Extraction of AlGaN/GaN heterostructure Schottky diode barrier heights from forward current-voltage characteristics

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Ni Schottky contacts on AlGaN/GaN heterostructures have been fabricated, and one of the prepared samples has been annealed at 700 °C for half an hour. The barrier heights for the prepared samples were measured by internal photoemission. Based on the measured forward current-voltage (I-V) characteristics and using the two-diode model, the Ni Schottky barrier height at zero bias has been analyzed and calculated by self-consistently solving Schrodinger's and Poisson's equations, and the correlation expression between the barrier height at zero electric field and that at zero bias has been derived for Schottky contacts on AlGaN/GaN heterostructures. The calculated Schottky barrier heights corresponding to zero electric field for the prepared Ni Schottky contacts on AlGaN/GaN heterostructures agree well with the photocurrent measured results. Thus, the method for extraction of AlGaN/GaN heterostructure Schottky barrier heights from forward I-V characteristics is developed and determined. © *2011 American Institute of Physics*. [doi:10.1063/1.3569594]

I. INTRODUCTION

Recently AlGaN/GaN heterostructure field-effect transistors (HFETs) have been the focus of intense research to improve device performance and reliability.[1–3] The Schottky barrier height of the AlGaN/GaN HFETs is of great importance for device performance and reliability. A large barrier height leads to small leakage currents and high breakdown voltage,[4] thus improving the noise level[5] and power performance of the device. Schottky barrier heights can be determined using current-voltage (I-V), capacitance-voltage (C-V), photocurrent and x-ray photoelectron spectroscopy (XPS) measurements.[6–10] However, for a heterojunction such as the AlGaN/GaN HFETs structure, the conventional I-V technique based on the thermionic emission model may not yield an accurate determination of the barrier height.[9] Currently, the barrier height for Schottky contacts on AlGaN/GaN heterostructures is mainly measured by internal photoemission. Whereas the measurement is not easily performed, because the two components of the photocurrent generated and diffused from the metal side or generated within the depletion region of the semiconductor by the incident photons need to be separated in the measurement, especially, when there are the deep level defects in the AlGaN barrier layer.[9] As a result, it is necessary to develop a method for extraction of AlGaN/GaN heterostructure Schottky barrier heights from forward I-V characteristics. As modeled by Chen *et al.*,[11] a structure consisting of a metal gate can be considered as two diodes connected in series back to back, one is a metal-AlGaN Schottky diode, and the other is an equivalent Schottky diode due to the heterojunction between the AlGaN and the GaN layer. With Chen's two-diode model, the effective Richardson constant needs to be determined. It is well known that the effective Richardson constant is very sensitive to the semiconductor material quality and the type of Schottky contact metal, and there is a large scattering in the measured values of the effective Richardson constant for GaN Schottky contacts.[12] Thus, an accurate determination of the effective Richardson constant is necessary for using the two-diode model to analyze and calculate the Schottky barrier height for Schottky contacts on AlGaN/GaN heterostructures. In addition, the barrier height calculated by the two-diode model corresponds to the barrier height at zero bias. To our knowledge, there has not been a correlation expression between barrier heights at zero bias and those at zero electric field for Schottky contacts on AlGaN/GaN heterostructures. Corresponding to zero electric field, the semiconductor bands are flat, and the barrier heights at zero electric field are also called flat-band barrier heights.[13] Since the flat-band barrier height must be a property of only the metal-semiconductor interface and is not affected by the electric field,[14] the flat-band barrier height as the fundamental barrier height for Schottky contacts on AlGaN/GaN heterostructures should be extracted and calculated from forward I-V characteristics. In order to obtain the barrier height at zero electric field (the flat-band barrier height), the correlation expression between the zero bias and zero electric field barrier heights for Schottky contacts on AlGaN/GaN heterostructures needs to be determined.

