Hindawi Publishing Corporation
Advances in Condensed Matter Physics
Volume 2010, Article ID 526929, 7 pages
doi:10.1155/2010/526929

Research Article

Analysis of Reverse-Bias Leakage Current Mechanisms in Metal/GaN Schottky Diodes

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Received 13 May 2010; Accepted 28 July 2010

Academic Editor: Jörg Fink

Temperature-dependent reverse-bias current-voltage characteristics obtained by other researchers for Schottky diodes fabricated on GaN are reinterpreted in terms of phonon-assisted tunneling (PhAT) model. Temperature dependence of reverse-bias leakage current is shown could be caused by the temperature dependence of electron tunneling rate from traps in the metal-semiconductor interface to the conduction band of semiconductor. A good fit of experimental data with the theory is received in a wide temperature range (from 80 K to 500 K) using for calculation the effective mass of 0.222 m_e. and for the phonon energy the value of 70 meV. The temperature and bias voltages dependences of an apparent barrier height (activation energy) are also explicable in the framework of the PhAT model.

1. Introduction

GaN is a wide direct band gap semiconductor which has unique applications in the fabrication of blue light-emitting diodes, lasers, ultraviolet detectors, field effect transistors, and high power rectifiers [1, 2]. Metal-semiconductor contact is one of the most widely used rectifying contacts in the electronics industry. However, GaN-based Schottky contacts suffer from abnormal leakage currents under reverse bias, which is one factor presently limiting device performance.

Due to the technological importance of Schottky diodes, a full understanding of the nature of their electrical characteristics is of great interest. Recently a number of papers on reverse-bias leakage current mechanisms in M/GaN Schottky diodes appeared [3–16]. In papers [17–20], the investigation of Schottky contact on GaN nanowires were presented.

Suggestions of investigators about the reverse-bias leakage current mechanism are very different. For instance, Miller et al. [3] claimed that two dominant leakage current mechanisms in Ni/n-GaN Schottky diode (SD) fabricated on GaN grown by molecular-beam epitaxy can be identified. One associated with field-emission tunneling and another with an exponential temperature dependence, consistent with either trap-assisted tunneling or one-dimensional hopping conduction. However, for the fitting of the experimental data with the tunneling current model, the authors [3] have used unphysically low the effective mass ($9.8 \times 10^{-3}\,m_e$) and the value for the effective Richardson's constant A^* ($0.001\,\mathrm{A/cm^2\,K^2}$). Zhang et al. [4] analyzed the leakage current mechanisms in the Schottky contacts of both n-GaN and AlGaN/GaN epitaxial layer structures at different temperatures and concluded that tunneling current dominates at temperatures below 150 K whereas the Frenkel-Poole emission dominates at temperatures higher than 250 K. Huang et al. on the basis of current-voltage measurements between 27 and 350°C in Au/Ni/GaN SDs concluded that thermionic-emission model with a Gaussian distribution of barrier heights is responsible for the electrical behavior of the diodes at temperatures lower than 230°C, while the generation-recombination process takes place at temperatures above 230°C [7]. Arslan et al. [11] assumed that the reverse-bias leakage current mechanisms in SDs on $Al_{0.83}In_{0.17}N$/AlN/GaN heterostructures, in the temperature range of 250–375 K is based on the Frenkel-Poole emission model. Moreover, Iucolano et al. [13] claimed that one-dimensional variable-range hopping conduction was one of the dominant carrier transport mechanisms for the Ni/GaN Schottky sample annealed at 1150°C for 5 minutes.

A such variety of proposed conduction mechanisms involved to describe the leakage current in M/GaN diodes implies that fundamental properties of the conduction mechanisms are not to date fully understood.

Another problem which emerges in examining the practical diodes characteristics is observed dependence of the barrier height derived from *I-V/T* measurements on applied bias voltage and temperatures. In terms of a classical thermionic emission theory [21] the forward current density is given by

$$j = j_0\left[\exp\left(\frac{qV}{nkT}\right) - 1\right], \tag{1}$$

where

$$j_0 = A^* T^2 \exp\left(-\frac{q\Phi_{\mathrm{BO}}}{kT}\right) \tag{2}$$

is the saturation current density, A^* is the effective Richardson constant, Φ_{BO} is the Schottky barrier height (SBH), k is the Boltzmann constant, q is the electronic charge unit, and n is the ideality factor which describes the deviation of practical diodes from the pure thermionic-emission model characterized by $n = 1$.

