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Conduction mechanism of non-gold Ta/Si/Ti/Al/Ni/Ta ohmic contact in AlGaIn/GaN high-electron-mobility transistors

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This work investigates the conduction mechanism of non-gold Ta/Si/Ti/Al/Ni/Ta ohmic contact in un-doped AlGaIn/GaN high-electron-mobility transistors (HEMTs) grown on Si. The temperature dependent I-V measurement reveals that the conduction mechanism is primarily via Thermionic Emission(TE). The extracted mean barrier height(Φ_B) values are 0.113 and 0.121 eV and the mean contact resistance(R_c) values are 0.24 and 0.28 $\Omega\cdot\text{mm}$ respectively for annealing temperature at 850 °C and 900 °C. The low R_c is attributed to the formation of low work function Ti_xSi_y at the metal-semiconductor interface. The HR-TEM and EDX analysis also provide structural evidence to support the TE mechanism.

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AlGaN/GaN High-Electron-Mobility-Transistors (HEMTs) have emerged as excellent candidate for high-power electronics and switching applications due to their intrinsic material properties such as high electron saturation velocity, high sheet carrier charge density, and large band gap, etc.¹⁻⁴ In order to achieve transistors with high drain current (I_D) and low specific on-resistance (R_{on}), ohmic contacts with low contact resistance, sharp edge acuity, smooth surface morphology and high thermal stability are necessary.⁵ Recently, GaN HEMTs fabricated on large diameter (200mm) silicon substrates with CMOS-compatible processes have received much attention as such approach will allow high-volume and low-cost GaN HEMTs and integrated circuits for the huge commercial high-power electronic market.^{6, 7} To realize CMOS-compatible process, the conventional gold-based Ti/Al/X/Au (X = Ni, Mo, Ti, etc.) ohmic stacks used in typical III-V fabrication process must be replaced by non-gold schemes as the usage of gold will contaminate CMOS fab facilities. In order to facilitate the optimization of ohmic contact, it is useful to have a good understanding of the ohmic metal formation and the conduction mechanism. For gold-based ohmic contacts, such studies have been well reported. The formation of the low contact resistance (R_c) ohmic contact is mainly due to the inter-diffusion of gold and N-atoms, which forms a low resistivity Al-Ti-N alloyed layer and results in a Thermionic-Field Emission (TFE) dominated electron transport at the Metal-Semiconductor (M-S) interface.^{8, 9} In contrast, although non-gold ohmic contacts have been published with improved R_c in recent years,^{8, 10, 11} their ohmic metal formation processes and conduct mechanisms were not well understood. Based on a non-gold ohmic contact (Ta/Si/Ti/Al/Ni/Ta) we developed previously,¹² the conduction mechanism is systematically studied in this work using the temperature dependent I-V

measurement. This work provides a better insight of the conduction mechanism of a non-gold ohmic contact on AlGaIn/GaN HEMTs.

The AlGaIn/GaN heterostructure was grown on 4-inch high-resistivity Si (111) substrate by Metal Organic Chemical Vapor Deposition (MOCVD). Fig 1 shows the schematic diagram of the cross-sectional device structure used in this study. At room temperature, the 2DEG sheet density and mobility are $1.1 \times 10^{13} \text{ cm}^{-2}$ and $1450 \text{ cm}^2/\text{V.s}$, respectively.¹² After mesa isolation by BCl_3/Cl_2 plasma, ohmic metal patterns were defined by conventional lithography. Before the deposition of Ta/Si/Ti/Al/Ni/Ta (5/5/20/120/40/30 nm) metal stacks by electron beam evaporation, the surface native oxide was removed by buffered HF etching for 60 s followed by deionized water rinsing. The samples then underwent rapid thermal annealing at 850 °C and 900 °C in N_2 ambient for 30 s separately. Two annealing temperatures were used because they yielded the lowest R_c values as reported in [Ref #12]. A gold-based reference sample [Metal scheme: Ti/Al/Ni/Au (20/120/40/50 nm), annealing: 825 °C for 30 s in N_2 ambient] was also fabricated on a similar epi-wafer for comparison purpose. For all the samples, the R_c , sheet resistance (R_{sh}) and specific contact resistivity (ρ_c) were extrapolated using the transmission line model (TLM) at the temperature range of -25 °C to 150 °C, with a step increment of 25 °C. On each non-gold sample, the I-V measurement was carried out at three different sites to verify the uniformity. To inspect the elementary distribution after annealing, high-resolution transmission electron microscopy (HR-TEM) and energy-dispersive X-ray (EDX) spectroscopy analysis were also carried out on the 850 °C-annealed non-gold sample.

