Thermal annealing effect of Au- and Pt-based Schottky contacts on unintentionally and n-type doped Al_xGa_{1-x}N

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In this work, the effect of thermal annealing on electrical properties of Au- and Pt based Schottky contacts on unintentionally and n-type doped Al_xGa_{1-x}N (x = 0.24, 0.25) on Si(111) substrates grown by plasma-assisted molecular beam epitaxy (MBE) were studied and investigated. The electrical characteristics were found to be changed by the thermal treatment in each sample with different annealing temperatures. The results revealed that the Au and Pt metal Schottky contacts show the rectifying behavior at as-deposited for each sample, while the Au metal contact revealed that the Schottky barrier height at annealed temperature of 300 °C was higher than Schottky barrier height for sample annealed at 600 °C. Pt metal contact shows the high Schottky barrier heights with different annealing temperatures. A high Schottky barrier height of 0.76 eV with Pt contact was attained at 600 °C and 15 minutes of thermal annealing for n-type doped sample. Finally, the n-type doping enhanced the structural properties of AlGaN sample surface and resulted in good improvement of the electrical properties.

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1. Introduction

The Recently implementations in AlGaN Schottkybased photodetectors and AlGaN/GaN HEMTs show their great potential for optoelectronics and microelectronics [1-3]. In order to optimize the performance of these devices, it is essential to develop stable and reliable Schottky contacts. Moreover, the application of III-nitride devices at high temperatures requires a full understanding of the thermal behavior of contacts and the relevant degradation mechanisms.

Due to the ionic character of the Ga-N and Al-N bonding, no Fermi level pinning occurs at the metal-AlGaN interface. Thus, the barrier height, Φ_b , increases with the metal work function, φ_m [4, 5]. Therefore, a high quality Schottky contact to AlGaN must be found. In order to reduce the reverse-biased leakage current in Schottky diodes, the metal with high work function must be used. Metals such as Pt ($\varphi_m = 5.65 \text{ eV}$), Ni ($\varphi_m = 5.15 \text{ eV}$), Pd $(\varphi_m = 5.12 \text{ eV})$ and Au $(\varphi_m = 5.1 \text{ eV})$ are commonly used for Schottky contact processing [6]. However, these metals are tend to react with GaN after prolonged thermal treatments at 600 °C, forming stable gallides [7]. In this study, the effect of thermal annealing on electrical properties of Au- and Pt- based Schottky metals contacts on undoped and n-type doped $Al_xGa_{1-x}N$ (x = 0.24, 0.25) on Si(111) substrate grown by plasma-assisted molecular beam epitaxy (MBE) have been studied and investigated.

2. Experimental

The growth of undoped and n-type doped Al_rGa_{1-r}N/GaN/AlN heterostructures on Si (111) substrates were performed using Veeco model Gen II MBE system. Active nitrogen was supplied by a radio frequency (RF) plasma source operating at 300 W. The pressure during growth was 1.2×10^{-5} Torr. Effusion cells were used for Al, Ga and Si. Growing surfaces of epilayers were monitored by reflection high energy electron diffraction (RHEED). Following outgassing in the load lock and buffer chamber, the Si(111) substrate was transferred to the growth chamber. The substrate was then thermally cleaned at substrate temperature of 850 °C. A clean Si surface was obtained when RHEED images showed a typical Si surface with the presence of prominent Kikuchi lines. This verifies desorption of the native oxide. A few monolayers of Al were deposited using high Al flux before growing of the AlN buffer layer. This buffer layer plays an important role in determining the crystalline quality of the thin film [8]. A thin AlN buffer layer was grown for 15 minutes at 860 °C and then GaN epilayer was grown at 845 °C for 25 minutes. Subsequently, unintentionally doped and Si-doped of Al_xGa_{1-x}N epilayers were grown at 860°C for 25 and 27 minutes, respectively.