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In this paper, Ni Schottky contacts on AlGaN/GaN heterostructures have been prepared, and one of the prepared Ni Schottky contact samples has been annealed at 700 °C for half an hour in N_2 ambient. Based on the measured forward I-V curves and using the two-diode model, the effective Richardson constant and the Schottky barrier heights at zero bias for the prepared samples have been analyzed and calculated by self-consistently solving Schrodinger's and Poisson's equations. The correlation expression between the zero bias and zero electric field Schottky barrier heights was derived, and the Schottky barrier heights obtained at zero electric field were compared with the photocurrent measured results.

II. EXPERIMENTS

The heterostucture layer employed in this study was epitaxially grown by metal organic chemical vapor deposition (MOCVD) on a (0001) sapphire substrate. The heterostructure layer consists of a 40 nm AlN nucleation layer, followed by a 3 μm undoped GaN layer and a 21.5 nm thick undoped $Al_{0.3}Ga_{0.7}N$ barrier layer. Hall measurements indicate a sheet carrier density of around 1.36×10^{13} cm^{-2} and an electron mobility of 1200 cm^2/V.s at room temperature. For the device processing, Ohmic contacts of Ti/Al/Mo/Au were fabricated by e-beam evaporation and lift-off technique. These contacts were annealed at 850 °C for 30 s in a rapid thermal annealing system. Ni/Au (60 nm/200 nm) circular Schottky contacts with a diameter of 120 μm were then deposited by e-beam evaporation. The separation between the Ohmic contact and the circular Schottky contact was 20 μm. One sample of the prepared Schottky contacts was then annealed at 700 °C for 0.5 h in N_2 ambient and the other was left unannealed as a control. The C-V measurements of the prepared Schottky contacts were performed by using an Aglient 4284A LCR meter, and a combination of a dc-biased voltage was applied between the Schottky and Ohmic contacts and an ac-modulation voltage of amplitude of ±0.1 V at frequency of 10 kHz. The photoemission measurements of the two Schottky diodes were performed with a halogen lamp as a light source, a monochromator (ISA, model HR-320) and a lock-in amplifier (EG&G, model 5209) for the photocurrent measurement. The I-V measurements were performed using an Agilent 4156 semiconductor parameter analyzer.

III. RESULTS AND DISCUSSIONS

Figure 1 shows photocurrent spectra of the unannealed and annealed Ni Schottky contacts at 700 °C for half an hour. According to Fowler's theory,[15] the relationship between the photocurrent per photon, R, and the incident photon energy hν is given by[9,15]

$$R \sim (h\upsilon - q\phi_b)^2, \tag{1}$$

where $q\phi_b$ is the Schottky barrier height. This relation is valid when $(h\nu - q\phi_b) > 3$ kT. Therefore, the Schottky barrier can be obtained from the linear relationship of the square root of the photocurrent per photon versus the incident photon energy. With the photoemission measurements, the

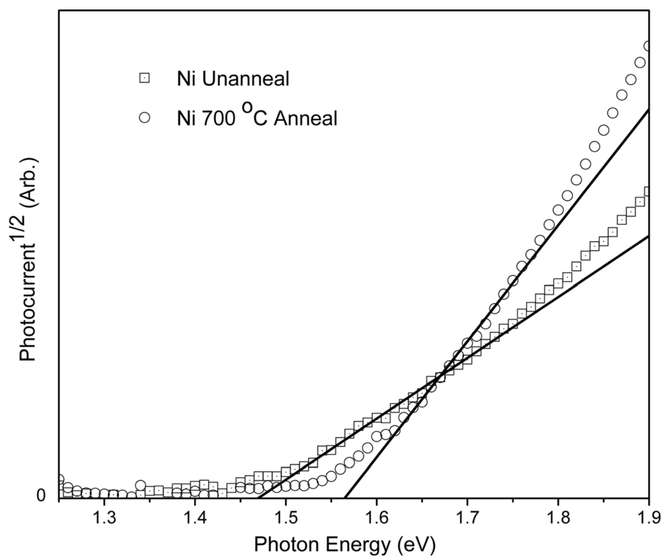

FIG. 1. Photoemission measurement curves for unannealed and 700 °C 30 min annealed Ni Schottky contacts.

