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Effects of Post Annealing on I-V-T Characteristics of (Ni/Au)/Al$_{0.09}$Ga$_{0.91}$N Schottky Barrier Diodes

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Abstract. Post annealing is a simple, effective and suitable method for improving the diode parameters, especially when the used chemically stable substrates like Si, III-N and ternary alloys. In our work, we were applied this method to (Ni/Au)/Al$_{0.09}$Ga$_{0.91}$N Schottky Barrier Diodes (SBDs) and investigated by temperature-dependent current-voltage (I-V-T) characteristics at optimum conditions. Optimum annealing temperature was 600°C, which it's determined with respect to have a highest barrier height value.

The temperature-dependent electrical characteristics of the annealed at 600°C (Ni/Au)/Al$_{0.09}$Ga$_{0.91}$N SBDs were investigated in the wide temperature range of 95-315K. The diode parameters such as ideality factor (n) and Schottky barrier height (Φ_{b0}) were obtained to be strongly temperature dependent. The observed variation in Φ_{b0} and n can be attributed to the spatial barrier inhomogeneities in Schottky barrier height by assuming a triple Gaussian distribution (TGD) of barrier heights (BHs) at 95-145K, 145-230K and 230-315K. The modified Richardson plots and T$_0$ analysis was performed to provide an experimental Richardson constants and bias coefficients of the mean barrier height. Furthermore, the chemical composition of the contacts was examined by the XPS depth profile analysis.

1. Introduction
GaN and its ternary alloys, especially AlGaN, are of interest in the fabrication of high-power, high-temperature and high-frequency electronic devices, as well as, transistors, light emitting and detecting devices. Devices based on AlGaN layers or bulk includes bipolar junction transistors [1], solar blind photodiodes [2], light emitting diodes and high electron mobility transistors [3]. These exciting applications brings numerous challenges, such as making reliable, high quality, efficient, thermally stable metal [4-7] contacts to nitride semiconductor, which is crucial for device performance. With respect to electronic devices such as metal semiconductor field effect transistor (MESFETs), metal oxide semiconductor field effect transistors (MOSFETs), modulation doped field effect transistors (MODFETs) and high power switching devices, main process improvements are needed in the areas of stable and reproducible Schottky and ohmic contacts to GaN based materials [8]. Also, for advancement of these devices, electrical properties and effect of post annealing have to be fully investigated. Especially, more detailed characterizations of metal/AlGaN interfaces seem to be necessary. Furthermore, the chemical structure of as-deposited and annealed metal/AlGaN interfaces also have to be investigated to give clear sight about properties of Schottky barrier diodes (SBDs).

In this work we focused on thermal annealing effects on the electrical characteristics of $(Ni/Au)/Al_{0.09}Ga_{0.91}N$ SBDs. Annealing treatment was performed at a temperature ranging from 100 to 600°C in increments of 100°C for 3 min in high purity argon ambient. The thermal stability of the Ni/Au Schottky contacts was evaluated by considering the change of the Schottky barrier height (SBH) with the annealing temperature. Also, the temperature-dependent electrical characteristics of the as-deposited and annealed at 600°C $(Ni/Au)/Al_{0.09}Ga_{0.91}N$ SBDs were investigated in the wide temperature range of 95-315K. Furthermore, the chemical composition of the contacts was examined by the XPS depth profile analysis.

2. Experimental

In this study, unintentionally doped (uid) n-type $Al_{0.09}Ga_{0.91}N$ epitaxial layers grown by MOCVD on a HPSI-SiC substrate were used. The epistructure of the wafer consists of 2 nm thin layer of GaN cap layer for protection purposes, $Al_{0.09}Ga_{0.91}N$ layer with a thickness of 21 nm, AlN layer with a thickness of 3 nm, Fe doped GaN buffer layer with a thickness of 1.8 µm and a 4H-SiC high-purity semi-insulating substrate. The AlGaN substrates were cleaned consecutively acetone, methanol, trichloroethylene, deionized water (18 MΩ) 5 min. using ultrasonic agitation in each step. The substrates were then dried with high-purity nitrogen. After cleaning organic residuals, the substrates were dipped in aqua regia (3:1 $HCl:HNO_3$) to remove the native oxide from the front surface of the substrate and boiling KOH (1 M) to reduce the surface roughness, respectively. The Ti/Al (25 nm/105 nm) Ohmic metallization was deposited using magnetron dc sputtering for Ti and thermal evaporation for Al and a standard lift-off process was used to pattern the contacts. The contacts were annealed at 850°C for 1 min in flowing high purity (6N) argon gas in a quartz tube furnace. The Ni/Au (30 nm/50 nm) Schottky metallization was then deposited using magnetron dc sputtering for Ni and thermal evaporation for Au and a standard lift-off process was used to pattern to form Schottky contacts with a diameter of 0.4 mm.

