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Effect of thermal annealing on electrical and structural properties of *Ni/Au/n-GaN* Schottky contacts

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A B S T R A C T

The effects of thermal annealing on the electrical and structural properties of *Ni/Au* Schottky contacts to *n*-type *GaN* were investigated by current–voltage (*I–V*) and capacitance–voltage (*C–V*) characteristics, atomic force microscopy (*AFM*), and X-ray photoelectron spectroscopy (*XPS*) depth profile analysis. The metallization patterns on *GaN* grown by metal organic chemical vapor deposition (*MOCVD*) on a (0 0 0 1) sapphire substrate were formed using the photolithography and lift-off techniques. The Schottky barrier height (*SBH*) for these contacts was obtained from *I–V* and *C–V* measurements. The value of *SBH* of the as-deposited contacts was found to be 0.560 ± 0.004 eV (from *I–V*) and 0.622 ± 0.018 eV (from *C–V*) with an ideality factor of 1.856 ± 0.085. The values of *SBH* obtained from the *C–V* measurements were found to be higher than that of obtained from the *I–V* measurements. This case was attributed to the presence of the lateral inhomogeneities of the barrier height. However, the values of *SBH* slightly increase after the annealing temperatures at 100, 200, 300, 400 and 500 °C. The *SBH* of the *Ni/Au* Schottky contact for the other annealing temperature of 600 °C was 0.617 ± 0.005 eV. The highest value of *SBH* for *Ni/Au* Schottky contact was obtained after annealing at 700 °C and the value was 0.910 ± 0.019 eV. The variations in the chemical composition of the contacts with the annealing process were examined by *XPS* depth profile analysis.

1. Introduction

Recently, group III-nitride semiconductors have been intensively studied for optoelectronic devices as well as high-temperature and high-power electronic devices due to their properties of wide band gap, high electron saturation velocity, large breakdown field and thermal stability [1–6]. Visible light-emitting diodes, ultraviolet (*UV*) photodetectors and high-electron-mobility transistors (*HEMTs*) have been fabricated by several researchers [5–9]. High quality ohmic and Schottky contacts are demanded in all of these devices. One of the key questions for both types of contacts is the poor reproducibility of the results obtained in different laboratories for similar metallization [10–12]. Another fundamental problem for Schottky contacts is the occurrence of high reverse leakage currents [10–12]. The barrier height of metal contacts to group III-nitride semiconductors strongly depends on the difference between the work function of the metal and the electron affinity of the semiconductor for *GaN* and other highly ionic semiconductors. Titanium-based metallization schemes have been used

to form ohmic contacts to *GaN* [12–14]. During annealing solid phase reactions between *Ti* and *GaN* have been reported. Nitrogen out-diffusing from the *GaN* lattice to form *TiN* and residual nitrogen vacancies act as donors in *GaN* [13]. The interfacial area thus becomes heavily doped providing the configuration needed for tunneling contacts [13].

Schottky barrier heights (*SBHs*) of a variety of elemental metals including *Au* [11], *Pt* [15], *Pd* [16], *Ni* [3] have been investigated. Published reports indicated that a barrier height was in between 0.53 and 1.05 eV which is dependent on the types of metals used. Wang et al. [15] investigated the thermal annealing effects on Schottky barrier height of the *Pt/n-GaN* Schottky contacts. They reported that the as-deposited *Pt/n-GaN* Schottky contact has a *SBH* and ideality factor of 0.82 eV and 1.40 respectively. The *SBH* of *Pt/n-GaN* Schottky contact was slightly increased after annealing at 500 °C and then degreased greatly after annealing above 600 °C. The temperature dependence change of the *SBHs* was attributed to changes of surface morphology of *Pt* films on the surface and variation of nonstoichiometric defects at the interface vicinity. Further improvements should be made in the Schottky contact to extract *GaN* robust material stability and to realize the long term integrity of *GaN* related devices. Therefore, various rare metals, alloys and

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multilayer systems have also been investigated and thermal annealing of the diodes in particular has been reported to be quite effective in some cases [17–22]. Dobos et al. [19] investigated the structural and electrical properties of *Au* and *Ti/Au* contacts on *n-GaN* and showed that the contacts were rectifying up to 700 °C, and the highest barrier height of 1.07 eV was obtained for *Au* single layer. Nickel also has a relatively large work function of 5.15 eV [23]. *Ni* is chemically more active than *Pt*, which can provide better adhesion on *GaN* [18]. The Schottky barrier height of *Ni/Au/n-GaN* contacts has been obtained with the values in between 0.58 and 1.07 eV by several research groups [20–22]. The obtained variation in the barrier height is mainly attributed to differences of material characteristics and measurement methods used [16–20].