Schottky barrier heights of the unannealed and thermally annealed Ni Schottky contacts are 1.47 eV and 1.57 eV, respectively.

The bandgap of $Al_xGa_{1-x}N$ at room temperature is given by[16]

$$E_g(x) = 6.13x + 3.42(1-x) - x(1-x)(\text{eV}). \tag{2}$$

The conduction-band offset is[17]

$$\Delta E_c = 0.7[E_g(x) - E_g(0)]. \tag{3}$$

In the calculation of (2) and (3), the Al content is taken as 0.3 at room temperature, and then ΔE_C was calculated to be 0.42 eV.

Figure 2 shows the measured C-V curves of the unannealed and annealed Ni Schottky contacts. The two dimensional electron gas (2DEG) sheet carrier density (n_{2D}) under Schottky contact metals at zero gate bias can be obtained by the C-V curve integration[18]

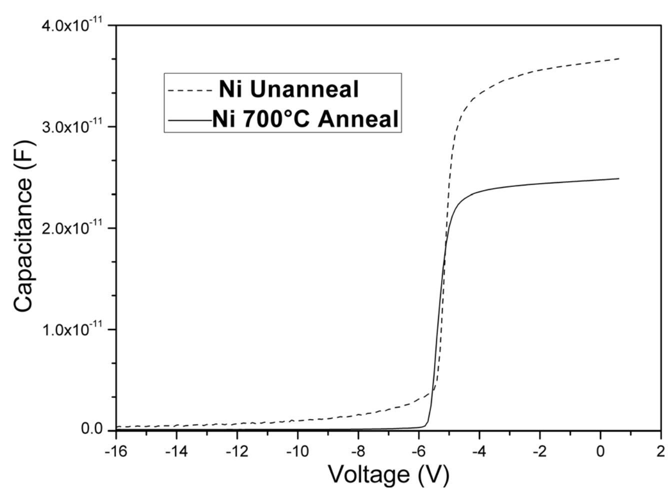

FIG. 2. The measured C-V curves at room temperature with frequency of 10 kHz for the unannealed and 700 °C 30 min annealed Ni Schottky contacts.

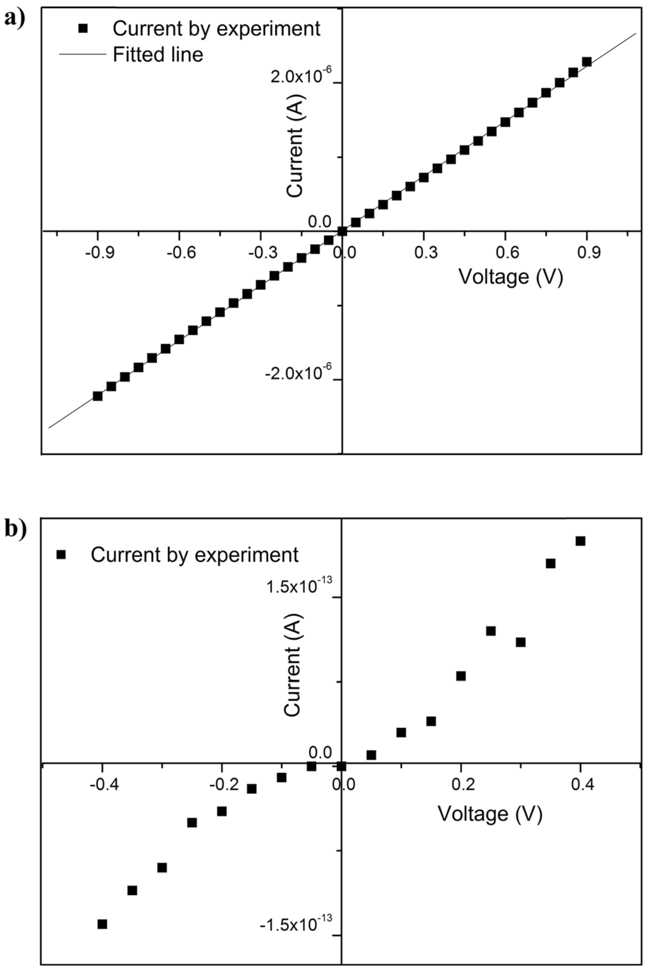

FIG. 3. The measured I-V characteristics at low bias for the (a) unannealed and (b) 700 °C 30 min annealed Ni Schottky contacts.