I-V-T measurements of the as-deposited and annealed $(Ni/Au)/Al_{0.09}Ga_{0.91}N$ SBDs were accomplished by employing a computer-controlled HP 4140B picoamperemeter with a LN_2 cooled cryostat. Annealing was performed in the quartz tube furnace with flow (~10 ccm/s) of high purity Ar gas ambient. Annealing time was 3 minutes.

3. Results and discussion

3.1. I-V measurements and effect of annealing on diode parameters

Fig. 1 shows the forward and reverse I-V characteristics of the as-deposited and annealed $(Ni/Au)/Al_{0.09}Ga_{0.91}N$ SBDs. For the as-deposited Ni/Au Schottky contact, the leakage current at -3 V is 7.18×10^{-7} A. For the diode annealed at temperature 400°C, 500°C and 600°C, the leakage currents are 2.06×10^{-7} A, 1.61×10^{-7} A and 1.21×10^{-7} A at -3 V, respectively. It can be seen from Fig. 1 that the thermal annealing effect on reverse bias current was small under the annealing temperature of 400°C.
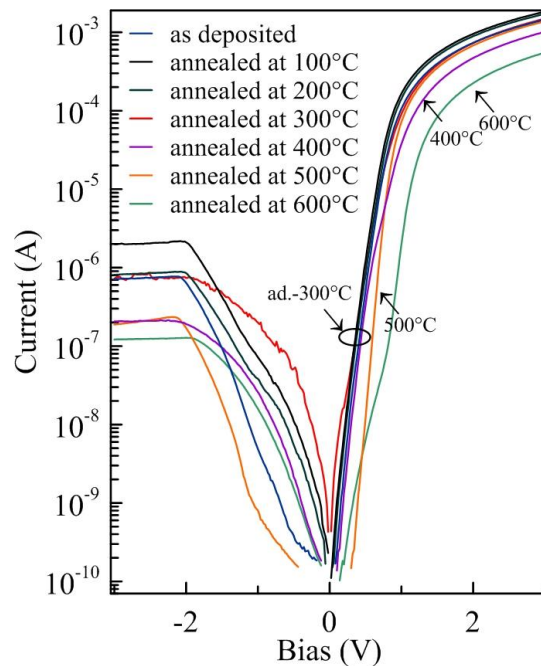
Fig. 1. I-V characteristics of the as-deposited and annealed (Ni/Au)/Al$_{0.09}$Ga$_{0.91}$N SBD.

However, the ratio of forward bias current/reverse bias current at given bias (rectification factor) was increased approximately 4 times after the annealing at 500°C (Fig 2.). Therefore, the annealing temperature of 500°C was crucial for the studied SBDs.
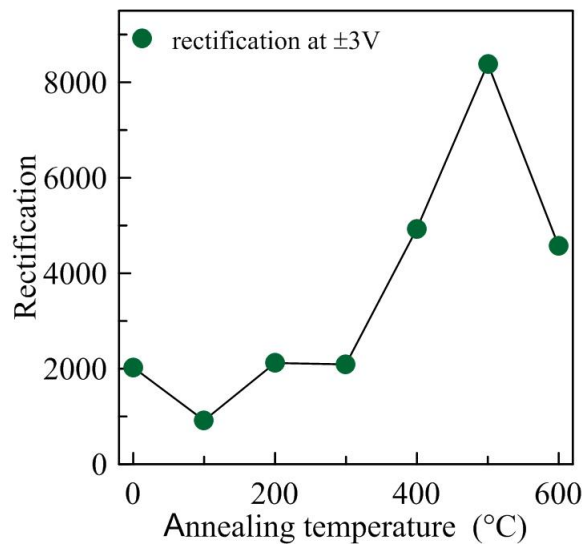

Fig 2. The variation of rectification factor of the as-deposited and annealed at ±3V.

I-V curves were analyzed using the thermionic emission theory (TET). According to the TET, the current flowing through the metal–semiconductor contact under forward bias V is given by (for V > 3kT/q) [9]

$$I = I_0 exp\left[{qV}/{nkT}\right] \tag{1}$$

where I_0 the saturation current is defined by

$$I_0 = AA^*T^2 exp\left[{-q\Phi_{b0}}/{kT}\right]. \tag{2}$$

The quantities V, n, T, A, A^*, q, k, and Φ_{bo} are the applied bias voltage, the ideality factor, the temperature in Kelvin, the effective diode area, the effective Richardson constant of 29.3 $\text{AK}^{-2}\text{cm}^{-2}$ for $\text{Al}_{0.09}\text{Ga}_{0.91}\text{N}$ [10], the electron charge, the Boltzmann constant, and the apparent barrier height at zero bias determined from the I-V data, respectively.

