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# Reverse leakage mechanism of Schottky barrier diode fabricated on homoepitaxial GaN

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ABSTRACT

In this work, Schottky barrier diodes with vertical geometry were fabricated on low-defect-density homoepitaxial GaN for studying the reverse leakage mechanism of GaN-based Schottky contact. A leakage current model based on electron transmission primarily through linear defects like dislocations was suggested to explain the reverse current–voltage characteristics measured between 300 and 410 K, in which electrons from contact metal overcome the locally height-reduced Schottky barrier through thermionic-field emission.

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## 1. Introduction

Schottky contact on GaN is a fundamental building block of many III-nitride-based high-power and high-frequency devices [1]. Nevertheless, even after many years' development, obtaining high-quality Schottky contacts on GaN with reproducible low leakage current and high reliability remains a major technological challenge [2]. One fundamental problem still under debate is its reverse leakage mechanism. It has been well accepted that classical thermionic emission (TE) model cannot explain the commonly-observed excessively large reverse leakage current of GaN-based Schottky junctions. There is strong evidence supporting that the high leakage current is caused by defect-related conduction, which flows very non-uniformly across the metal/GaN interface [2–5]. By studying with conductive atomic force microscopy, Hsu et al. suggests that dislocations, especially those with a screw component, are the primary leakage path in GaN grown by molecular beam epitaxy [3]. Based on the results obtained by other related characterization techniques, similar conclusion was also made on GaN materials grown by metal–organic chemical vapor deposition (MOCVD) and hydride vapor phase epitaxy (HVPE) [4,5]. If this is true, the leakage electrons should primarily move along a continuum of states associated with a conductive dislocation [6] within the forbidden band instead of on the conduction band.

Besides the mechanism of how electrons move through the depletion region, how electrons overcome the surface barrier and move into the semiconductor layer is another hot topic under debate. Frenkel–Poole (FP) emission has been suggested to explain the reverse leakage mechanism of AlGaN/GaN or AlInN/GaN-based Schottky junctions, which refers to electrical-field-enhanced thermal emission of electrons from trapped states onto a continuum of electronic states [7,8]. Unfortunately FP emission is a qualitative model and cannot be used to rigorously calculate current–voltage ($I$–$V$) characteristics for fitting experimental curves. Comparatively, electron tunneling through the Schottky barrier is a more frequently adopted model [9–11], which includes thermionic field emission (TFE) and field emission (FE) mechanisms [12]. However, similar to the situation of TE mechanism, because of the large barrier height and width of low-to-medium-doped GaN Schottky junctions, the magnitude of classical TFE and TE currents are normally orders of magnitude lower than that of the experimental leakage current as well. To resolve this contradiction, thin surface barrier (TSB) model has been proposed by Hasegawa et al., in which considerable thinning of the surface Schottky barrier is assumed due to the presence of unintentional surface defect

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donors [13]. Although TSB model is found effective to numerically reproduce the experimental curves, there are multiple adjustable model parameters involved, making the fitting process less persuasive. In addition, the basic assumption of the model – very high density surface donors (sometimes up to $10^{19}$ cm$^{-3}$) is not widely supported by material growth and characterization studies.

In this work, by fabricating a high-quality vertical Schottky barrier diode (SBD) on low-defect-density GaN homo-epilayer and fitting its temperature-dependent *I–V* characteristics, a modified tunneling model is proposed to explain the reverse leakage mechanism between 300 and 410 K. The model is based on electron tunneling through locally-height-reduced Schottky barrier and then moving along a continuum of states associated with a conductive dislocation.

## 2. Experiment

The freestanding conductive bulk GaN substrate used in this study was produced by HVPE technique with a thickness of 320 μm. The room temperature (RT) Hall mobility and electron concentration of the substrate are 260 cm$^2$/V s and $2 \times 10^{18}$ cm$^{-3}$, respectively. The device structure was grown by MOCVD under optimized growth conditions, consisting of a 0.5 μm n + GaN ($\sim 3 \times 10^{18}$ cm$^{-3}$) transition layer and a 3 μm n-GaN ($\sim 1 \times 10^{17}$ cm$^{-3}$) active layer [14]. Fig. 1a shows a typical panchromatic cathodoluminescence (CL) mapping image of the homoepitaxial GaN layer examined over a large surface area, in which each dislocation is represented by a small dark spot resulting from strong local non-radiative recombinations [15]. The dislocation density of the homoepitaxial GaN layer is estimated to be $\sim 5 \times 10^6$ cm$^{-2}$ in average, which is about 2–3 orders lower than the typical dislocation density of hetero-epitaxial GaN. The corresponding full width at half maximum of the GaN (0002) XRD rocking curve is 80–100 arcsec, which agrees with the low dislocation density determined by CL mapping. The doping concentration of the n-GaN active layer calculated from the capacitance–voltage (*C–V*) curve measured at 1 MHz confirms the growth design.