$$n_{2D} = \int_{V_T}^{0} \frac{CdV}{(Sq)}, \tag{4}$$

where q is the electron charge, C is the measured capacitance between the ohmic contact and the Ni Schottky contact, V_T is the threshold voltage and can also be obtained by the C-V curve integration,[18] S is the Ni Schottky contact area. The calculated 2DEG electron density for the unannealed and annealed Ni Schottky contacts is 9.732×10^{12} and $6.968 \times 10^{12}\ \text{cm}^{-2}$, respectively.

The I-V characteristics of the unannealed and annealed Ni Schottky contacts at low biases are shown in Fig. 3. As shown from Fig. 3(a), for the unannealed Ni Schottky contact, in the region of low forward and reverse voltages, the I-V curve is almost linear. The linear characteristics can not be explained by either the thermionic emission or the vertical tunneling models.[19,20] This shows the existence of a shunt conduction path in the unannealed Schottky diode sample, and the shunt conduction path is related to hopping conduction through high density surface electronic states in AlGaN.[21,22] Figure 3(b) is the I-V curve at low forward and reverse biases for the annealed Ni Schottky contact. It is shown that the value of the current for the annealed sample is many orders of magnitude smaller than that of the unannealed, and the I-V curve deviates from linearity. This can be attributed to the decrease of the surface electronic state density in the AlGaN barrier layer by annealing, which results in a great increase of the shunt path resistance. As a result, the current of the shunt conduction path can be neglected for the annealed Ni Schottky contact. The conductance (ρ) of the shunt path for the unannealed Schottky diode sample can be obtained by the slope of the I-V curve at low bias as shown in Fig. 3(a). Then, the current of the shunt conduction path is calculated by

$$I_{path} = \rho V, \tag{5}$$

where I_{path} is the shunt path current, and V the applied bias. Figure 4 shows the measured forward I-V curves for the unannealed and annealed Ni Schottky contacts. According to Chen's model,[11] the two linear regions marked with dash dot line (Fig. 4) correspond to the applied voltage drop across diode 1 and diode 2 (Fig. 5), respectively. And at the current value of around 10^{-7} A (Fig. 4), a small platform occurs, which is possible to be related to the thin insulating interfacial layer between the Schottky metals and the AlGaN barrier layer, or the defects in AlGaN/GaN heterostructures. Combining with (5), the current of the shunt conduction path for the unannealed Ni Schottky contact is deducted from the