However, the realization of these devices not only depends on the quality of the material properties, but also relies seriously on the performance of metal contacts. Fabrication of electrical contacts to these devices requires the deposition of metals on semiconductors with subsequent annealing. Interfacial reactions between metals and *GaN* are important since the electrical properties of such contacts are influenced by the phases formed directly on the *GaN* surface because of process annealing or high-temperature service. High quality, thermally stable contacts to *GaN*-based semiconductors are required for the fabrication of reliable and high-performance devices. The structure of metal/semiconductors interfaces is of vital importance to all microelectronic and optoelectronics devices.

In this work, we have investigated the thermal annealing effects on the electrical and structural properties of the *Ni/Au* contacts on *n-GaN*. Annealing treatment was performed at a temperature ranging from 100 to 800 °C in increments of 100 °C for 2 min in argon ambient. The thermal stability of the *Ni/Au* Schottky contacts was evaluated by considering the change of the *SBH* with the annealing temperature. The variations in the chemical composition of the contacts with the annealing temperature were examined by *XPS* depth profile analysis.

2. Experimental procedure

In this study, unintentionally doped (uid) *n*-type *GaN* epitaxial layers grown by metalorganic chemical vapor deposition (*MOCVD*) on a sapphire (0 0 0 1) substrate were used. The structure of the samples consists of a 2.5 μm thick *n*-type *GaN* layer on top of a 3.5 μm thick nucleation *GaN* layer on a sapphire substrate.

The *GaN* samples were cleaned consecutively acetone, methanol, trichloroethylene, deionised water (18 MΩ) 5 min. using ultrasonic agitation in each step. The samples were then dried with high-purity nitrogen. After cleaning organic residuals, the substrates were dipped in aqua regia to remove the native oxide from the front surface of the substrate and boiling *KOH* solution (0.5 M) to reduce the surface roughness, respectively. Stripe of a bilayer of *Ti/Al* (25 nm/105 nm) was deposited using magnetron dc sputtering for *Ti* and thermal evaporation for *Al* on *n-GaN* as ohmic contact. The contact was annealed at 850 °C for 1 min in flowing high purity (5 N) argon gas in a quartz tube furnace. The *Ni/Au* (30 nm/50 nm) metallization was then deposited using magnetron dc sputtering for *Ni* and thermal evaporation for *Au*. Conventional photolithography lift-off technique was used to deposit metalized dots with a diameter of 0.5 mm for Schottky contacts. All contact metals were deposited in the same environment without breaking the vacuum using a high vacuum metallization system (NANOVAK-NVTS400) and back pressure better than 1×10^{-6} mTorr and 20 mTorr during the thermal evaporation and sputtering process respectively. AZ 400K Developer, AZ 5214 E image reversal photoresist and optical mask with UV lamp were used in conventional photolithography technique. Following the metallization, metals lift-off was performed in acetone.

In order to study the thermal annealing effects of *Ni/Au* Schottky contacts on *n-GaN*, samples were annealed in a quartz tube furnace for 2 min. in flowing argon (5N) ambient from 100 to 800 °C with step of 100 °C. Prior to the all annealing process, tube furnace carefully swept with high argon flow to prevent undesired oxidation of metals at high temperatures and residual humidity effects (if exist).

The current–voltage (*I–V*) and capacitance–voltage (*C–V*) measurements of the *Ni/Au/n-GaN* Schottky contacts were accomplished by employing a computer-controlled *HP 4140B* picoamperemeter and *Agilent E4980A* Impedance Analyzer, respectively. The surface morphology of the annealed Schottky contacts was investigated using atomic force microscopy (*AFM*). The variations in the chemical composition of the contacts with the annealing process were examined by *XPS* depth profile analysis. Prior to *XPS* measurements the *GaN* substrates were ex situ degreased in isopropanol, next washed in distilled water and dried in air, then were mounted with copper strips on molybdenum plates. The *XPS* spectra for the as-deposited and annealed *SBDs* were recorded using a Thermo Scientific system equipped with a monochromatic *Al* K_α source and 180° double focusing hemispherical analyzer. X-ray spot size was 250 μm, take-off angle 60° and back pressure better than 8×10^{-8} mTorr. *XPS* depth profiles recorded by alternating sputtering with argon ion-sputter (2 keV energy). The ion beam was raster over an area of 1×1 mm^2. Due to the insulating nature of substrate, a defocused low energy electron gun was used to stabilize the surface potential. *XPS* peak refinement and peak defining were performed with Avantage Data System.