The SBDs were fabricated by using standard optical photolithography and e-beam evaporation. The fabrication process starts with the formation of ohmic contact by evaporating Ti/Al/Ti/Au (30/150/50/300 nm) metal stack at the wafer backside followed by rapid thermal annealing in $N_2$ at 650 °C for 2 min. The reason that a relatively lower annealing temperature was chosen here compared with the conventional value of 800–850 °C for ohmic contact formation on GaN is to prevent the fresh GaN epi-surface from possible decomposition and oxidation. After cleaning and a short HCl-solution dip, a layer of Schottky metal consisting of Ni/Au (40/250 nm) was deposited on the wafer front side. Then, Schottky electrodes of 125 × 125 μm$^2$ in size were defined by photolithography and formed by wet chemical etching (Transene™ Au and Ni etchants). Compared with lift-off process, chemical etching for contact patterning has less chance for surface contamination. Fig. 1b shows a schematic of the device structure.

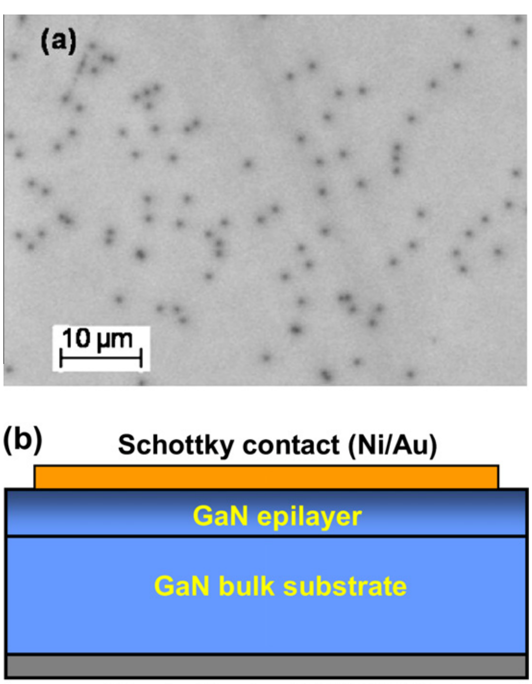


**Fig. 1.** (a) Panchromatic CL image of the homoepitaxial GaN layer grown by MOCVD on bulk GaN; (b) schematic of the vertical Schottky barrier diode fabricated on bulk GaN substrate.

## 3. Results and discussion

Temperature-dependent *I–V* characteristics of the SBDs fabricated on GaN homo-epilayer were measured between 300 and 410 K. As shown in Fig. 2, the diode shows typical rectification behaviors in all temperature range with a low RT reverse leakage current of ~mid-$10^{-11}$ A under −10 V bias, which is considerably lower than the typical reported values of Schottky diodes fabricated on heteroepitaxial GaN [6,16–17]. The reverse leakage current also increases rapidly as a function of both reverse bias and temperature. Meanwhile, the RT built-in potential of the Ni/GaN Schottky junction deduced from the CV curve is 1.00 eV (see inset of Fig. 2), resulting an average Schottky barrier height (SBH) $q\Phi$ of 1.08 eV.

As has been pointed out, TE-induced leakage current is many orders of magnitude lower than the experimental leakage current. A rough calculation based on electron tunneling directly through the Schottky barrier indicates that leakage current induced by simple TFE mechanism is also too small to explain the excessive leakage current (not shown). The problem of the above two classical models is that the contribution of structural defects (especially dislocations) to leakage current are not considered, which could

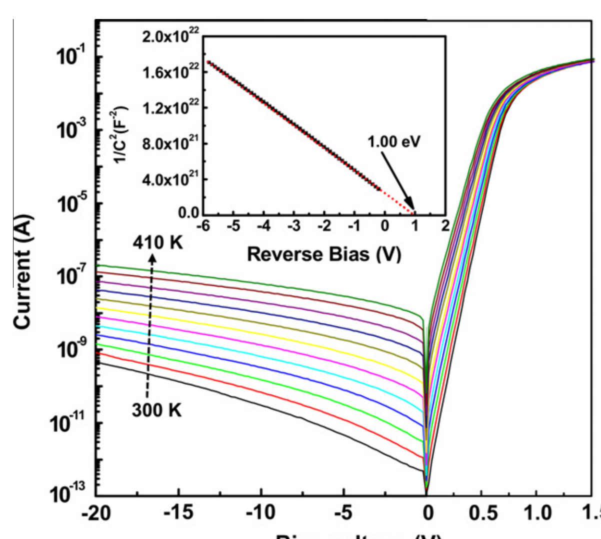


**Fig. 2.** Measured *I–V–T* characteristics of a 125 × 125 μm$^2$ Schottky barrier diode fabricated on homoepitaxial GaN from 300 to 410 K. The inset shows the 1 MHz 1/$C^2$–*V* curve at 300 K.

