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Ti/Al/Ni/Au Ohmic contacts for AlInN/AlN/GaN-based heterojunction field-effect transistors

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The microstructure of AuNiAlTi/Al_{0.84}In_{0.16}N/AlN/GaN Ohmic contacts annealed from 700 to 900 °C has been determined using transmission electron microscopy and associated analytical techniques. Intermixing and phase separation of the metal contact layers was observed to degrade the surface roughness. An optimal contact performance was obtained for contacts annealed at 800 °C and was attributed to the formation of TiN contact inclusions that had penetrated through the AlInN layers into the GaN layers underneath. These TiN contact inclusions had an inverted mushroom shape with a density of $\sim 10^8$ cm⁻², and they were invariably located at the positions of mixed-type threading dislocations. These inclusion defects would act as a conduction path between the metal contacts and the two-dimensional electron gas of heterojunction field-effect transistor devices. The AlInN layer remained intact in dislocation-free areas of all samples. © 2010 American Institute of Physics. [doi:10.1063/1.3275241]

I. INTRODUCTION

The lattice-matched AlInN/GaN system offers much promise for the fabrication of heterojunction field-effect transistors (HFETs) not only because of the formation of a high density two-dimensional electron gas (2DEG) at the AlInN/GaN interface, but also due to the possibility of strain-free device fabrication with improved reliability.^{1,2} AlInN/GaN high electron mobility transistor heterostructures grown on sapphire substrates with a 2DEG density of $\sim 2.6 \times 10^{13}$ cm⁻² have been reported.³ The Ohmic contact resistance (CR) is critical to the performance of any HFET in general, and AlInN-based HFETs in particular. Thus, it is imperative to understand the relationship between electrical properties and interfacial reactions of the Ohmic contacts used for AlInN HFETs. However, unlike the well-studied AlGaIn/GaN system,^{4–8} there are no published reports about the structural characterization of Ohmic contacts for the AlInN/GaN system. In this study, the microstructure of near-lattice-matched Al_{0.84}In_{0.16}N/GaN heterostructures with Ti/Al/Ni/Au contacts annealed from 700 to 900 °C, have been examined by a range of electron microscopy methods, including conventional transmission electron microscopy (TEM), high-resolution transmission electron microscopy, high-angle annular-dark-field (HAADF) scanning transmission electron microscopy (STEM), and energy-dispersive x-ray spectroscopy (EDXS). The relationship between microstructure and electrical transport properties has also been determined.

II. EXPERIMENTAL

The HFET device structures were grown on (0001) sapphire substrates in a vertical low-pressure metal-organic

chemical-vapor deposition system. A 300-nm-thick AlN layer was first deposited at 1050 °C as a nucleation layer, followed by growth of a 3- μ m-thick undoped GaN buffer and a thin AlN spacer layer with a thickness of ~ 1 nm. The Al_{0.84}In_{0.16}N barriers were then grown and capped with a 2-nm-thick undoped GaN layer. Transmission line measurement patterns were defined on the samples, and stacks of Ti/Al/Ni/Au (30/100/40/50 nm) were then deposited by evaporation. Following a standard liftoff procedure, the samples were heated using rapid thermal annealing for 1 min in N₂ ambient at temperatures ranging from 700 °C to 900 °C. Table I summarizes details of the annealing temperature (AT) (T_a) for the samples labeled A to F which were examined in this study.

Samples suitable for cross-sectional TEM observation were prepared by mechanical wedge polishing, followed by short periods of Ar ion milling. Plan-view TEM samples were prepared by mechanical polishing and Ar ion milling from the substrate side until a small hole was formed. TEM images of the contacts were then taken. Subsequently, the plan-view TEM samples were briefly Ar ion milled from both the substrate and metal contact sides to reveal the metal/AlInN interface region. The Ar ion milling for both cross-sectional and plan-view TEM samples was performed at 3.2 keV with a liquid-nitrogen-cooled specimen stage to minimize any phase-segregation artifacts. A Philips-FEI CM200 FEG was primarily used for microstructural analysis, and a JEOL 2010F with a focused probe size in the range of 0.2–1 nm was used for HAADF STEM imaging and microanalysis.