Prior to the metallization, AlGaN wafers are cleaned by the following steps; first, the removal of native oxide in 1:20 NH4OH:H2O solution for 15 second, followed by a 10 second dip in a 1:50 HF:H2O solution. The last step of the cleaning process was a 10 minutes etch in boiling aqua regia (HCI:HNO3 = 3:1). In this experiment, two wafers were used and they were divided into 12 small pieces to minimize possible variability between different metallization runs. In addition, Au and Pt metals contacts with thickness of about 300nm and targets purity of 99.99% were sputtered onto Al_xGa_{1-x}N samples through a metal mask, which consists of an array of dots with diameter of 250 µm using Edwards A500 RF sputtering unit. The first set of current-voltage (I-V) measurements were taken for all samples for the as-deposited Schottky contacts. After that, samples were than annealed under flowing nitrogen gas environment in the furnace at 300 and 600 °C for 15 minutes. The MBE grown Al_xGa₁. xN/GaN/AlN heterostructure thin films were characterized by a variety of tools. High-resolution XRD (PANalytical X'pert Pro MRD) with a Cu-K α l radiation source (λ = 1.5406Å) was used to assess and determine the crystalline quality of the epilayers and the aluminum composition of $Al_xGa_{1-x}N$. The current voltage (I-V) measurements were performed with a Kiethley High-voltage-source-measureunit model 237.

3. Results and discussion

Figs. 1(a and b) shows the XRD scans of Al_xGa_{1-x}N /GaN/AlN heterostructure for unintentionally and n-type doped samples, respectively. The XRD results confirmed that the heterostructures of III-nitrides were epitaxially grown on Si (111). This can be seen from the presence of the peaks at 34.52°, 34.88° and 36.01° for unintentionally doped sample and 34.54°, 34.90° and 36.02° for n-type doped sample. These peaks diffraction correspond to GaN(0002), AlGaN(0002) and AlN(0002), respectively. From the XRD spectra, the lattice constant c for the GaN and AlN layers as determined by using the Bragg diffraction law is about 5.190 and 4.982 Å for unintentionally doped sample and 5.189 and 4.982 Å for n-type doped sample, respectively. These values are in good agreement with the relevant literature where the lattice constant c for the bulk GaN and AlN, are respectively, 5.186 and 4.978 Å [9].

XRD rocking curve (RC) was also carried out to determine the crystalline quality of the epilayers as shown in Figure 2. From the XRD symmetric RC ω scans of (0002) AlGaN plane and applying the Vegard's law, the Al-mole fraction and FWHM of Al_xGa_{1-x}N samples are found to be 0.24 and 0.69° for unintentionally doped sample and 0.25 and 0.52° for n-type doped sample, respectively [10]. The RC results show that the Si-doping of Al_xGa_{1-x}N/GaN revealed good crystalline quality [11]. Additionally, the results for the two samples demonstrated a high Al-mole fraction with a good crystalline quality of Al_xGa_{1-x}N thin films layers. This is in disagreement with relevant literature [12-14] which reported that the growth of III nitrides on Si (111) produce relatively low crystalline quality when the Al-mole fraction increases.



Fig 1. XRD scans of $Al_xGa_{1,x}N/GaN/AlN$ grown on Si (111) substrate: (a) unintentionally doped sample and (b) n-type doped sample.

Schottky barrier height (SBH) can be determined by using I-V curves as shown in Figures 3 and 4. For thermionic emission under V>3KT, the Schottky diode barrier height can be calculated from the following equations [15]:

$$I = I_0 \exp\left[qv / (nKT)\right] \tag{1}$$

$$I_0 = A^* A T^2 \exp\left[-q\Phi_B / (KT)\right]$$
(2)

where I_o is the saturation current, *n* is the ideality factor, *K* is the Boltzmann's constant, *T* is the absolute temperature, Φ_B is the barrier height, *A* is the area of the Schottky contact, and A^* is the effective Richardson coefficient. The theoretical value of A^* can be calculated as below:

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

where *h* is Planck's constant and m^* is the effective electron mass for AlGaN. In this study, the effective mass of electron m^* for Al_xGa_{1-x}N with different *x* was estimated by linear interpolation from the theoretical value of $m^*=0.35$ m_o for AlN and $m^*=0.22$ m_o for GaN [16].

These results are in good agreement with the literature [17].

Based on Equation (1), the plot of $\ln[I \exp(qV/KT)]$ versus V which gives a straight line, I_o is derived from the intercept with y-axis. By substituting of I_o value in Equation (2), the Schottky barrier height for all the samples can be obtained. The results of the Schottky barrier heights Φ_B of the Au- and Pt-based Schottky contacts for each sample are summarized in Table 1.