3. Results and discussion

3.1. Electrical properties of Ni/Au Schottky contacts on n-GaN

Fig. 1 shows the forward and reverse *I–V* characteristics of the as-deposited and annealed *Ni/Au/n-GaN* Schottky diodes. For the as-deposited *Ni/Au* Schottky contact, the leakage current at −1.0 V is 7.82×10^{-5} A. For the diode annealed at temperature 400 °C, 500 °C and 600 °C, the leakage currents are 3.11×10^{-5}, 1.50×10^{-5} and 1.71×10^{-6} A at −1.0 V, respectively. It can be seen from Fig. 1 that the thermal annealing effect was small under the annealing temperature of 500 °C. However, the annealing effect on the leakage current reduction was revealed to be more significant at the annealing temperature of 700 °C. The reverse leakage current was drastically reduced to the order of 10^{-7} A. Therefore, the annealing temperature of 700 °C is crucial for the studied *Ni/Au* Schottky contacts.

The experimental *I–V* curves were analyzed using the thermionic emission theory (*TET*). According to the *TET*, the current
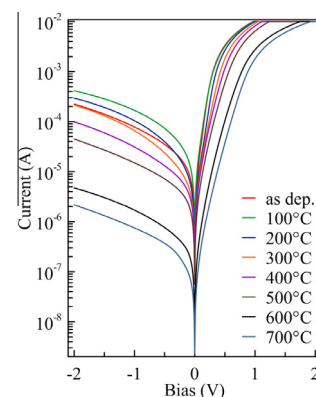

Fig. 1. The current–voltage characteristics of the as-deposited and annealed (*Ni/Au*)/*n-GaN* Schottky diodes.

flowing through the metal–semiconductor contact under forward bias V is given by (for $V > 3kT/q$) [23,24]

$$I = I_0 \exp\left[\frac{qv}{nkT}\right] \qquad (1)$$

where I_0 the saturation current is defined by

$$I_0 = AA^*T^2 \exp\left[-\frac{q\Phi_{bo}}{kT}\right]. \qquad (2)$$

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 26.4 A K^{-2} cm^{-2} for n-type GaN [4], the electron charge, the Boltzmann constant, and the apparent barrier height at zero bias determined from the $I–V$ data, respectively. In Eq. (1), the ideality factor n is a dimensionless parameter introduced to account for the departures from the TET and is given by

$$n = \frac{q}{kT}\left(\frac{dv}{d\ln I}\right). \qquad (3)$$

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. (2) and (3), 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 barrier height of the Ni/Au Schottky contacts as a function of annealing temperature is shown in Fig. 2. Table 1 shows that the Schottky barrier height determined of the as-deposited Ni/Au Schottky contact was 0.560 ± 0.004 eV which agrees well with the 0.58 eV reported in the literature [22]. 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 GaN [1–6,13,25]. The barrier heights of the Ni/Au Schottky contact for the other annealing temperatures of 200, 300, 400, 500 and 600 °C were 0.574 ± 0.006, 0.561 ± 0.005, 0.559 ± 0.003, 0.563 ± 0.006, and 0.617 ± 0.005 eV, respectively. The highest SBH was obtained for Ni/Au Schottky contact is to be 0.910 ± 0.019 eV after annealing at 700 °C. Moreover, the rectification feature of the diode after annealing at 800 °C was deteriorated (not shown here). It can be seen in Table 1 that the values of ideality factor determined from the slope of linear region of semilog forward bias $I–V$ plots were found to be 1.856 ± 0.085 for as-deposited, 2.086 ± 0.0068 for annealed at 100 °C, 2.125 ± 0.128 for annealed at 200 °C, 2.880 ± 0.175 for annealed at 300 °C, 3.379 ± 0.070 for annealed at 400 °C, 3.728 ± 0.076 for annealed at 500 °C, 3.578 ± 0.046 for annealed at 600 °C and 1.523 ± 0.095 for annealed at 700 °C. The results 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
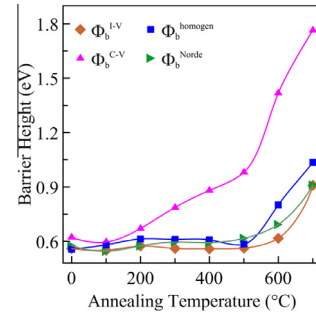

Fig. 2. The variation of the barrier height as a function of annealing temperature for the (Ni/Au)/n-GaN Schottky diodes.

[26–28]. These effects invariably increase the ideality factor. Moreover, even if the semiconductor surface was devoid of an oxide layer, a native oxide layer would form by exposure to air in the time taken to transfer the semiconductor to a vacuum chamber, as would be the case if it was prepared by cleaving a crystal so as to expose a fresh surface [26]. The formation of such a thin interfacial layer is inevitable during the fabrication of the device. The above observations reveal that before the value of the ideality factor increases by annealing temperature up to 600 °C and then decreases at the above annealing temperatures of 600 °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 [28–30]. 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 GaN.