A so-called Richardson plot of $\ln(j_0/A^*T^2)$ versus inverse temperature $1/T$ is often used to determine the SBH from the slope of the thermally activated behavior. According to (2)

$$\ln\left(\frac{j_0}{A^*T^2}\right) = -\frac{q\Phi_{\mathrm{BO}}}{kT} \tag{3}$$

and the plot $\ln(j_0/A^*T^2)$ versus $1/T$ (Richardson plot) should yield a straight line with an activation energy $E_T = -q\Phi_{\mathrm{BO}}$ if the SBH Φ_{BO} is temperature dependent. But in most cases these plots do not yield straight lines (see e.g., [15, 16]). The curving in these plots results in (determines) dependence of E_T on temperature.

In the case of reverse bias voltage when $(qV/kT) \gg 1$ for the current density jr from (2) one obtains

$$j_r = A^* T^2 \exp\left(-\frac{q\Phi_{\mathrm{br}}}{kT}\right). \tag{4}$$

The apparent SBH Φ_{br} calculated from the gradient of the Richardson plot lines will be lower than Φ_{BO} due to the lowering of the barrier height caused by image-force, but temperature dependence of both Φ_{BO} and Φ_{br} has the same shape [14].

Analysis of the *I-V/T* characteristics of Schottky diodes on the basis of thermionic emission theory reveals a decrease in the apparent barrier height Φ_{BO} and an increase in the ideality factor n with a decrease in temperature [5, 6, 12, 15, 16, 19]. The temperature dependence of the apparent barrier height is frequently explained by invoking a Gaussian distribution of the SBH values at the interface between the Schottky metal and the semiconductor [15, 16, 19].

In previous work [22], we have shown that in Ni/n-GaN SD the leakage current dependence on temperature in a wide range of temperatures can be described in the framework of phonon-assisted tunneling (PhAT) model. The purpose of this work is on the basis of this model to explain the peculiarities of the reverse-bias current dependence on bias voltage and their temperature behavior in the M/GaN Schottky diodes presented by various authors in recent publications. Dependence of the apparent SBH on temperature discussed by many investigators is also explained in the framework of the PhAT model.

2. Theory and Comparison with Experimental Data

2.1. The Phonon-Assisted Tunneling Model. In accordance with phonon-assisted tunneling model, the current transport through the barrier is governed by a process of tunneling from states nearby metal-semiconductor interface to the conduction band of the semiconductor. The electron population in the states is assumed to be independent of bias voltage due to the continuous filling of interface states from the metallic electrode (see Figure 1). If the electrons released from these centers dominate the current through the diode, the current density, neglecting scattering of electrons by phonons and recombination process, will be equal to

$$I_r = qN_S WS, \tag{5}$$

where N_S is the charged states density at the interface, S is the area of barrier electrode, and W is the electron tunneling rate from these states into the conduction band which is a function of field strength E and temperature T. Therefore, $I_r \approx W(E,T)$, and we can fit the current dependences obtained by measurements with the theoretical tunnel transition through the barrier rate dependences on temperature.

The electrons tunneling rate $W(E,T)$ from centers of ε_T depth at the metal/semiconductor interface is [22, 23]

$$\begin{aligned} W(E,T) = {} & \frac{qE}{(8m^*\varepsilon_T)^{1/2}}\left[\left(1+\gamma^2\right)^{1/2} - \gamma\right]^{1/2}\left[1+\gamma^2\right]^{-1/4} \\ & \times \exp\left\{-\frac{4}{3}\frac{(2m^*)^{1/2}}{qE\hbar}\varepsilon_T^{3/2} \times \left[\left(1+\gamma^2\right)^{1/2} - \gamma\right]^2 \right. \\ & \left. \times \left[\left(1+\gamma^2\right)^{1/2} + \frac{1}{2}\gamma\right]\right\}, \\ \gamma = {} & \frac{(2m*)^{1/2}\Gamma^2}{8q\hbar E\varepsilon_T^{1/2}}. \end{aligned} \tag{6}$$