The experimental values of the barrier height Φ_{bo} and the ideality factor n after each annealing step were calculated from the intercepts and slopes of the straight-line portions of the semilog forward bias I-V characteristics using Eqs. (1) and (2), respectively. The values of n and Φ_{bo} obtained depending on the annealing temperature for the diodes are given in Table 1. The variation of SBH of the Ni/Au Schottky contacts as a function of annealing temperature is shown in Fig. 3.
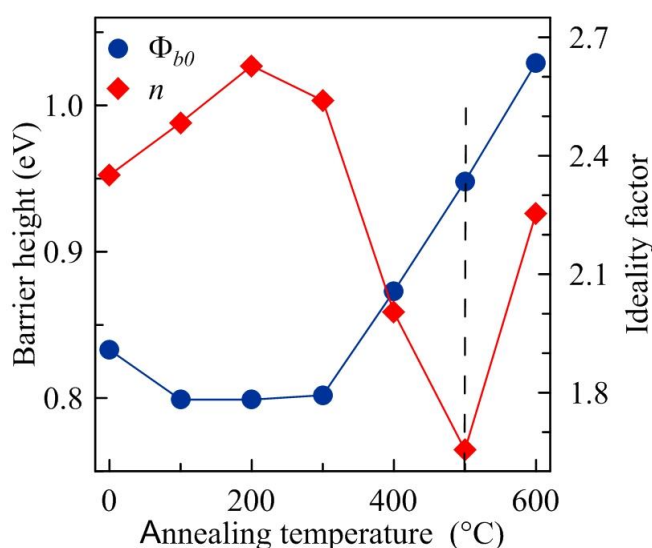

Fig 3. The variation of SBH and ideality factor of the as-deposited and annealed (Ni/Au)/$\text{Al}_{0.09}\text{Ga}_{0.91}\text{N}$ SBD.

Table 1 show that the Schottky barrier height determined of the as-deposited (Ni/Au)/$\text{Al}_{0.09}\text{Ga}_{0.91}\text{N}$ SBD was 0.833 eV which agrees with the literature [11]. The SBH is lower than the theoretical value which can be explained by the existence of the interfacial layer, structural defects such as the stacking faults, and dislocations on the AlGaN [11, 12]. The highest SBH was obtained to be 1.029°eV after annealing at 600°C for Ni/Au Schottky contact. Moreover, the rectification feature of the diode after annealing at 700°C was deteriorated (not shown here). The results in Table 1 show that the values of ideality factor are higher than unity for all contacts. For an ideal diode, the value of ideality factor should be nearly equal to one. A departure from the ideality could be caused by the image force lowering, generation and recombination of carriers in the space charge region, interface states, interfacial layer, and thermionic field emission [13-15]. These effects invariably increase the ideality factor [11].

The above observations reveal that before the values of the ideality factor fluctuate around 2 by annealing temperature up to 400°C and then decreases at the above annealing temperatures of 500°C. This situation encountered may be due to the change of the interface state distribution and/or chemical composition formed between the metal and the semiconductor at the interface [15-17]. This is confirmed by XPS analysis, as will be seen later. Therefore, it can be said that the performance and reliability of Schottky contacts depend on the nature of interfacial layer at the MS contacts which affected by annealing temperature. The nature of interfacial reactions between the metal and semiconductor plays an important role in determining the quality of Schottky barrier in AlGaN.

The SBHs and serial resistance (Rs) of the Ni/Au/n-GaN Schottky diodes are determined using the Norde method [18]. The plots of $F(V)$ versus V for the SBD using data in Fig. 1 at the different annealing temperatures are shown in Fig. 4. The values of obtained Rs of the SBDs are also given in

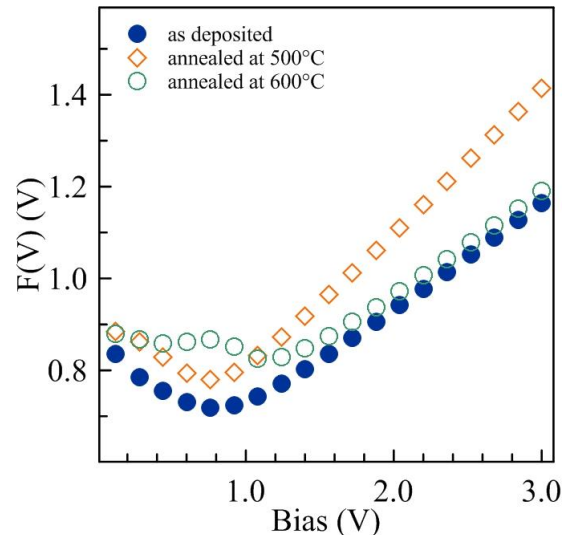Table 1. As can be seen from Table 1, the obtained *Rs* values of the diodes are nearly constant up to 500°C.