The $SBHs$ of the $Ni/Au/n$-GaN Schottky diodes are also determined using the Norde method [31]. In this method, the Norde function is expressed by

$$F(V) = \frac{V}{2} - \frac{kT}{q} \ln\left[\frac{I(V)}{AA^*T^2}\right] \qquad (4)$$

where $I(V)$ is current obtained from the $I–V$ curve. The plots of $F(V)$ versus V for the $Ni/Au/n$-GaN Schottky diode using data in Fig. 1 at the different annealing temperatures is shown in Fig. 3. From the plot of $F(V)$ versus V, the values of the SBH of the diode can be obtained

$$\Phi_b = F(V_{min}) + \frac{V_{min}}{2} - \frac{kT}{q}, \qquad (5)$$

where $F(V_{min})$ is the minimum value of $F(V)$ and V_{min} is the corresponding voltage. Fig. 3 shows a plot of $F(V)$ versus V for the $Ni/Au/n$-GaN Schottky diode. The obtained $SBHs$ are 0.576 ± 0.007 eV for as-deposited, 0.545 ± 0.005 eV, 0.575 ± 0.011 eV, 0.596 ± 0.013 eV, 0.593 ± 0.005 eV, 0.616 ± 0.010 eV, 0.693 ± 0.005 eV and

Table 1
The obtained characteristics diode parameters of the (Ni/Au)/n-GaN Schottky diodes, before and after thermal annealing. Each value represents the average of ten diodes.

Annealing temperature (°C)	$I–V$						$C–V$	
	n	I_0 (A)	Φ_b (eV)	Φ_b^{Norde} (eV)	Φ_b^{Homo} (eV)	R_s (Ω)	Φ_b (eV)	N_d ($\times 10^{16}$ cm^{-3})
As-dep.	1.856 ± 0.085	7.82×10^{-5}	0.560 ± 0.004	0.576 ± 0.007	0.593	39.3 ± 5.4	0.622 ± 0.018	3.218 ± 0.249
100	2.086 ± 0.068	1.68×10^{-4}	0.551 ± 0.005	0.545 ± 0.005	0.593	46.5 ± 5.4	0.596 ± 0.012	3.196 ± 0.237
200	2.125 ± 0.128	1.04×10^{-4}	0.574 ± 0.006	0.575 ± 0.011	0.622	45.1 ± 8.4	0.671 ± 0.009	3.202 ± 0.220
300	2.880 ± 0.175	6.59×10^{-5}	0.561 ± 0.005	0.596 ± 0.013	0.628	30.8 ± 5.1	0.787 ± 0.015	3.143 ± 0.147
400	3.379 ± 0.070	3.11×10^{-5}	0.559 ± 0.003	0.593 ± 0.005	0.638	29.2 ± 5.2	0.881 ± 0.007	2.997 ± 0.131
500	3.728 ± 0.076	1.50×10^{-5}	0.563 ± 0.006	0.616 ± 0.010	0.656	28.9 ± 3.9	0.981 ± 0.026	2.846 ± 0.090
600	3.578 ± 0.046	1.71×10^{-6}	0.617 ± 0.005	0.693 ± 0.005	0.701	40.6 ± 12.5	1.418 ± 0.065	2.831 ± 0.077
700	1.523 ± 0.095	7.49×10^{-7}	0.910 ± 0.019	0.911 ± 0.010	1.007	88.2 ± 8.5	1.765 ± 0.055	2.811 ± 0.075
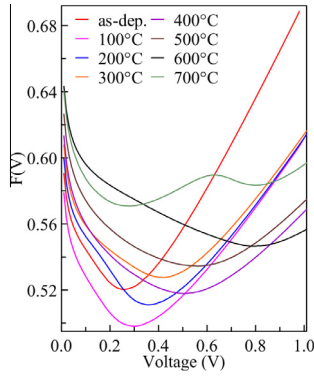
Fig. 3. The plot of F(V) versus V for the as-deposited and annealed (Ni/Au)/n-GaN Schottky diodes.

0.911 ± 0.010 eV for the samples annealed at 100 °C, 200 °C, 300 °C, 400 °C, 500 °C, 600 °C and 700 °C, respectively. The variation of barrier height obtained from Norde method of the Ni/Au Schottky contacts as a function of annealing temperature is shown in Fig. 2. As can be seen from Table 1 and Fig. 2, the determined SBH values are in agreement with those obtained by the I–V method. In this method, series resistance is given by

$$R_s = \frac{kT(\gamma - n)}{qI_{min}} \qquad (6)$$

where γ is a dimensionless integer larger than ideality factor ($\gamma > n$, I_{min} is the corresponding current at the lowest voltage. The values of obtained series resistance (R_s) of the Ni/Au/n-GaN Schottky diode are also given in Table 1. As can be seen from Table 1, the values of the obtained R_s of the Ni/Au/n-GaN Schottky diode are in the range of 30.312–88.223 Ω. It was found that the series resistance of the diode increased with an increase in the annealing temperature.