Here, $\Gamma^2 = \Gamma_0^2(2n+1) = 8a(\hbar\omega)2(2n+1)$ is the width of the centre absorption band caused mainly by interaction with optical phonons of energy $\hbar\omega, n = [\exp(\hbar\omega/kT) - 1]^{-1}$ is the temperature distribution of phonons, m^* is the effective density mass of the electron in the semiconductor, and a is the electron-phonon coupling constant. The parameter γ provides the temperature dependence for tunneling process. If γ is very small due to a very large electrical field or low temperature, the tunneling process is temperature independent, and in this case PhAT is similar to classical tunneling.

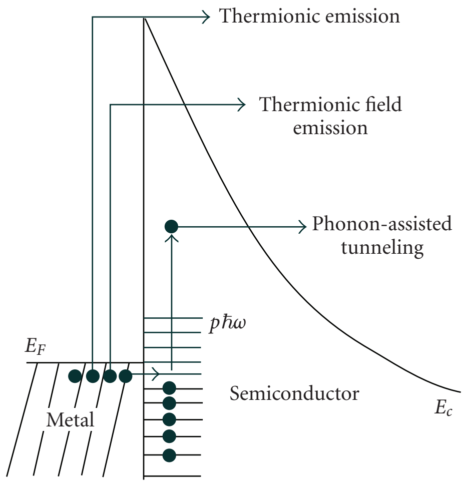

FIGURE 1: Energy diagram of the metal/semiconductor contact.

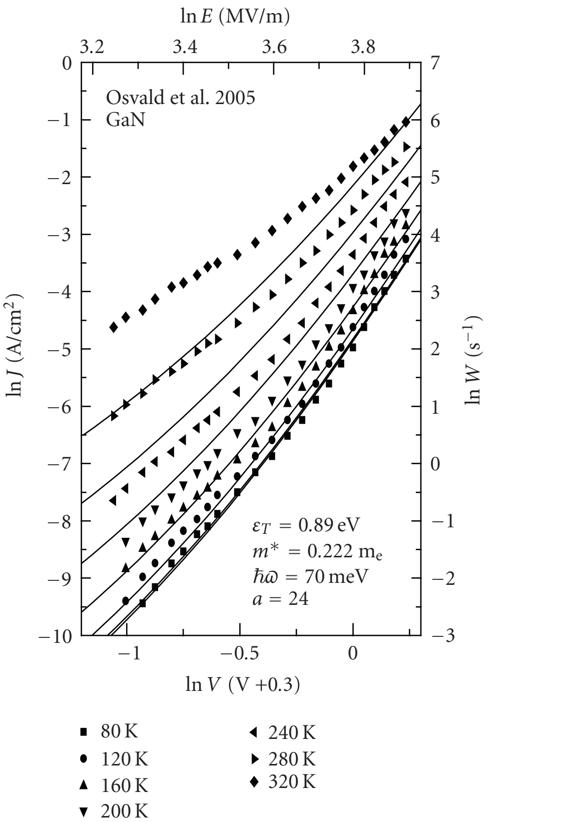

FIGURE 2: Comparison of *I-V* dependences for metal/n-GaN Schottky diode from Figure 2 [5] (symbols) with theoretical $W(E,T)$ against E dependences (solid curves), computed using parameters: $\varepsilon_T = 0.89$ eV, $m^* = 0.222$ m$_e$, $\hbar\varpi = 70$ meV, $a = 2.4$.