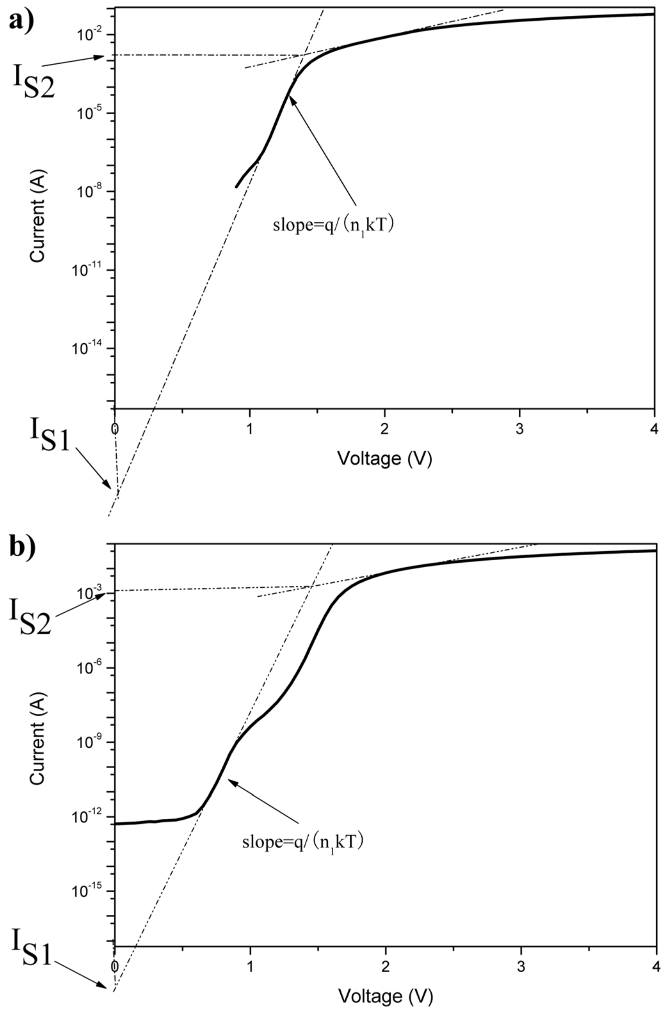

FIG. 4. The measured forward I-V curves for the (a) unannealed and (b) 700 °C 30 min annealed Ni Schottky contacts.

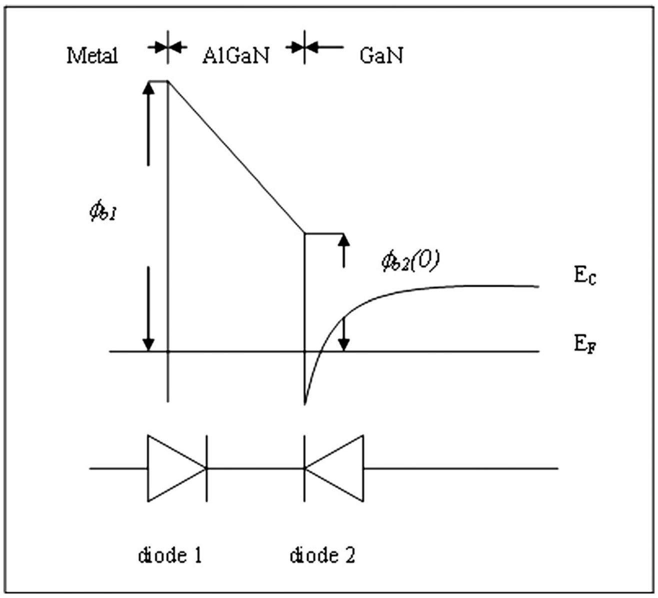

FIG. 5. Conduction band diagram of the AlGaN/GaN heterostructure at zero bias and the two-diode equivalent circuit.

measured I-V curve (Fig. 4(a)). Figure 5 shows the conduction band diagram of AlGaN/GaN heterostructures, according to Chen's model[11] in which the equivalent circuit of a Schotty AlGaN/GaN diode can be visualized as two diodes back-to-back in series. The left diode (diode 1) represents the Schottky contact between the Schottky metals and the AlGaN barrier layer. The right diode (diode 2) represents the effective Schottky contact between the two dimensional electron gas and the AlGaN barrier layer.[11,23] The current through diode 1 can be written as[11]

$$I = I_{s1}[\exp(qV_1/n_1KT) - 1], \tag{6}$$

where V_1 is the voltage across diode 1, n_1 is the ideality factor of diode 1, k is Boltzmann's constant, T is the temperature, and

$$I_{s1} = SA^*T^2 \exp(-q\phi_{b1}/KT), \tag{7}$$

where A^* is the effective Richardson constant and ϕ_{b1} is the barrier height of diode 1 at zero bias.

The current through diode 2 is

$$I = I_{s2}[\exp(qV_2/n_2KT) - 1], \tag{8}$$

where V_2 is the applied voltage across diode 2, and

$$n_2 = \frac{1}{|\partial\phi_{b2}/\partial V_2|}, \tag{9}$$

ϕ_{b2} is the barrier height of diode 2

$$I_{S2} = SA^*T^2 \exp[-q\phi_{b2}(0)/KT], \tag{10}$$

$\phi_{b2}(0)$ is the barrier height of diode 2 at zero bias.