nevertheless be a dominant leakage factor for GaN Schottky junctions. To include dislocation-related leakage, a modified tunneling model is proposed in this work and its schematic band diagram is illustrated in Fig. 3. Since modeling of leakage current through individual dislocations is difficult, which depends on many factors such as the exact type and local surrounding of the dislocations, the model treats the influence of various dislocations combinative as a continuum of states associated with conductive dislocations within the forbidden band. Thus, in defective regions, leakage current can be caused by electron tunneling onto the dislocation states and then moving along the continuum of states instead of the conduction band. Compared with other possible transport mechanisms, TFE-related tunneling is a more straightforward mechanism for electrons to overcome the locally reduced Schottky barrier under the influence of electrical field. Meanwhile, FP emission is not supported by the FP plots of the experimental reverse *I–V* curves, which exhibit non-linear characteristics (not shown).

To validate the purposed reverse leakage current model, numerical simulation of the experimental reverse *I–V* curves was conducted analytically. Since the continuum of states associated with conductive dislocations is below and parallel to the conduction band, the corresponding energy barrier $q\Phi_D$ for electron tunneling onto the continuum of states is considerably reduced compared with the average SBH deduced from *C–V* measurement. The tunneling current density from metal to semiconductor within the defective regions can be expressed by the following equation [11,18]:

$$J_{TU} \approx \frac{A^*T}{k}\int_{-q(V_r-V_b)}^{q\Phi_D} F_m P(E)[1-F_s(E)]dE \tag{1}$$

where $A^*$ is the effective Richardson constant, $T$ is the temperature, $k$ is the Boltzmann constant, $q$ is the fundamental electronic charge, $V_b$ is the built-in potential at zero bias, $V_r$ is the reverse bias, $F_m$ and $F_s$ are the Fermi–Dirac distribution functions of electrons in metal and in semiconductor respectively. Here $F_m$ is given by

$$F_m = \frac{1}{1+\exp\left(\frac{E-E_{fm}}{kT}\right)} = \frac{1}{1+\exp\left(\frac{E}{kT}\right)} \tag{2}$$

Since under reverse bias, the defect states within the depletion region are mostly empty, it is reasonable to assume $1 - F_S \approx 1$ .

The tunneling probability $P(E)$ of electrons with energy of $E$ can be calculated using the WKB approximation

$$P(E) = \exp\left[-2\frac{\sqrt{2m^*}}{\hbar}\int_{x_1}^{x_2}\sqrt{q\phi_D(x)-E}dx\right] \tag{3}$$

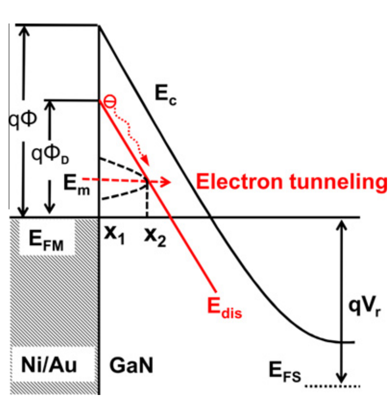


**Fig. 3.** Energy band diagram showing the suggested localized electron tunneling model.

where $m^*$ is the electron effective mass, $\hbar$ is the reduced Planck constant, $x_1 - x_2$ is the tunneling distance, and $\phi_D(x)$ is the electrostatic potential of dislocation as a function of distance $x$. If the energy barrier is approximated as being a triangular shape, $\phi_D(x)$ can be expressed as $q\phi_D(x) = -q\xi x + q\Phi_D$, in which $\xi$ is the uniform electric field over the triangular barrier. By substituting $x_1 = 0,\ x_2 = \frac{\phi_D - E}{\xi}$ into Eq. (3), $P(E)$ can be calculated as:

$$P(E) = \exp\left[-\frac{4}{3}\frac{\sqrt{2m^*}}{\hbar}\frac{(q\phi_D-E)^{\frac{3}{2}}}{q\xi}\right] \tag{4}$$

Based on Eqs. (2) and (4), it is clear that $P(E)$ and $F_m(E)$ would rapidly increase and decrease as a function of $E$ respectively. Thus, as illustrated in Fig. 3, their product $P(E)F_m(E)$ would form a Gaussian peak at a certain energy $E_m$, at which the tunneling current is maximum.