2.2. The Comparison of the Leakage Current Dependences on Bias for Different Temperatures with Theoretical W(E,T) Dependences. Now let us represent the comparison of some *I-V/T* characteristics measured on diodes fabricated both on epitaxial GaN and on GaN nanowires with the PhAT rate dependence on field strength computed using (6). The fit of the leakage *I-V/T* curves obtained by Osvald et al. [5] in the temperature range from 80 to 320 K for metal/n-GaN diode fabricated on N-polarity GaN grown by molecular-beam epitaxy to the tunneling rate dependences on field strength $W(E,T)$ is shown in Figure 2. The fit is performed under the assumption that the field strength is proportional to the square root of applied voltage, that is, the tunneling occurs in the high field region. The theoretical $W(E,T)$ versus E dependences were computed using for the barrier height ε_T the value of 0.89 eV estimated from the *C-V* data [5], and for the electron effective mass the the value of 0.222 m$_e$ [24] was used. For the phonon energy the value of 70 meV (i.e., somewhat lower than the energy of LO phonon, which in GaN is equal to 91 meV [25]) was selected. The coupling constant a was chosen in order to get the best fit of the experimental data with the calculated dependences. As is seen in Figure 2, the theoretical $W(E,T)$ dependences fit reasonably well with the experimental data for entire range of the measured temperatures. It is possible to notice that the higher the reverse bias is, the weaker is the temperature dependence. The estimated density of charged states in the interface was found to be equal to 1.5×10^{15} cm^{-2}.

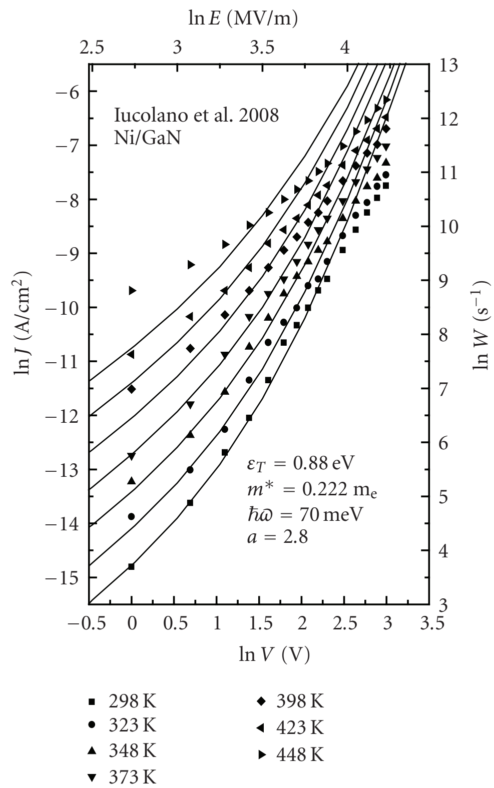

FIGURE 3: The *I-V* characteristics of Ni/GaN diode extracted from Figure 6 in [13] (symbols) fitted to the theory (solid curves). Parameters for computation: $\varepsilon_T = 0.88$ eV, $m^* = 0.222$ m$_e$, $\hbar\varpi = 70$ meV, $a = 2.8$. Estimated states density $N_s = 6.2 \times 10^{10}$ cm^{-2}.

Figure 3 shows the *I-V/T* data measured by Iucolano et al. [13] for Ni/GaN Schottky diode made on epitaxial n-GaN layer fitted to the theoretical $W(E,T)$ curves. As is seen from Figure 3, the theoretical curves describe well the

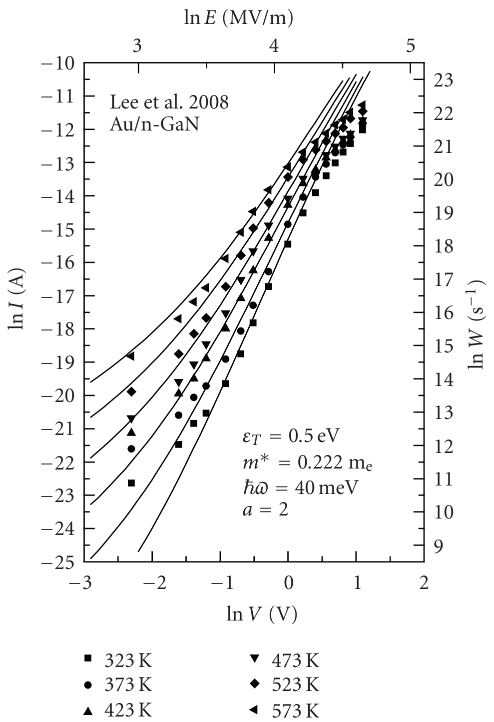

Figure 4: The I-V characteristics of Au/n-GaN nano-Schottky diode represented from Figure 2 [19] (symbols) fitted to theoretical $W(E, T)$ against E dependences (solid curves). Parameters for computation: $\varepsilon_T = 0.5$ eV, $m^* = 0.222\ \mathrm{m_e}$, $\hbar\varpi = 40$ meV, $a = 2.0$.