Fig. 4. The plot of *F(V)* versus *V* for the as-deposited and annealed (Ni/Au)/Al$_{0.09}$Ga$_{0.91}$N SBDs.

Another way to determine diode parameters is to use Cheung's functions [19]. In this method, the slope and y-axis intercept of a plot of *dV/d(lnI)* vs. *I* give *Rs* and *nq/kT* and a plot of *H(I)* vs. I gives also a straight line with the y-axis intercept equal to *nΦ$_b$* (Fig. 5b) The slope of this plots also provides a second determination of *Rs*, which can be used to check the consistency of Cheung's approach [19]. The values of obtained *Rs*, *n* and *Φ$_b$* of the SBDs are given in Table 1.
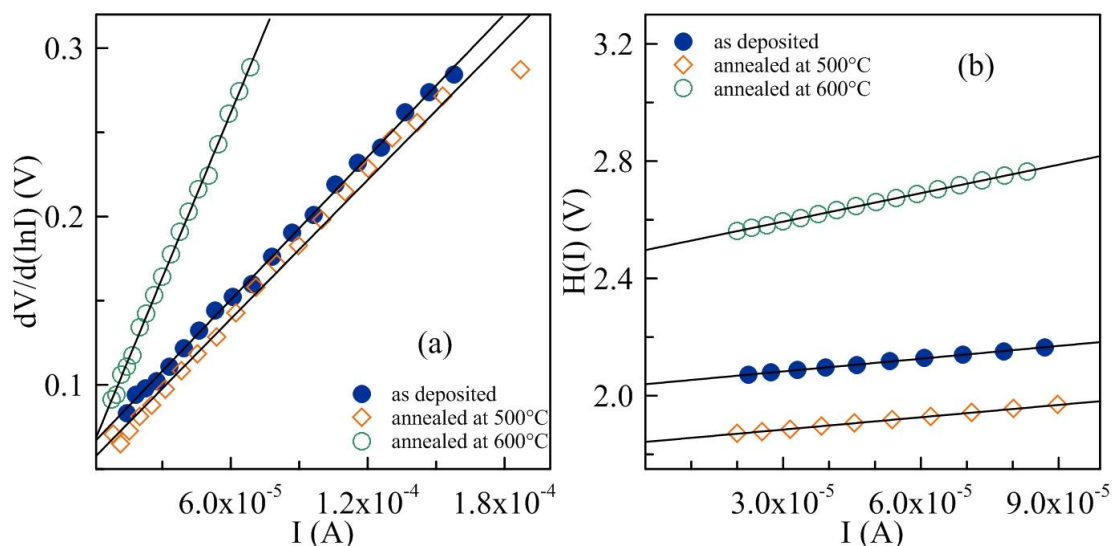

Fig. 5. The experimental *dV/d(ln I)* versus *I* (a) and *H(I)* versus *I* plots (b) for one of the as-deposited and annealed (Ni/Au)/Al$_{0.09}$Ga$_{0.91}$N SBD.

Table 1. The obtained characteristics diode parameters of the (Ni/Au)/$Al_{0.09}Ga_{0.91}N$ SBDs before and after thermal annealing.

AT (°C)	n	Φ_{b0} (eV)	I_0 (A)	Cheung				Norde	
				n	Rs (kΩ)	Φ_{b0} (eV)	Rs (kΩ)	Φ_{b0} (eV)	Rs (kΩ)
-	2.351	0.833	1.39×10^{-10}	2.472	1.445	0.825	1.442	0.892	1.558
100	2.484	0.799	5.07×10^{-10}	2.335	1.142	0.819	1.138	0.865	1.102
200	2.628	0.799	5.23×10^{-10}	2.294	1.207	0.836	1.2018	0.877	1.095
300	2.540	0.802	4.51×10^{-10}	3.391	1.289	0.747	1.286	0.900	1.290
400	2.004	0.873	2.94×10^{-11}	3.459	1.877	0.778	1.868	0.970	1.781
500	1.655	0.948	1.64×10^{-12}	2.114	1.416	0.871	1.422	1.014	1.371
600	2.254	1.029	7.16×10^{-14}	2.589	3.214	0.964	3.228	1.088	3.166

Kim et al. [20] have investigated the Schottky behavior of Ni/AlGaN/GaN (x=0.29) Schottky diodes under time dependent and fixed annealing temperature conditions by I-V measurements. They have reported that the barrier height change from 0.74°eV (as-deposited) to 0.82°eV under 170°min annealing at 400°C in N_2 ambient. They have explained the variation of barrier height upon annealing by the post annealing reduced the density of the electrically active states at the Schottky metal/AlGaN surface, leading to decrease of reverse leakage current, n, and saturation current and increase of SBH.