Fig 2(a) shows the total resistance (R_{total}) versus the TLM gap length at different measurement temperatures for the sample annealed at 850 °C. As shown in the graph, the measured R_{total} data points can be well fitted linearly for all measurement temperatures. For the sample annealed at 900 °C, similar trend was observed for the R_{total} versus the TLM gap length plot. The R_c values were extracted from the y-intercept of the linear fits given in Fig 2(a). Fig 2(b) gives the ρ_c ($= R_c^2/R_{sh}$) values of the ohmic contact versus measurement temperature. The R_c and ρ_c of all samples at 25 °C are given in Table I. The non-gold Ta/Si/Ti/Al/Ni/Ta ohmic contacts again exhibited low R_c in all measured TLM patterns.

Typically, there are three possible models used to explain the conduction mechanisms at an M-S interface in ohmic contacts. These are Thermionic Emission (TE), Thermionic-Field Emission (TFE), and Field Emission (FE, or tunneling), which exhibit different temperature dependencies. Theoretically, the dominant mechanism can be identified by using the conduction model to fit the ρ_c values measured at various temperatures. The non-gold ohmic contact exhibit larger ρ_c values (850 °C: $\sim 2.3 \times 10^{-6}$, 900 °C: $\sim 3.3 \times 10^{-6}$, gold-based: $\sim 1.4 \times 10^{-6} \text{ } \Omega \cdot \text{cm}^2$) at -25 °C in Fig 2(b). As the measurement temperature increased, ρ_c of both non-gold samples decreased more rapidly and became smaller than that of gold-based contact since the measurement at 100 °C. The calculated mean ρ_c of non-gold ohmic contact can be fitted well using the TE model given by the following equation¹³

$$\rho_c = \frac{k_B T}{q A^* T^2} \exp\left(\frac{q \Phi_B}{k_B T}\right) \quad \text{Eqn (1)}$$

where Φ_B denotes the Schottky barrier height at the M-S interface, A^* represents the Richardson constant, and q , k_B , T are the electron charge, the Boltzmann constant and

the temperature in unit K, respectively. The Richardson constant $A^* = 4\pi m_n^* q k_B^2 / h^3$ (27.12 A/cm²-K²), where m_n^* is the electron effective mass (2.06×10^{-31} Kg) and h is the Planck constant. The extracted Φ_B values for the samples annealed at 850 °C and 900 °C range from 0.109 ~ 0.116 eV (mean value: 0.113 eV) and 0.117 ~ 0.124 eV (mean value: 0.121 eV), respectively, as given in Table I. These parameters were not only verified the good uniformity of the non-gold ohmic contact across devices but were also consistent with the reported R_c values.¹² The extrapolated mean Φ_B values are only ~4.5 times of the thermal energy at room temperature (kT @ 300 K = 0.026 eV). The extremely low barrier energies make the electron transport by surmounting the barrier with sufficient energy possible. Using a same measurement at the temperature range of -113 °C to 27 °C, Kim, et al, reported the TE mechanism of 700 °C annealed Ti/Si/Ti/Au ohmic contacts on n-GaN (7×10^{16} cm⁻³). The low energy barrier at the M-S interface was also attributed to the formation of low work function Ti_xSi_y .¹⁴ The reason for the slight increase in R_c (from ~ 0.24 to ~ 0.28 $\Omega \cdot mm$) and in Φ_B at 900 °C could be the instability of $TiSi_2$ at high annealing temperature. Lanerrolle, et al, have realized the decomposition of formed alloy $TiSi_2$ into TiN and Si when it annealed at ~ 925 °C in N_2 ambient.¹⁵ This possibly explains the slight degradation of our non-gold ohmic contacts annealed at 900 °C.¹²

Several conduction mechanisms for gold-based ohmic contacts in GaN HEMTs have been postulated recently.^{5, 16-18} These include (1) Tunneling conduction due to heavily n-doped region resulting from the out-diffusion of Ga- and N-atoms;^{5, 16} (2) Direct link due to the penetration of conductive TiN alloy through AlGaN barrier until 2DEG;¹⁷ (3) Low Schottky barrier resulting from the formation of metal alloys.¹⁸ However, no clear conclusion has been made except for the widely acknowledged

tunneling component due to the large concentration of N-vacancies. Liu, et al, proposed a TFE based mechanism for the annealed Ti/Al/Ni/Au ohmic contact annealed at 850 °C.⁸ In addition to the TFE mechanism for Ti/Al/Ni/Au ohmic contacts annealed at 750°C, Lucolano, et al, even observed a ‘metal-like’ ($\rho_c \propto T^{1.8}$ relationship) behavior for the sample subject to 850 °C annealing.⁹ In our study, the calculated ρ_c values of gold-based contacts exhibited a distinctively different trend comparing to the non-gold contacts as shown in Fig 2(b), which suggests that it is due to a different type of conduction mechanism. The ρ_c versus temperature plots can be fitted well using the TFE conduction model given by the equation (2)¹⁹