Based on above, the tunneling current density from metal into the dislocation-related continuum of states can be rewritten as:

$$J_{TU} = \frac{A^*T}{k}\int_{-q(V_r-V_b)}^{q\Phi_D}\frac{1}{1+\exp\left(\frac{E}{kT}\right)} \times \exp\left[-\frac{4}{3}\frac{\sqrt{2m^*}}{\hbar}\frac{(q\phi_D-E)^{\frac{3}{2}}}{q\xi}\right]dE \tag{5}$$

which has a strong dependence on both the junction electrical field as well as the effective barrier height $q\Phi_D$. To simulate the experimental leakage current, clearly $q\Phi_D$ is a key fitting parameter. Meanwhile, another unknown parameter is the effective leakage area of dislocations ($A_D$), as the total dislocation-related leakage current $I_{TU} = A_D J_{TU}$. Here we approximate that all threading dislocations in the homo-epilayer conduct leakage current equally and define the Debye length $\lambda_D$ as the effective radius of leakage area of each dislocation. Thus, $A_D = AN_{DD}\pi\lambda_D^2$, in which $N_{DD} \sim 5\times10^6\ \text{cm}^{-2}$ is the dislocation density revealed by CL mapping and A is the Schottky contact area. $\lambda_D$ is calculated as being 13.1 nm at 300 K, which is on the same order of magnitude as the radius of leakage spots on GaN measured by conductive atomic force microscopy [3]. The corresponding RT fill factor of the defective region to the total Schottky contact region is $\sim 4.9\times10^{-6}$. Here it should be noted that in real situation, the ability to conduct leakage current by each dislocation strongly depends on its individual microstructure and could varies considerably among different dislocations, leading to an uncertainty of $A_D$ [19]. Fortunately, as $I_{TU}$ is only a linear function of $A_D$ and given the fact that the experimental reverse leakage current varies many orders of magnitude as a function of both reverse bias and temperature, a deviation of $A_D$ from the real value, if not too much, would not invalid the simulation result.

Finally, the theoretical total reverse current $I_r$ of the SBD should include leakage current from the defective low-barrier regions ($I_{rL}$) as well as leakage current from the dislocation-free high-Schottky-barrier regions ($I_{rH}$). Since both TE and TFE-related leakage current through dislocation-free regions are negligibly small, the total leakage current can be approximated as:

$$I_r = I_{rL} + I_{rH} \approx I_{rL} \approx I_{TU} \tag{6}$$

Fig. 4 shows the simulated reverse *I–V* curves along with the experimental curves at various temperatures using the reduced barrier height $q\Phi_D$ as the only fitting parameter. A good agreement between the two groups of curves is obtained, indicating the applicability of our suggested leakage current model. The fitting values of $q\Phi_D$ as a function of temperature are shown in the insert of Fig. 4. Its RT value is 0.612 eV and decreases nearly linearly to 0.514 eV at 410 K with a negative temperature coefficient of $\alpha \approx -8.9\times10^{-4}$ eV/K, which is close to the temperature coefficient of GaN's bandgap ($\sim -5.6\times10^{-4}$ eV/K) [20]. As a result, the en-

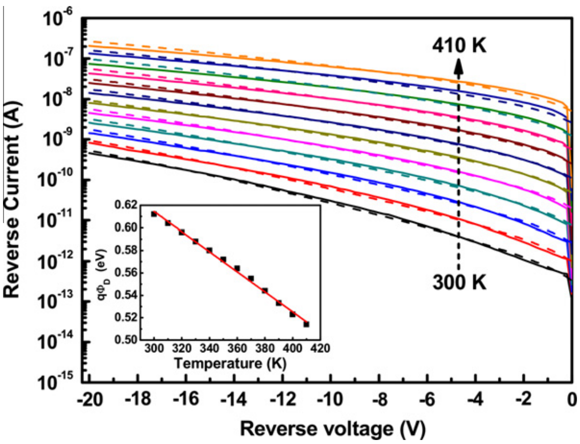


**Fig. 4.** Simulated reverse *I–V* curves (dashed line) along with the experimental curves (solid line) at various temperatures ranging from 300 to 410 K. The insert shows the fitted effective local barrier height $q\Phi_D$ as a function of temperature.

hanced reverse leakage current at elevated temperatures can be explained by bandgap-shrinkage-induced effective tunneling barrier height reduction.

## 4. Summary

In summary, a phenomenological leakage current model focusing on defect-related conduction is purposed to explain the experimental temperature-dependent reverse *I–V* characteristics of SBDs fabricated on low-defect-density GaN homo-epilayer. The model suggests that linear defects like dislocations would form a continuum of states within the forbidden band on which leakage electrons could move. Electrons from the contact metal could overcome the locally reduced Schottky barrier and tunnel onto the dislocation-related continuum of states through thermionic-field emission. Good agreement between the simulated *I–V* curves and the experimental results is obtained. In addition, besides the suggested dominant leakage mechanism, other minor or parasitic leakage mechanisms could co-exist in the real reverse transport process [7,21–23].

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