The reverse bias capacitance–voltage (C–V) characteristics of the as-deposited and annealed Ni/Au/n-GaN Schottky diodes were measured at room temperature. Fig. 4 shows a plot of $1/C^2$ as a function of bias voltage for the Ni/Au Schottky contacts at a frequency 1 MHz. The primary objective of the C–V measurements was to uncover the nature of the depletion region of the Schottky diodes. The C–V relationship for a Schottky diode is given by [24]

$$\frac{1}{C^2} = \frac{2\left(V_{bi} - \frac{kT}{q} - V\right)}{A^2 q N_d \varepsilon_s} \qquad (7)$$

where A is the Schottky contact area of the diode, N_d is the doping concentration of the GaN substrate, V_{bi} is the built-in potential, ε_s is the dielectric constant of the semiconductor (ε_s for GaN) and k, T
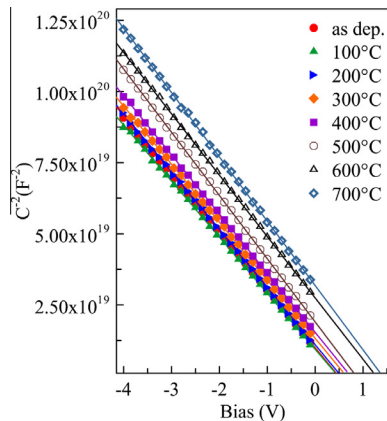
Fig. 4. The experimental reverse bias C^{-2}–V plots of the (Ni/Au)/n-GaN Schottky diodes at 1 MHz.

and q have their usual definitions. The plot of ($1/C^2$) versus V should be a straight line with a slope of $2/q\varepsilon_s N_d$ and the x-intercept of the plot, V_0 is related to the built-in potential V_{bi} by the equation $V_{bi} = V_0 + kT/q$. The barrier height Φ_b is given by equation $\Phi_b = (V_{bi} + V_n)$, where V_n is the potential difference between the Fermi level and the bottom of the conduction band in the neutral region of n-GaN and $V_n = (kT/q)\ln(N_c/N_d)$, where N_c is the effective density of states in the conduction band and is calculated from the slope of the experimental C^{-2} versus V plots. The density of states in the conduction band is given by $N_c = 2(2\pi m^* kT/h^2)^{3/2}$, where $m^* = 0.22m_0$, and its value is found to be 2.6×10^{18} cm^{-3} for GaN at room temperature [2]. The values of Φ_b (C–V) and N_d for the Ni/Au Schottky contacts on n-GaN are given in Table 1. Fig. 2 shows the variation of barrier height as a function of annealing temperature. As can be seen clearly in Table 1 that the barrier heights obtained by C–V method of the Ni/Au Schottky contact are 0.622 ± 0.018 eV for as-deposited, 0.596 ± 0.012 eV, 0.671 ± 0.009, 0.787 ± 0.015, 0.881 ± 0.007, 0.981 ± 0.026, 1.418 ± 0.065, and 1.765 ± 0.055 eV after the annealing temperatures at 100 °C, 200 °C, 300 °C, 400 °C, 500 °C, 600 °C and 700 °C, respectively. Fig. 2 and Table 1 show that the values of barrier height obtained from I–V measurements are lower than those obtained from C–V measurements. The difference in the values of Φ_b obtained by I–V and C–V measurements may be attributed to the possible existence of lateral inhomogeneity in the SBH at MS interfaces [32–37]. As reported by Werner and Güttler [34], the lateral distribution of potentials and barriers influence capacitance and dc current measurements differently. The capacitance C arises from the displacement current in which turn originates at frequency w from the time periodic change of the width of the space charge region. These widths depend on the mean electric field E at MS interface. Short-wavelength potential fluctuations at the MS interface are screened at the edge of the space charge region. Consequently, capacitances are expected to measure only the mean values of the SBH. The capacitance is insensitive to potential fluctuations on a length scale of less than the space charge width. On the other hand, the dc current across the interface depends exponentially on the SBH and thus sensitively on the detailed barrier distribution at the interface. Any lateral variation in the SBHs causes the current I to flow preferentially through the barrier minima. Therefore, the values of SBH obtained from I–V measurements are lower than those obtained from C–V measurements [34].

Other possible reason for this difference is the existence of excess capacitance at the interfacial layer due to deep level traps in the semiconductor [14,38]. The lateral inhomogeneity in the SBH formed at the MS interface are possibility caused by some effects such as inhomogeneities of thickness and composition of the layer, non-uniformity of the interfacial charges, the presence of a thin insulating layer between the metal and semiconductor [33–37]. Furthermore, there are numerous structural defects, grain boundaries, dislocations, stacking faults at the GaN layer [39], and these may also contribute to SBH inhomogeneity.