$$\rho_c = \frac{1}{qA^*} \cdot \frac{k_B^2}{\sqrt{\pi(\Phi_B + V_n)E_{00}}} \cdot \cosh\left(\frac{E_{00}}{k_B T}\right) \cdot \sqrt{\coth\left(\frac{E_{00}}{k_B T}\right)} \cdot \exp\left(\frac{\Phi_B + V_n}{E_0} - \frac{V_n}{k_B T}\right)$$

Eqn (2)

in which V_n denotes the energy difference of Fermi level and conduction band, the E_0 and E_{00} are calculated using the equation (3) and (4)

$$E_0 = E_{00} \coth(E_{00}/k_B T) \quad \text{Eqn (3)}$$

$$E_{00} = qh\sqrt{N_D/m_n^* \varepsilon / 4\pi} \quad \text{Eqn (4)}$$

where N_D is the semiconductor doping concentration. The dielectric constant $\varepsilon = 8.9\varepsilon_0$. The TFE model fitted N_D , Φ_B and V_n values of gold-based contact are given in Table I. Compare to the parameters in [Ref #8], a much lower Φ_B (0.233 eV) and a similar N_D ($8.42 \times 10^{18} \text{ cm}^{-3}$) are obtained. This is consistent with the observed smaller R_c value of our gold-based sample. Unlike TE which has a strong dependence on temperature, TFE typically exhibits a weaker temperature dependency because it is a combination of TE

and FE mechanism. For FE which is mainly due to tunneling, it is almost independent of temperature.

The schematic diagram of the band structure is used to explain the formation process and the conduction mechanism of ohmic contacts on AlGaN/GaN HEMTs. Fig 3(a) shows the band diagram of as-deposited metal stack in contact with GaN cap/AlGaN/GaN heterostructure. As the work functions of first metal layer are close to each other [$\Phi_M(\text{Ti}) \sim 4.33$ eV, $\Phi_M(\text{Ta}) \sim 4.26$ eV]²⁰, the band structure of gold-based and non-gold samples can be qualitatively illustrated by Fig 3(a). Before annealing, both contacts are non-ohmic due to the thick Schottky barrier at the M-S interface. Fig 3(b) shows the band diagram of TFE model for 850 °C annealed Ti/Al/Ni/Au contact proposed by Liu, et al.⁸ The three regions of the contact included two barriers and a high conductive layer. The first barrier (region I) locates at the metal and the modified GaN/AlGaN interface, and the second barrier (region III) is formed between the modified GaN/AlGaN and the 2DEG. The term “modified GaN/AlGaN” (region II) was used because the material properties of GaN/AlGaN sandwiched in between the two barriers had been significantly modified. This is the prominent change in the band diagram of gold-based Ti/Al/Ni/Au ohmic contacts after thermal annealing. The chemical reactions (mainly Ti with GaN cap/AlGaN) caused large amount of N-atoms diffusion hence resulted in the region II with high density of N-vacancies. These N-vacancies can act as n-type dopant with which the tunneling conduction was greatly enhanced. In contrast, our non-gold ohmic contacts yielded a totally different band diagram, as shown in Fig 3(c). The annealing was helping for the formation of metal alloys. At the same time, no reaction was occurred between the metal and the GaN cap layer. This is confirmed by the

HR-TEM and EDX analysis (See Fig 4). As the AlGaIn/GaN heterostructure was well separated by the bottom refractory Ta layer, the Ti didn't react with (Al)GaN thus the cap/barrier layer was kept intact. The most notable change during annealing was at the M-S interface. When the Ti_xSi_y was alloyed then it diffused downwards and touched the GaN cap/AlGaIn interface, the Fermi level was re-aligned due to the smaller work function of Ti_xSi_y .^{12, 14} Subsequently, a small barrier height value (0.113 eV) was obtained for 850 °C annealed contacts from the TE model fitting (See Table I). A band bending of GaN cap at the interface was assumed. Because of the dipole effect, small amount of electrons could be gathered at the GaN cap surface.²¹ However, the localized electrons and band bending would not affect the electron transport as the GaN cap is very thin (2-nm). Compare to the Fig 3(b), the high conductive region (II) due to high density N-vacancies which appears in gold-based ohmic contact does not exist in the non-gold ohmic contacts, by which an alternative mechanism can be inferred.