Akkaya et al. [21] have reported that the value of SBH of the as-deposited Ni/Au Schottky contact on n-GaN substrate was 0.560°eV (obtained from I-V) and 0.622°eV (obtained from C-V) and SBH increases with increase in the annealing temperature. After the annealing at 700°C, the value of the SBH of Ni/Au Schottky contact was found to be 0.911°eV (I-V) and 1.765°eV (C-V). In this study, increment in barrier height by as much as % 62.5 was successfully recorded by thermal annealing at 700°C. Furthermore, the variation of Schottky barrier heights and ideality factors with annealing temperature was attributed to the interfacial reactions of Ni/Au with GaN layer.

3.2. I-V-T Measurement results
The semi-logarithmic forward I-V characteristics of the as-deposited and annealed at 600°C (Ni/Au)/$Al_{0.09}Ga_{0.91}N$ SBDs in the temperature range of 95–305°K by the step of 10°K are shown in Fig. 6. The experimental values of the apparent SBH and the ideality factor were determined from intercepts and slopes of the linear regions of the forward-bias *lnI* versus *V* plots according to the TET at each temperature, respectively. Least square fittings and other calculations are performed via computer program SeCLaS [22, 23]. The values of the SBH and the ideality factor of the as-deposited Ni/$Al_{0.09}Ga_{0.91}N$ SBD varied from 0.268 eV and 7.727 at 95 K to 1.873°eV and 0.913 at 315°K, respectively. The values of the SBH and the ideality factor of the annealed at 600°C (Ni/Au)/$Al_{0.09}Ga_{0.91}N$ SBD varied from 0.256°eV and 5.386 at 95 K to 0.772°eV and 2.000 at 315°K, respectively.

Fig. 7 shows the variation of the SBH and the ideality factor as a function of temperature for as-deposited and annealed SBD. As can be seen from Fig. 7, the values of ideality factor decrease while the values of SBH increase with increasing temperature. Such a temperature dependent behavior of the SBH and the ideality factor is commonly observed in real SBD and attributed to the lateral inhomogeneity of the SBH at the MS interface [24-26]. Similar trends have been reported for diodes on AlGaN [17, 21, 23, 27-31] as well as any other semiconductors [24, 32, 33].
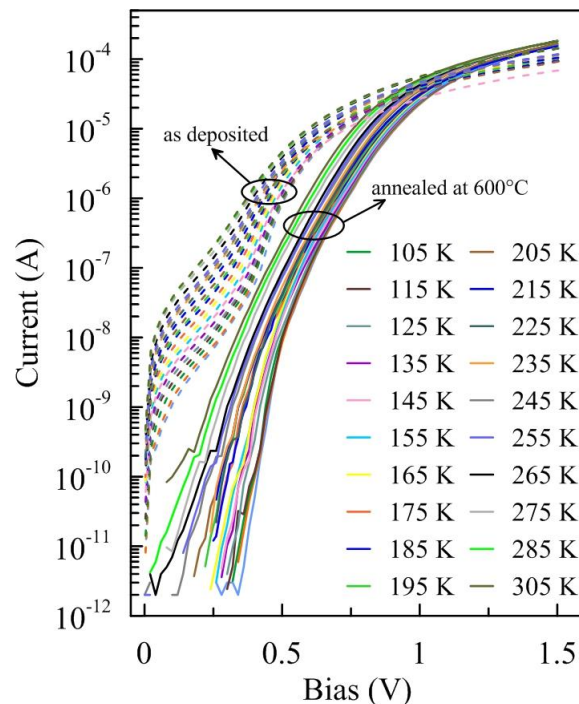
Fig. 6. The semi-logarithmic forward bias I-V characteristics for the as-deposited and annealed (Ni/Au)/Al$_{0.09}$Ga$_{0.91}$N SBDs in the temperature range of 105–305°K.
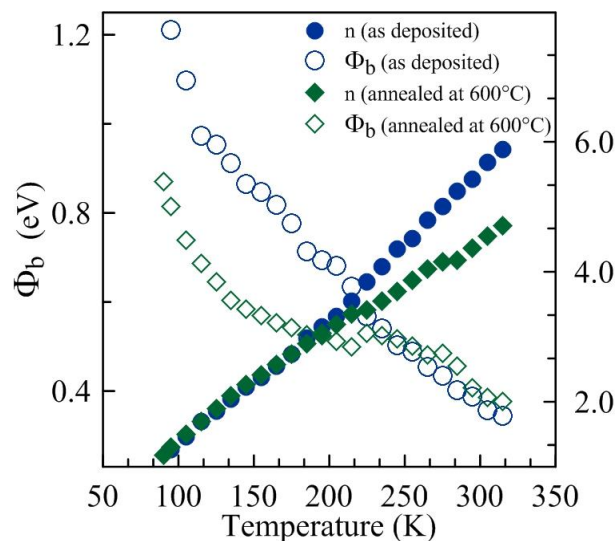