The extrapolations of the experimental SBHs versus ideality factors plot (not shown in here) to an ideality of 1.0 have given laterally homogeneous SBH of the Ni/Au/n-GaN Schottky diodes approximately 0.593 eV, 0.622 eV, 0.628 eV, 0.638 eV, 0.656 eV, 0.701 eV and 1.007 eV for the as-deposited and annealed at 200, 300, 400, 500, 600 and 700 °C, respectively. Fig. 2 shows a plot of the homogeneous SBH of the Ni/Au/n-GaN Schottky diodes as a function of the annealing temperature. According to I–V measurement, Norde function and C–V measurements, the barrier heights are enhanced with an increase in the annealing temperature, as shown in Fig. 2. The SBH of device improved upon annealing at 700 °C, as also obtained from other methods.

Sun et al. [20] investigated the Schottky behavior of Ni/Au contact on n-GaN under various annealing conditions by I–V measurements. They reported that the barrier height change from 0.689 eV

(as-deposited) to 0.860 eV under 5 min annealing at 600 °C in N_2 ambient. The variation of barrier height upon annealing has been attributed to interfacial reactions of *Ni/Au* with *GaN* and the phase transitions of *Ni/Au* during annealing. Miura et al. [21] reported that the barrier heights of *Ni/Au* Schottky contacts on c-plane *n-GaN* were 0.85 eV and 0.88 eV at the as-deposited condition and after the thermal treatment at 500 °C, respectively. A high work function metal such as *Pt, Ir, Pd* or *Mo* was inserted to the conventional *Ni/Au* Schottky contact to *n-GaN* in order to increase the *SBH* of the device. The diodes with *Ni/Pt/Au* electrodes showed the best electrical performance after annealing at 500 °C which was found to be 1.09 eV. Furthermore, they stated that all the devices deteriorated after annealed at 700 °C, which would be due to the formation of some metal–gallides and/or metal–nitrides at the interface [21]. Jung et al. [22] investigated the electrical and structural properties of *Ni/Au* metallization on a-plane *GaN*. They reported that while the Schottky barrier height of as-deposited *Ni/Au* on a-plane *GaN* was 0.58 eV, the *SBH* was increased up to 0.83 eV after an accumulative anneal up to 500 °C under an N_2 ambient. Dobos et al. [19] investigated the structural and electrical properties *Au* and *Ti/Au* contacts on *n-GaN* and showed that the contacts were rectifying up to 700 °C, and the highest barrier height of 1.07 eV was obtained for *Au* single layer. Moreover, they revealed that the barrier height of contacts decreased due to the formation of several intermetallic phases after high-temperature annealing at 900 °C. Reddy et al. [40] investigated the electrical and structural properties of *Ni/Pd* Schottky contacts on *GaN* as a function of annealing temperature. They stated that *Ni/Pd* Schottky contact exhibits excellent electrical properties after a rapid thermal annealing at 600 °C. They also reported that the formation of gallide phases at the *Ni/Pd/n-GaN* interface according to the secondary ion mass spectrometer (*SIMS*) and X-ray diffraction (*XRD*) analysis could be the reason of the *BH* increase at elevated annealing temperatures.

As generally known, chemical reactions between the metal and the semiconductor play an important role in the electrical properties of the metal/semiconductor contact. The change in the barrier height of *Ni/Au/n-GaN* Schottky contact with annealing temperature may also be ascribed to the interfacial reaction occurring between metals and *GaN*, as will be shown below. These interfacial layers may have different work functions than the *Ni/GaN* contact layers, which is responsible for the increase of barrier height.

3.2. XPS and AFM measurements

The *XPS* depth profile was employed in order to investigate the interfacial reaction between *Ni/Au* metal layers and *GaN*. Fig. 6 shows the *XPS* depth profiles of the *Ni/Au* Schottky contacts on *n-GaN* as-deposited and after annealing at 700 °C and 800 °C for 2 min under argon ambient. Fig. 5(a) shows the interface of as-deposited *Ni/Au* Schottky contacts on *n-GaN*. The as-deposited layer reveals a relatively sharp interface, which indicates that there is no significant inter-diffusion between the metal layers and *GaN*. The depth profile of the contact annealed at 700 °C is shown in Fig. 5(b). 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 *GaN*, resulting in the formation of gallide phases (*GaNi*) at the interface. For the contact annealed at 800 °C, as shown from Fig. 5(c), a considerable change in the interface is observed with an increase in an *AuNi* phase and a decrease in a *GaNi* phase.