Fig 2. XRD rocking curve (RC) of (0002) plane of $Al_xGa_{1-x}N/GaN/AlN$ grown on Si (111) substrate for unintentionally and n-type doped samples.

Table 1: Schottky barrier heights (SBH) for Au and Pt metal contacts on unintentionally and n-type doped samples with different annealing temperatures.

Annealing temperature (°C)	u-A b 24Ga 0,76 N Au-SBH (eV)	u-A l_{0.24}Ga_{0.76}N Pt-SBH (eV)	n-A 1_{0.25} Ga _{0.75} N Au-SBH (eV)	n-Al _{0.25} Ga _{0.75} N Pt-SBH (eV)
As-deposited	0.51	0.58	0.54	0.61
300	0.61	0.62	0.58	0.66
600	0.55	0.67	0.63	0.76

Fig. 3 (a and b) shows the I-V characteristic of Au based Schottky contact with 300 and 600 °C annealing temperatures for unintentionally and n-type doped of $Al_xGa_{1-x}N$ samples, respectively. Because of the Au metal contact has a high work function (5.1 eV), therefore, it exhibited rectifying behavior with SBH equal to 0.51 eV for as-deposited metal as shown in Figure 3(a). When the sample was annealed at 300 °C, the Au-Schottky contacts revealed good rectifying behavior with SBH equal to 0.61 eV indicating the intimate contact between metal and semiconductor. SBH become less rectifying at 600 °C as

shown in Table 1 due to degradation of electrical properties. The degradation could be ascribed to the formation of oxide layers and poor surface morphology of the contacts which reduced the amount of current flow into the thin films. From Figure 3(b) the SBHs of n-type doped samples were 0.54, 0.58 and 0.63 eV for as-deposited, 300 and 600 °C annealing temperatures, respectively. It can be seen that all curves show rectifying behavior and this rectifying improved with heat treatment indicating that the heat treatment produced strong chemical reaction and better contact, resulting in a layer of a compound at the interface [18, 19].



Voltage (V) Fig 3. The I-V characteristic of Au-Schottky contact with different annealing temperatures on (a) unintentionally doped $Al_xGa_{1-x}N$ sample and (b) n - type doped $Al_xGa_{1-x}N$ sample.

Fig. 4 (a and b) shows the I-V characteristic of Ptbased Schottky contact for the as-deposited, 300 and 600 °C annealing temperatures of the unintentionally and n-type doped $Al_xGa_{1-x}N$ samples. Also the Pt has a high work function (5.65 eV) and high thermal stability, therefore, Figure 4 (a) and (b) exhibited rectifying behavior for all samples, and also show the improvements in the electrical properties for unintentionally and n-type doped samples before and after heat treatment. The SBH of unintentionally doped samples were 0.58, 0.62 and 0.67 eV for as-deposited, 300 and 600 °C annealing temperatures, respectively, and SBH of n-type doped samples were 0.61, 0.66 and 0.76 eV for as-deposited, 300 and 600 °C annealing temperatures, respectively (Table 1).

From all these results for Au- and Pt-Schottky contacts, it can be found that the SBH for the contact on ntype doped sample was higher than the SBH for unintentionally doped sample, which indicate that the ntype doping enhanced the structural properties of AlGaN sample surface which resulted in improvement of the electrical properties [20].





Fig 4: The I-V characteristic of Pt-Schottky contact with different annealing temperatures on (a) unintentionally doped $Al_xGa_{1-x}N$ sample and (b) n-type doped $Al_xGa_{1-x}N$ sample.

3. Conclusions

Unintentionally doped and Si-doped $Al_xGa_{1-x}N$ /GaN/AlN layers on Si (111) substrates have been successfully been grown by PA-MBE. The effect of thermal annealing on electrical properties of Au- and Pt based Schottky contacts on unintentionally and n-type doped $Al_xGa_{1-x}N$ (x = 0.24, 0.25) have been studied and investigated. The Au metal contact revealed that the Schottky barrier height at temperature of 300 °C was higher than Schottky barrier height for sample annealed at 600 °C. A high Schottky barrier height at 600 °C and 15 minutes of thermal annealing for n-type doped sample. Finally, the n-type doping has enhanced the structural properties of AlGaN sample surface, resulting in the good improvement of the electrical properties.

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