Fig. 7. The SBH and the ideality factor of the as-deposited and annealed (Ni/Au)/Al$_{0.09}$Ga$_{0.91}$N SBDs as a function of temperature.

As explained in [34, 35], since the current transport across the metal-semiconductor (MS) interface is a temperature-activated process, electrons at low temperatures are able to surmount the lower barriers. Therefore, the current transport will be dominated by the current flowing through the patches of lower SBH, leading to a larger ideality factor. As the temperature increases, more and more electrons have sufficient energy to surmount the higher barriers. As a result, both SBH and n are strongly dependent on temperature. The nature and origin of these anomalies in some studies have been explained on the basis of the TET which takes into account the lateral barrier distribution of the SBHs due to inhomogeneities prevailing at the MS interface [23].

3.3. Triple Gaussian distribution of barrier heights

There are two main method used to explain the Schottky barrier inhomogeneity. One of is Tung's pinch-off model [25, 36] and other approach is the parallel conduction model based on different patches having different barrier height which do not affect each other. According to the latter model, the total current through the diode is the sum of the currents flowing all of these patches in the present of the whole contact area and at thermodynamic equilibrium (V=0), the temperature dependence barrier height and variation of the ideality factor with temperature can be described by the following equations [37]

$$\Phi_b = \overline{\Phi_b} - {q\sigma_{s0}^2}/{2kT} \tag{3}$$

$$1/n - 1 = -\rho_2 + {a\rho_3}/{2kT}. \tag{4}$$

σ_{s0}, ρ_2 and ρ_3 can be found by using a changing in the Φ_b and $1/n$-1 with $1/2kT$, respectively (Fig. 8 and Table 2). In our case, these graphics indicates SBH can be modeled with three set Gaussian distributions.
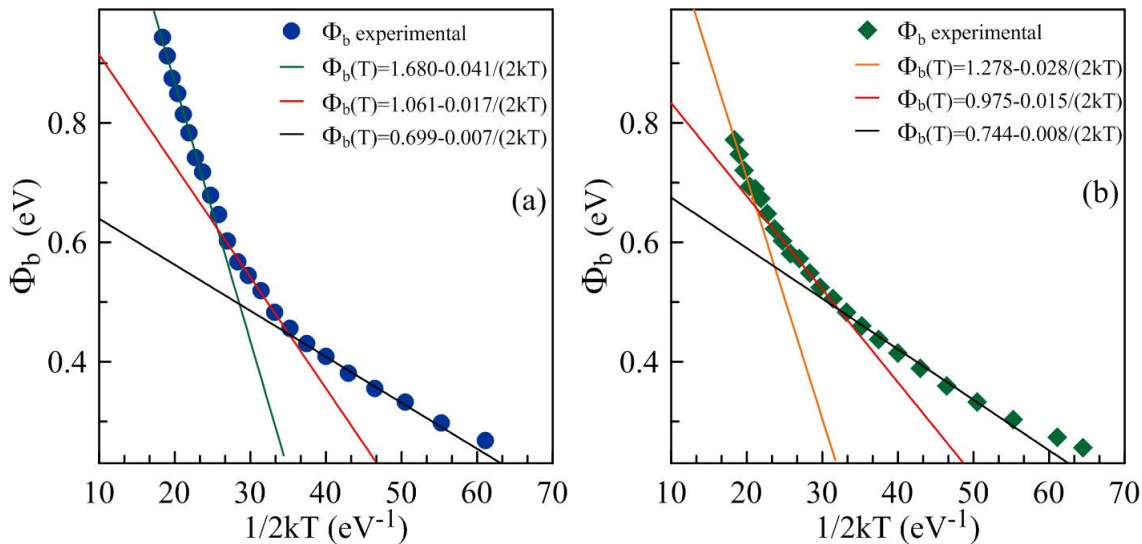

Fig. 8. The Φ_b values of the as-deposited (a) and annealed (b) (Ni/Au)/Al$_{0.09}$Ga$_{0.91}$N SBD as a function of $1/2kT$.