Combining (6), (7), (8), (9) and (10), the parameters I_{s1}, I_{s2}, n_1, and n_2 can be obtained from the measured forward I-V curves (Fig. 4), and the detailed analysis for characterizing these parameters is reported in the literature.[11] For the unannealed Ni Schottky contact, the values of I_{s1}, I_{s2}, n_1, and n_2 are calculated and obtained, they are 6.85×10^{-21} A, 1.36×10^{-3} A, 1.35 and 15.29, respectively, and with the annealed Ni Schottky contact, the values of I_{s1}, I_{s2}, n_1, and n_2 are 3.08×10^{-20} A, 2.68×10^{-3} A, 1.42, and 24.29, respectively. Both under unannealed and annealed conditions, the values of n_2 are very high. With Chen's model,[11] n_2 reflects the degree of barrier height change (diode 2) due to the change of voltage across it. The large n_2 means the barrier height change for diode 2 is small, otherwise the current increment will be large. In order to obtain the barrier height of ϕ_{b1}, the effective Richardson constant A^* is determined by the iterative calculation shown below. First, the value of $\phi_{b2}(0)$ is assumed to be equal to the value of ΔE_C (0.42 eV), and with the known value of I_{s2}, the effective Richardson constant A^* is calculated by (10). Then we take the calculated value of A^* into (7) with the known value of I_{s1}, and obtain the value of ϕ_{b1}. Based on the calculated ϕ_{b1} and the values of n_{2D} and ΔE_C, we calculate the value of the Fermi level E_F at zero bias (Fig. 5) by self-consistently solving Schrodinger's and Poisson's equations.[24] From Fig. 5, it is shown that the relationship between $\phi_{b2}(0)$ and E_F obeys

$$\phi_{b2}(0) = \Delta E_C - E_F. \tag{11}$$

We then replace the initial $\phi_{b2}(0)$ by the new calculated value and operate iteratively the above process until the difference between the latest $\phi_{b2}(0)$ and the prior $\phi_{b2}(0)$ value is less than a specified value. With this iterative calculation, the value of the effective Richardson constant A^* is determined, and the values of ϕ_{b1} and $\phi_{b2}(0)$ are also determined.

It is well known that the barrier height of a Schottky barrier diode is electric field dependent.[25,26] The obtained ϕ_{b1} is the barrier height of Ni Schottky contacts on AlGaN/GaN heterostructures at zero bias. For a Schottky diode, if we take the barrier height ϕ_{BF} as the barrier height when the electric field is zero and the barrier height ϕ_{B0} as the barrier height at zero bias, the correlation between the ϕ_{BF} and ϕ_{B0} is[14]

$$\phi_{BF} = n\phi_{B0} - (n-1)\frac{kT}{q}\ln\frac{N_C}{N_D}, \tag{12}$$

where n is the ideality factor for the Schottky diode, N_C is the effective conduction-band density of states, and N_D is the n-type semiconductor donor density. However, the correlation expression of (12) is not correct for Schottky contact diodes on AlGaN/GaN heterostructures. For Schottky contacts on AlGaN/GaN heterostructures, ϕ_{BF} and ϕ_{B0} correspond to the barrier heights of the metal-AlGaN Schottky diode (diode 1) at zero electric field and zero bias, respectively, and ϕ_{B0} equals the above calculated ϕ_{b1}. The new correlation expression between the ϕ_{BF} and ϕ_{b1} for the Schottky diodes on AlGaN/GaN heterostructures can be derived as follows. First, we have the identification[14]

$$\phi_{BF} = \phi_{b1} + \left(\frac{n_1 - 1}{n_1}\right)V_0, \tag{13}$$

TABLE I. The calculated and measured parameters for the unannealed and the annealed samples.