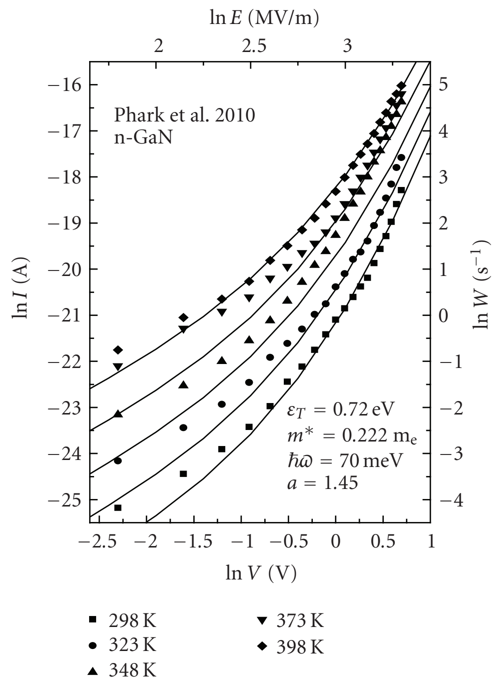

Figure 5: Reverse bias I-V characteristics of the Pt Schottky contacts to a-plane n-GaN extracted from Figure 2 [26] (symbols) fitted to theory (solid curves) Parameters: $\varepsilon_T = 0.72$ eV, $m^* = 0.222\ \mathrm{m_e}$, $\hbar\varpi = 70$ meV, $a = 1.45$. Assessed state density $N_S = 1.4.\ 10^{13}\ \mathrm{cm^{-2}}$.

experimental data in the temperature range from 298 K to 448 K. Only the I-V curve measured at 448 K signally deviates from theoretical ones. Other discrepancy between the theory and experiment emerges at higher voltages/fields when the current approaches to saturation. The observed trend to saturation of the current at higher electric field could be due to limitation of the filled centers in the interface when their exhaustion rate is very high (approximately $10^{10}\ \mathrm{s^{-1}}$). The assessed traps density for this diode was found to be equal to $6 \times 10^{10}\ \mathrm{cm^{-2}}$.

I-V/T characteristics for Au/n-GaN nano-Schottky diode measured by Lee et al. [19] in the temperature range from 323 to 573 K are shown in Figure 4. The temperature behavior of the I-V curves are very similar to the curves in Figure 3 and are also well described by the PhAT model. The electrical characteristics of a single GaN nanowire Schottky diode by authors of [19] were explained by a thermionic-field emission and an enhancement of the tunneling effects.

In a very recent paper, the temperature-dependent I-V characteristics of Pt Schottky contacts to a-plane n-type GaN were presented [26]. A notable deviation from the theoretical Richardson constant value was observed in the conventional Richardson plot. The authors of [26] have concluded that the thermionic emission model is inapplicable for these diodes. To explain the observed electrical behaviors, defect-assisted tunneling was necessary to invoke.

In Figure 5, the fit of the reverse bias branch of I_r-V/T characteristics from Figure 2 [26] with PhAT model is exposed. As can be seen the theoretical curves describe well the experimental data for all measured temperatures using the same value of $\varepsilon_T = 0.72$ eV assessed in [26]. From the fit of the experimental data with the theory and using (5) (S = $4.2 \times 10^{-4}\ \mathrm{cm^2}$) estimated states density at the interface was found to be equal to $1.4 \times 10^{13}\ \mathrm{cm^{-2}}$.

2.3. Apparent Barrier Height Dependence on Temperature. In this section, we present a comparison of the apparent barrier height dependence on temperature with envisaged for such dependence by PhAT model.