According to the results of *XPS* depth profile, the out-diffusion of the *Ga* from the *GaN* into *Ni/Au* layers participates in the formation of gallide phases at the interface. The formation of gallide phases leads to the accumulation of gallium vacancies at the vicinity of the interface. This induces an increase in the Schottky barrier
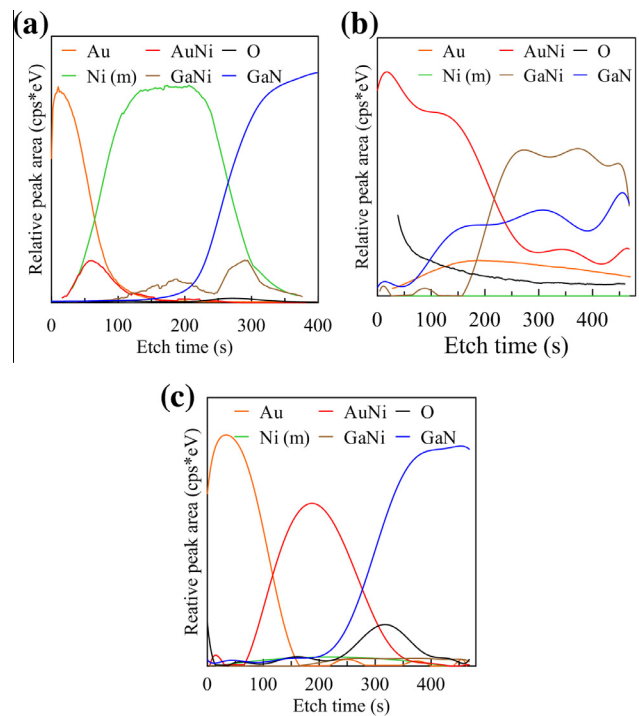

Fig. 5. *XPS* depth profiles of *Ni/Au* Schottky contact on *n-GaN* (a) as-deposited sample, (b) 700 °C annealed sample, and (c) 800 °C annealed sample.

heights of the *Ni/Au* contact which are observed from *I–V* characteristics of the *Ni/Au* contact annealed at 700 °C. The increase in the Schottky barrier heights always corresponds to a decrease of the reverse leakage current [23,24].

In addition, *Au* diffuses through the *Ni* layer and forms an *Au–Ni* alloy layer while a *GaNi* alloy layer resides at the surface. The *Au–Ni* layer underneath may prevent further diffusion of *Ni* toward the *GaN* surface. At high annealing temperature, on the other hand, formation of the *Au–Ni* alloy might prevent in-diffusion of *Ni* into the *GaN* layer to form a *GaNi* alloy. It has been reported that the *GaNi* compounds can be form when *Ni/Au* and *Ni/Pd* Schottky contacts on *n-GaN* is annealed around 600 °C [22,40].

Moreover, there is also the existence of a small amount of oxygen in the interface for all contacts, which may be introduced during the fabrication process, and it also partially originates from the *GaN* surface.

Indeed, atom diffusion is enhanced along dislocation cores so that dislocations might be considered as pipes for metal atom migration [13].