		n_1	ϕ_{b1} (ev)	$\phi_{b2}(0)$ (ev)	ϕ_{BF} (ev)	Φ_B (Photo) (ev)	A^* A/(K^{2}m^2)
Unannealed	A^*obtained by iterative calculation	1.35	1.13	0.10	1.49	1.47	120.3
	A^* calculated from theoretical formula	1.35	1.36	0.10	1.80	1.47	3.58×10^5
700 °C, 30 min annealed	A^*obtained by iterative calculation	1.42	1.18	0.17	1.60	1.57	1.54×10^3
	A^* calculated from theoretical formula	1.42	1.32	0.17	1.80	1.57	3.58×10^5

where V_0 is the flat-band voltage, and V_0 can be written as

$$V_0 = \phi_{BF} - \phi_{b2}(0). \tag{14}$$

Substituting (14) into (13), we obtain

$$\phi_{BF} = n_1\phi_{b1} - (n_1 - 1)\phi_{b2}(0). \tag{15}$$

Equation (15) is the correlation expression between ϕ_{BF} and ϕ_{b1} for the Schottky contacts on AlGaN/GaN heterostructures. It has been shown that the barrier height for Schottky contacts obtained by internal photoemission is in better agreement with the flat-band barrier height ϕ_{BF}.[7,8] With the determined parameters of $\phi_{b1,}$ $n_{1,}$ $\phi_{b2}(0)$, the value of ϕ_{BF} can be obtained by using (15). Thus, the parameters of $\phi_{b1,}$ n_1, $\phi_{b2}(0)$, A^* and ϕ_{BF} for the prepared unannealed and annealed Ni Schottky contacts are determined and summarized in Table I.

The value of the effective Richardson constant A^* can also be determined by the theoretical formula[27]

$$A^* = 4\pi q m^* k^2/h^3, \tag{16}$$

where m^* is the electronic effective mass in the $Al_{0.3}Ga_{0.7}N$ barrier layer, and $m^* = 0.298\ m_0$,[28] m_0 is the free-electron mass, h is the Plank' constant, and k is Boltzmann's constant. The effective Richardson constant A^* calculated by (16) is 3.58×10^5 (A/(K^{2}m^2)). Based on the known parameters of I_{s1} and n_1 determined by the measured forward I-V curves, and substituting the value of A* (3.58×10^5 A/(K^{2}m^2)) into (7), the value of ϕ_{b1} is obtained. Then, with the known ϕ_{b1} and n_{2D}, the value of $\phi_{b2}(0)$ is determined by self-consistently solving Schrodinger's and Poisson's equations. At last, the value of ϕ_{BF} is calculated using (15). These calculated parameters for the prepared unannealed and annealed Ni Schottky contacts on AlGaN/GaN heterostructures are also listed in Table I. As seen from Table I, with the values of A^* determined by the iterative calculation, the calculated values (1.49 eV and 1.60 eV) of the Schottky barrier height ϕ_{BF} for both the unannealed and the annealed Ni Schottky contacts on AlGaN/GaN heterostructures agree well with the values obtained by photocurrent measurements (1.47 eV and 1.57 eV, respectively), whereas those obtained by the theoretical values of A^* are larger by 0.33 eV (the unannealed sample) and 0.23 eV (the annealed sample) than the corresponding photocurrent measured results. It is shown that the method for extraction of AlGaN/GaN heterostructure Schottky barrier heights from forward I-V characteristics is valid.

IV. CONCLUSION

In summary, Ni Schottky contacts on AlGaN/GaN heterostructures have been fabricated, and one of the prepared samples was annealed at 700 °C for half an hour. With the measured I-V and C-V characteristics for the prepared samples, the barrier heights at zero bias for the Ni Schottky contacts on AlGaN/GaN heterostructures have been analyzed and calculated by self-consistently solving Schrodinger's and Poisson's equations, and the correlation expression between the zero electric field and zero bias barrier heights has been derived for Schottky contacts on AlGaN/GaN heterostructures. Using the effective Richardson constant determined by the iterative calculation, the calculated Schottky barrier heights corresponding to zero electric field for the prepared unannealed and the annealed Ni Schottky contacts on AlGaN/GaN heterostructures are in good agreement with those obtained by photocurrent measurements. This demonstrates that the method for extraction of AlGaN/GaN heterostructure Schottky barrier heights from forward current-voltage characteristics is developed and determined.

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