To study and analyze the ohmic contacts formation between metals and the GaN/AlGaIn epi-layer, HR-TEM and area EDX characterizations have also been carried out. As shown in the inset of Fig 4(a), the narrow dark layer at the M-S interface of non-gold contacts annealed at 850 °C consists of bottom Ta and Ti_xSi_y alloy. Because of a 5nm-thick bottom Ta layer, the rest of the metal (Si/Ti/Al/Ni/Ta) cannot diffuse into the GaN/AlGaIn layers.¹² The boundary of M-S interface is very clear in Fig 4(a). The EDX area mapping in Fig 4 (b) indicates that there is no out-diffusion of N-atoms from the GaN/AlGaIn into the ohmic metals as there were no traces of elementary N_2 species in the metal alloy. Without the heavily doped region to assist FE conduction, we can thus attribute the conduction mechanism to be mainly TE. In most gold-based ohmic contacts,

the penetration of metal alloy (e.g. metallic TiN) into GaN/AlGaN was observed.²² As a result, the AlGaN barrier was damaged even partially consumed.^{22, 23} The interfacial reaction caused large amount of out-diffusion of *N*-atoms,^{5, 16, 17} which has been detected by EDX area mapping⁵ or by Auger Electron Spectroscopy (AES) line scanning.^{14, 24} The *N*-vacancies left behind enhanced the tunneling conduction.^{5, 23} This explains the FE component in the conduction of gold-based ohmic contacts as the TFE can be regarded as a combination of TE and FE.^{8, 9}

In summary, temperature dependent I-V measurements were carried out to investigate the conduction mechanism for non-gold Ta/Si/Ti/Al/Ni/Ta ohmic contacts on un-doped AlGaN/GaN HEMTs. The TLM measurement shows different temperature dependency of ρ_c for the gold-based Ti/Al/Ni/Au and the non-gold ohmic contacts. The measured ρ_c of gold-based ohmic contact agreed well with the reported TFE mechanism. However, the conduction mechanism of non-gold ohmic contact is found to be dominated by TE. The fitted mean energy barriers at the M-S interface are 0.113 eV and 0.121 eV for the annealing temperatures at 850 °C and 900 °C, respectively. The low R_c value of the non-gold ohmic contact is mainly due to the formation of low work function Ti_xSi_y at the M-S interface as supported by the HR-TEM and area EDX mapping.

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Table I Fitted conduction parameters (Φ_B , V_n , N_D) and measured R_c and ρ_c values at 25 °C of gold-based and non-gold ohmic contacts on un-doped AlGaIn/GaN HEMTs grown on silicon.

Sample	TLM Patterns	$R_c@25^\circ\text{C}$ ($\Omega\cdot\text{mm}$)	$\rho_c@25^\circ\text{C}$ ($10^{-6}\Omega\cdot\text{cm}^2$)	Φ_B (eV)	Cond. Model
850 °C	A1	0.22	0.82	0.109	TE
	A2	0.25	1.09	0.113	
	A3	0.25	1.06	0.116	
	Mean	0.24	0.99	0.113	
900 °C	B1	0.27	1.34	0.124	
	B2	0.28	1.37	0.117	
	B3	0.29	1.45	0.123	
	Mean	0.28	1.39	0.121	
Gold-based	C1	0.18	0.86	0.233	TFE*

*For the gold-based contact, fitted $V_n = 0.008$ eV and $N_D = 8.42 \times 10^{18} \text{ cm}^{-3}$ in TFE model

Figure 1 (Color online) Schematic diagram of as-deposited non-gold stacks onto the AlGaIn/GaN HEMTs.

Figure 2 (Color online) (a) R_{total} versus gap length of a TLM pattern on 850°C -annealed non-gold sample, and (b) calculated ρ_c values of gold-based and non-gold (with error bar) ohmic contacts versus measurement temperature with the TE and TFE mechanism fitted curves.

Figure 3 (Color online) The band diagram of (a) as-deposited metal stacks (b) annealed gold-based ohmic contacts with TFE mechanism, and (c) annealed non-gold ohmic contacts with TE mechanism onto the AlGaN/GaN.

Figure 4 (Color online) (a) The cross-sectional view of HR-TEM image, and (b) the EDX elementary mapping of 850 °C-annealed non-gold ohmic contacts [The EDX scan area is marked in (a) with dashed border].

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Captions

Table I Fitted conduction parameters (Φ_B , V_n , N_D) and measured R_c and ρ_c values at 25 °C of gold-based and non-gold ohmic contacts on un-doped AlGaIn/GaN HEMTs grown on silicon.

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Figure 4 (Color online) (a) The cross-sectional view of HR-TEM image, and (b) the EDX elementary mapping of 850 °C-annealed non-gold ohmic contacts [The EDX scan area is marked in (a) with dashed border].