The reason for SBH derived from I-V/T characteristics depends on temperature lies in the fact that Φ_{br} is calculated from the gradient of Richardsons' plots which, in general, are not straight lines. The steepness of $\ln(I_R/T^2)$ versus $1/T$ curves at higher voltages was found to decline at lower temperatures, and the bowing of these curves is observed [15, 16]. The phonon-assisted theory predicts, namely, the same value of decrease in Φ_{br} as obtained from I-V/T characteristics. The correctness of this assertion will be confirmed by the comparison of the theoretical activation energy E_T dependences upon temperature with the apparent barrier height dependence on the same parameter. E_T was

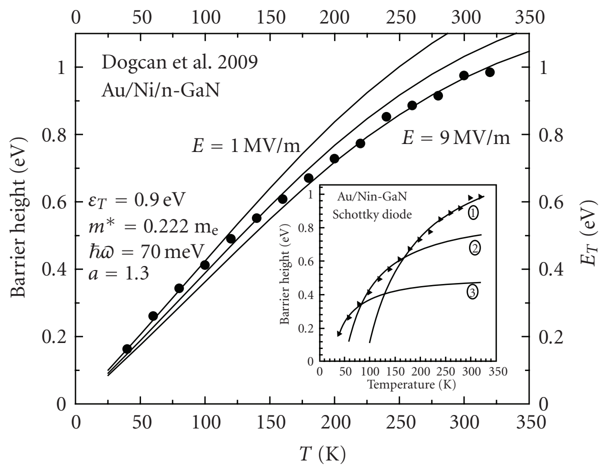

Figure 6: Temperature dependence of the barrier height for Au/Ni/n-GaN from [16] (symbols), fitted to the theoretical E_T versus T (solid lines) computed for field strengths of 1, 5, 9 (MV/m). Note that theoretical E_T is higher at lower fields. The inset shows barrier height versus T from the same work. The continuous curves in the inset correspond to Φ_b computed by authors of [16] using TE model for the three Gaussian distributions of the barrier height.

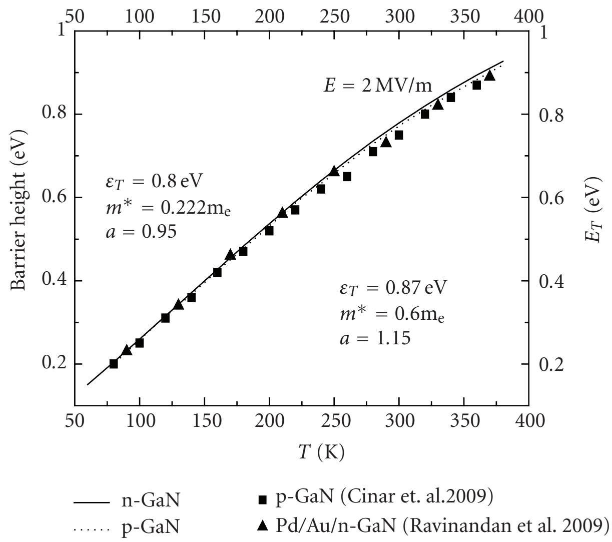

Figure 7: Variation of the barrier height with temperature for Pd/Au/n-GaN from [12] and Ag/p-GaN [14] (symbols), fitted to the E_T versus T exposed by solid line for n-type and dot line for p-type GaN.

calculated as the gradient of theoretical "Richardon plot" using

$$E_T = \frac{k}{q}\frac{d\ln(W/T^2)}{d(1/T)}. \tag{7}$$

In Figure 6 the apparent SBH dependence on temperature assessed by Doğan et al. for Au/Ni/n-GaN Schottky diodes from references [16] fitted to E_T dependence on temperature is shown. As is seen in Figure 6 the theoretical E_T versus T dependence reflects well the apparent barrier height dependence on temperature. An abnormal temperature dependence of the barrier height the authors of [16] have explained by invoking three sets of Gaussian distributions of barrier heights at 320–160 K, 160–80 K, and 80–40 K (see inset of Figure 6).

Figure 7 shows the fit of temperature-dependent SBH for Pd/Au/n-GaN from [12] and Ag/p-GaN/ SDs [14] with the theoretical E_T versus T dependence. One can see that theoretical curves both for n-type and p-type GaN describe very well the strong temperature dependence of apparent SBH observed for these diodes. Such the SBH behavior in [12] was attributed to barrier inhomogeneities by assuming a Gaussian distribution of barrier heights at the interface. Temperature variation of the experimental value of the SBH derived from the reverse bias characteristics from 0.17 eV at 80 K to 0.84 eV at 360 K for the Ag/p-GaN SD; the authors of [14] ascribed to the charge transport tunneling mechanism.

