reduced reverse-bias leakage current compared to diodes fabricated on unmodified areas, confirming that the dislocation-related leakage paths are a major contributor to the reverse-bias leakage current. By modeling the leakage paths as a network of resistors in parallel, it was determined that the modification of the surface was incomplete and that further reduction in reverse-bias leakage current should be possible. The incomplete modification of the surface was most likely a result of an insufficient amount of time spent on each dislocation with a tip-sample bias applied. Further experiments are in progress to devise means by which to reduce the reverse-bias leakage current using other surface treatments to block current flow along the dislocation-related leakage paths.

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