As is known, the condition of the surface of metal contacts on the semiconductor plays an important role in determining the electrical properties. Atomic force microscopy (*AFM*) was used to examine the surface morphology of the *Ni/Au* Schottky contacts on *n-GaN*. Fig. 6 shows the *AFM* images of the *Ni/Au* Schottky contacts on *n-GaN* as-deposited and after annealing at 700 °C and 800 °C. As shown in Fig. 6(a), the surface morphology of the as-deposited Schottky contact is fairly smooth with a root mean square (*RMS*) roughness of 2.9 nm. When the contact was annealed at 700 °C, the surface roughness is increased with an *RMS* roughness of 9.2 nm as compared to the as-deposited Schottky contact, as shown in Fig. 6(b). The increase of surface roughness may be because of island formation due to thermal annealing. However, it is observed that the surface morphology of the Schottky contact annealed at 800 °C is increased with a *RMS* roughness of 17.9 nm as compared to the contact annealed 700 °C (Fig. 6(c)).
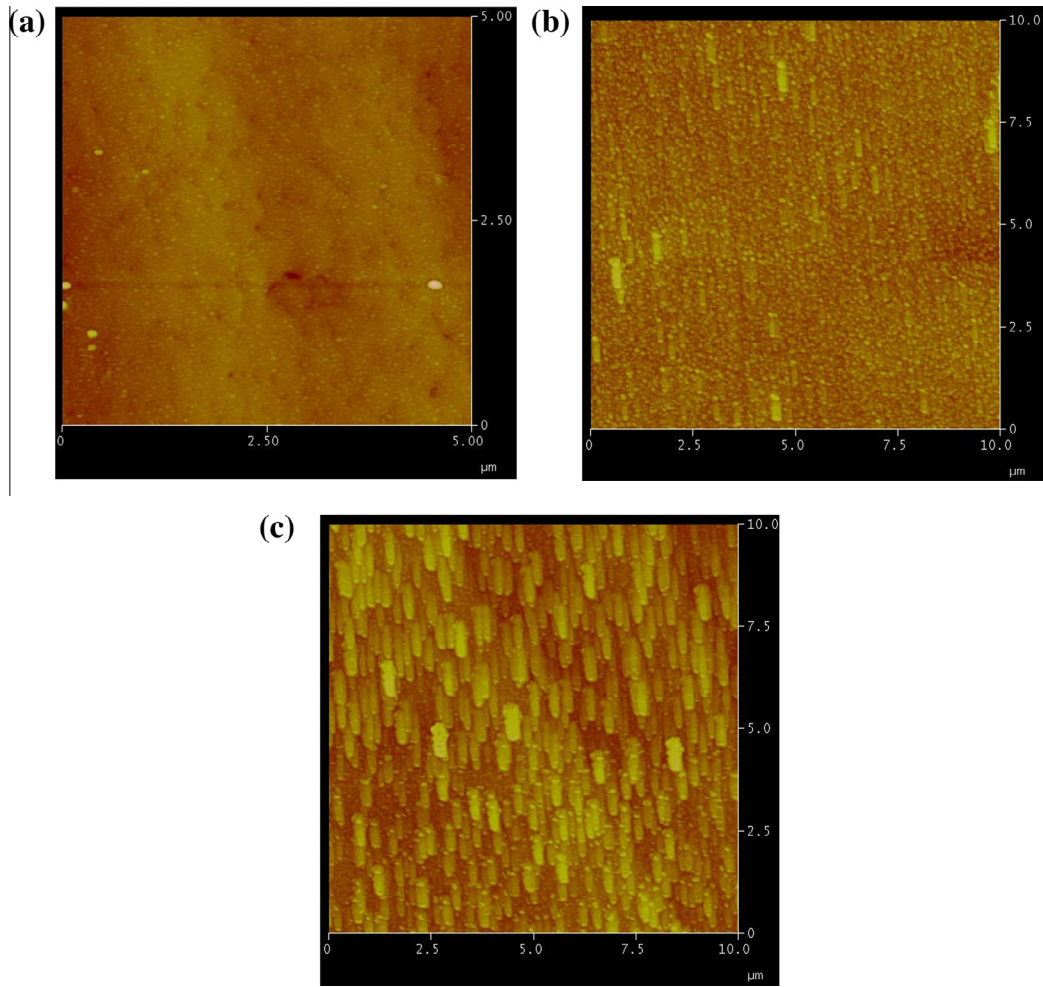
Fig. 6. *AFM* micrographs of the *Ni/Au* Schottky contacts to *n*-type *GaN*: (a) as-deposited sample, (b) 700 °C annealed sample, and (c) 800 °C annealed sample.

The phenomenon of island formation is typically observed for interfaces between thin metal films and ceramics [41]. The dewetting occurs because the ceramic has a very low surface energy whereas the metal has a fairly high surface energy. In order to minimize the total surface energy of the system, the metal agglomerates to minimize its surface area and exposes more surface area of the low surface energy ceramic. We conclude from this behavior that *GaN* has a low surface energy, as also reported in the literature [41].

4. Conclusion

The effect of thermal annealing on electrical and structural properties of the *Ni/Au/n-GaN* Schottky diodes were investigated using *I–V*, *C–V*, *XPS* and *AFM* measurements. The value of Schottky barrier height of the as-deposited *Ni/Au* Schottky contact on *n-GaN* substrate was found to be 0.560 ± 0.004 eV (obtained from *I–V*) and 0.622 ± 0.018 eV (obtained from *C–V*). The values of the *SBH* obtained from the *C–V* measurements were found to be higher than that of obtained from the *I–V* measurements. This case was attributed to the presence of the lateral inhomogeneities of the barrier height. Furthermore, it is shown that the value of Schottky barrier height 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 ± 0.010 eV (*I–V*) and 1.765 ± 0.055 eV (*C–V*). The obtained results are shown that the

optimum annealing temperature for the *Ni/Au* Schottky contact is 700 °C. The variation of Schottky barrier heights and ideality factors with annealing temperatures may be attributed to the interfacial reactions of *Ni/Au* with *GaN* layer. The analysis of *XPS* depth profile showed that the formation of the gallide phases at metal/*GaN* interface upon annealing temperature could be the reason for the increase in the barrier heights of *Ni/Au* Schottky contact. Increment in barrier height by as much as % 62.5 was successfully recorded by thermal annealing at 700 °C, Furthermore, the *AFM* measurements showed that the surface morphology of the as-deposited Schottky contact was fairly smooth with a root mean square (*RMS*) roughness of 2.9 nm. However, it was observed that the surface morphology of the Schottky contact annealed at 800 °C was increased with a *RMS* roughness of 17.9 nm. It was concluded that the *Ni/Au* Schottky contact is a suitable choice for the fabrication of *GaN*-based high power device applications.

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