It is worth mentioning that the strong temperature dependence of the apparent Schottky barier height is also peculiarity for SDs made on the basis of other semiconductors. For instance in Figure 8 we represent the temperature dependence of SBH assessed from I-V/T data for SD made on n-type Si [27] and on p-type Si [28] ones. As can be seen the theoretical curves E_T versus T computed using

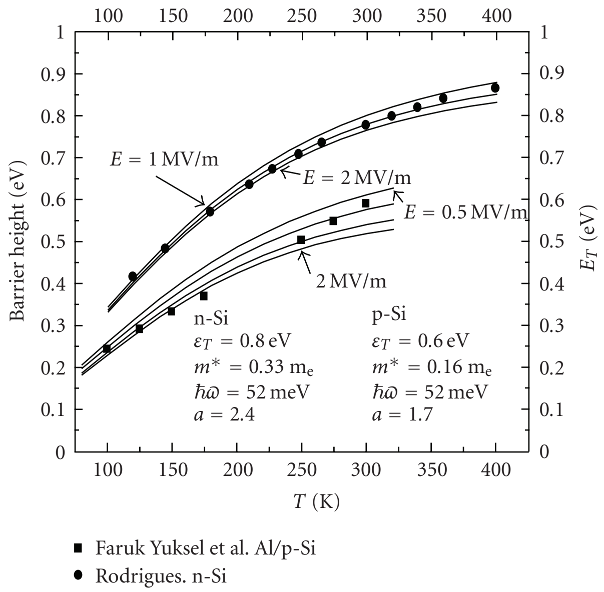

Figure 8: Temperature dependence of the barrier height for n-Si from [26] and Al/p-Si [27] symbols, fitted to the E_T versus T dependences (solid lines).

(6) and (7) and inherent for silicon parameters describe the experimental SBH dependence on temperature very well. The temperature dependence of the apparent SBH in these SDs by authors of [27, 28] have been explained invoking the Schottky barrier height inhomogeneity model [29]. Under their opinion, in presence of inhomogeneities of SBH electrons at low temperatures are able to surmount the lower barriers, and therefore the current transport will be dominated by current flowing through the patches of lower Schottky barrier height. As the temperature increases,

an increasing number of electrons will have sufficient energy to surmount the higher barriers; consequently, the dominant barrier height will increase with increasing both temperature and bias voltage. However, actual decrease in barrier height with increasing bias is observed for many diodes (see, e.g., [30] and references therein). We want to emphasize that PhAT theory predicts the SBH decrease as a bias voltage increases. This assertion is proved by E_T dependence on temperature computed for different values of field strength (see Figures 6 and 8).

The physical essence of the apparent barrier height dependence both on temperature and bias voltage in the framework of the PhAT theory is comprehensible. According to this model, the apparent SBH/(activation energy) depends on the quantity of phonons taken part in the tunneling process. At low temperatures the number of phonons according to the equation $n = [\exp(\hbar\omega/kT) - 1]^{-1}$will be less in determining lower energy activation and herewith barrier height. At higher temperatures the number of phonons is greater, and apparent SBH will be higher. Likewise is explicable dependence of SBH on bias voltage. At high voltages for the tunneling less quantity of phonons is required then at low ones. Hence, at low bias voltages the apparent SBH will be higher. Thus, the actual barrier height can be determined from the C-V measurements but not from I-V/T measurements using thermionic emission theory.

3. Conclusion

In conclusion, the phonon-assisted tunneling model describes well the peculiarities of reverse-bias current-temperature dependence in Schottky diodes fabricated either on GaN epitaxial layer or on GaN nanowires. The fit of experimental data to computed tunneling rate allows to estimate the field strength at which the free charge carriers are generated, and the density of charged states near the interface between metal and semiconductor. In the terms of this model the bias voltage and temperature dependence of apparent SB height evaluated from I-V/T measurements is explained as well. Thus, phonon-assisted tunneling mechanism must be taken into account in explaining the reverse leakage current characteristics for diodes with Schottky barriers.

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