Table 2. Three set Gaussian distribution parameters of the as-deposited and annealed (Ni/Au)/Al$_{0.09}$Ga$_{0.91}$N SBDs.

	Φ_b^1 (eV)	Φ_b^2 (eV)	Φ_b^3 (eV)
As deposited			
	1.680	1.061	0.699
σ_{si}	0.202	0.132	0.086
Annealed at 600°C			
	Φ_b^1 (eV)	Φ_b^2 (eV)	Φ_b^3 (eV)
	1.278	0.975	0.744
σ_{si}	0.168	0.123	0.090

Richardson plots (*ln(I₀/T²) vs. 1000/T*) have bowing of the curve. That is impossible to linear fit our data in the whole temperature range. However, for T>210 K, the experimental data lie on a straight line. The value of *A** obtained from the intercept of the straight portion at the ordinate is equal to 1.859 Acm^{-2}K^{-2} for as-deposited SBD and 1.951 Acm^{-2}K^{-2} for annealed SBD, which is much smaller than the theoretical value of 29.3 Acm^{-2}K^{-2} for electrons in undoped Al$_{0.09}$Ga$_{0.91}$N.

As above mentioned, the conventional Richardson plots have showed nonlinearity at low temperatures. To explain these discrepancies in Richardson plot can be rewritten as [38]

$$ ln\left(I_0/T^2\right) - \left(q^2\sigma_{s0}^2/2k^2T^2\right) = ln(AA^*) - \left(q\overline{\Phi_b}/2kT\right). \tag{5}$$

Using the experimentally obtained I_0 data, the $ln(I_0/T^2)-q^2\sigma_{s0}^2/2k^2T^2$ values were calculated for both three values of σ_{s0} associated with the Gaussian distributions of SBHs. The best linear fitting to these modified experimental data are exhibited by the solid curves in Fig. 9 which represent the true activation energy plots in the respective temperature regimes. The obtained Richardson constant values are very close to the theoretical value for n-type Al$_{0.09}$Ga$_{0.91}$N.
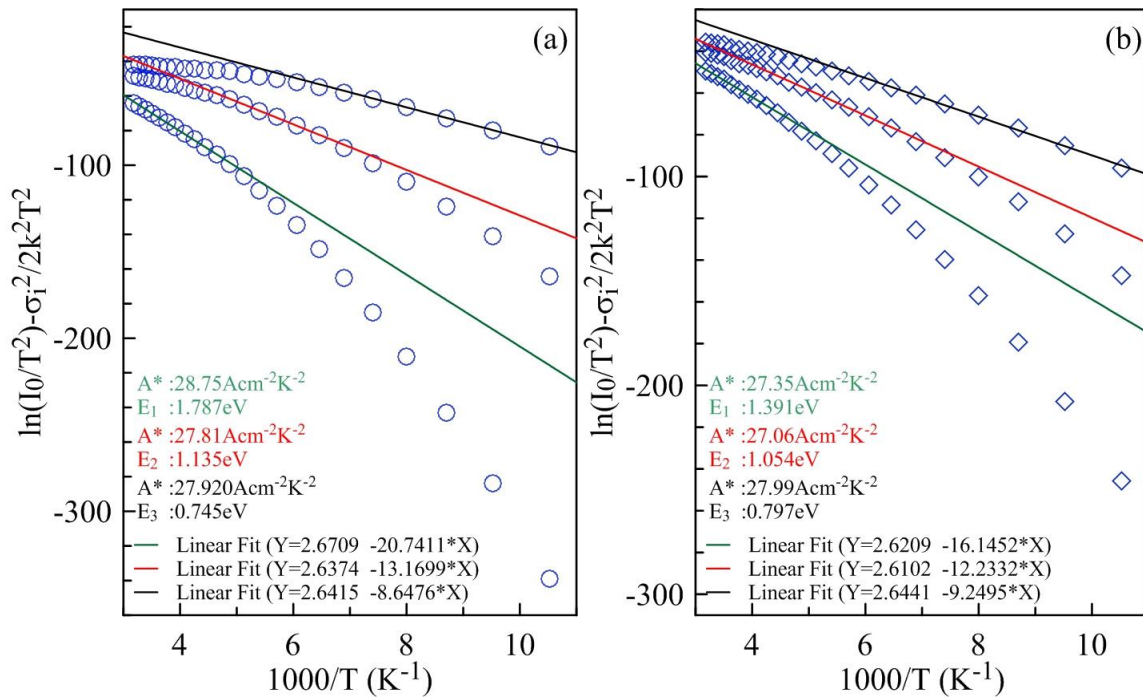

Fig. 9. The modified Richardson plot for the as-deposited (a) and annealed (b) (Ni/Au)/Al$_{0.09}$Ga$_{0.91}$N SBDs according to the three set Gaussian distribution of SBHs. The solid lines show the best fitting of the data in the corresponding temperature regime.

3.4. XPS measurements results

The XPS depth profile was employed in order to investigate the interfacial reaction between Ni/Au metal layers and AlGaN. Fig. 10 shows the XPS depth profiles of (Ni/Au)/Al$_{0.09}$Ga$_{0.91}$N SBD as-deposited and after annealing at 600°C. The as-deposited layer reveals a relatively sharp interface, which indicates that there is no significant inter-diffusion between the metal layers and AlGaN. The depth profile of the contact annealed at 600°C is shown in Fig. 10b. It should be noted that some amount of Ga out-diffused into the metal layers. This is indicative of possible reaction between the Ni/Au layers and the AlGaN, resulting in the formation of gallide phases (GaNi) at the interface.

When the XPS spectra evaluated one by one for Al, Ga, N, Au and Ni peak shifting point out a intermetallic compounds (such as gallide phases and NiAu alloys) exist in interface even the contact was not anneal. Furthermore these findings indicate a few clues about interface. One of its Au was

spread to almost all contact and small shift in binding energy could be caused from reaction between the Au and excess Ga and Ni. Shift in binding energy of Ni was verified by this situation. Secondly, when the diode annealed, significantly amount of Ga out diffused from substrate to the contact [21].
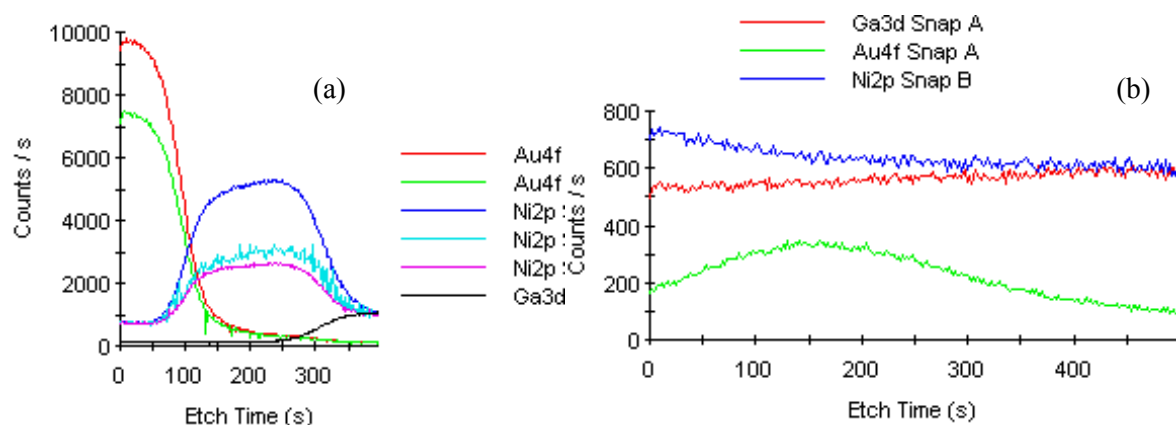

Fig. 10. XPS depth profiles of (Ni/Au)/$Al_{0.09}Ga_{0.91}N$ SBD (a) as-deposited sample and (b) 600°C annealed sample.

4. Conclusion

The effect of thermal annealing on electrical and structural properties of the (Ni/Au)/$Al_{0.09}Ga_{0.91}N$ SBD were investigated using I-V and XPS measurements. The value of SBH of the as-deposited (Ni/Au)/$Al_{0.09}Ga_{0.91}N$ SBD was found to be 0.833°eV. Furthermore, it is shown that the value of SBH increases with increase in the annealing temperature. After the annealing at 600°C, the value of the SBH was found to be 1.029°eV. The obtained results are shown that the optimum annealing temperature for the Ni/Au Schottky contact is 500-600°C. In other word, the partial stability observed up to the 400°C annealing temperature. Gaussian distribution parameters of as-deposited and annealed (Ni/Au)/$Al_{0.09}Ga_{0.91}N$ SBD indicates that annealed SBD become a more homogeneous. It was concluded that the Ni/Au Schottky contact is a suitable choice for the fabrication of AlGaN based high power device applications. Also, the analysis of XPS depth profile revealed that the formation of the gallide and intermetallic phases exist at metal/GaN/AlGaN interface. The variation of SBH and ideality factors with annealing temperatures may be attributed to the interfacial reactions of Ni/Au with GaN/AlGaN layer.

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