III. RESULTS AND DISCUSSION

A. Metal contact morphology

After annealing, the color of all sample contacts changed from gold to silver gray. Figure 1 shows plan-view TEM

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TABLE I. AT, microstructure, and CR of samples A–F (the width of the contact pads is 120 μm).

Sample	AT ($^{\circ}\text{C}$)	CI density (cm^{-2})	t_{TiN} (nm)	$t_{\text{GaN capping}}$ (nm)	t_{AlInN} (nm)	CR (Ω)
A	700	0	1.5	~ 2	~ 14	7.4
B	750	0	2.5	~ 1	~ 14	3.0
C	780	$\sim 2 \times 10^6$	~ 3.5	~ 0.5	~ 14	2.4
D	800	$\sim 7 \times 10^7$	~ 3.5	0	~ 14	0.45
E	850	$\sim 2 \times 10^7$	~ 3.5	0	~ 14	1.3
F	900	$\sim 2 \times 10^7$	~ 3.5	0	~ 14	1.5

images of samples B, C, D, and F illustrating the change in the contact morphology for different T_a . For T_a equal to or below 750 $^{\circ}\text{C}$, small light and dark regions were observed, indicating some intermixing of metal layers. The morphology changed markedly for sample C with the appearance of large dark patches, while regions between these patches had relatively uniform contrast [Fig. 1(b)]. Further increase in T_a led to an increase in size of the black patches and the appearance of a distinctive network structure, as visible in Fig. 1(d).

Figure 2 shows HAADF STEM images of samples B, D, and F. EDXS point analysis of sample B [Fig. 2(a)] indicated that the contact multilayers had mixed together and formed different intermetallic phases. The black regions were identified as Ni–Al alloys and the bright regions were Au–Al alloys with small amounts of Ti. With increasing T_a , the contact surface bulged upwards due to the formation of ellipsoidal Ni–Al intermetallic particles (black patches in Fig. 1) embedded in the Al–Au matrix. These particles were ~ 400 nm tall in sample F [Fig. 2(c)]. The formation of these Ni–Al particles might be driven by the minimization of interface energy, as reported for the Au/Mo/Al/Ti system.⁹ The EDXS line profile of sample A (lowest T_a) showed relatively uniform Ti distribution in the Al–Au regions. However, a strong Ti signal was observed at the Al–Au alloy surfaces

with increasing T_a . Furthermore, a ~ 25 -nm-thick porous layer was observed below the Ni–Al and Au–Al alloys in samples A, B, C, and D [as indicated by the black arrow shown in Fig. 4(b), sample D]. This layer was only observed underneath the Ni–Al particles for samples E and F, while it was replaced by a ~ 80 -nm-thick Al–Au porous structure in other regions with a Ti-rich layer above. EDXS mapping and line profiles indicated that the ~ 25 -nm-thick porous layer was mostly Ti mixed with some Au and Al. The porous structure may be caused by diffusion of Ti. There was also a strong N signal close to the surface of the contact metal, which could be due to reaction between Ti and N_2 during annealing.

The abrupt change in contact morphology with increasing T_a is likely to be caused by the formation of a liquid Al–Au phase in some regions at temperatures above ~ 800 $^{\circ}\text{C}$. According to the Al–Au phase diagram,¹⁰ a liquid $\text{Al}_{0.2}\text{–Au}_{0.8}$ phase can be formed at ~ 800 $^{\circ}\text{C}$, and a liquid Al–Au phase can also be formed for Au mole fractions from

FIG. 1. Plan-view TEM images showing the morphology of Ti/Al/Ni/Au contacts for samples B (a), C (b), D (c), and F (d).

FIG. 2. HAADF STEM images of samples B (a), D (b), and F (c) showing bulging up of Ni–Al intermetallic phase (indicated by black arrows) at higher T_a . The Au–Al intermetallic phase (indicated by white arrows) is transformed into a network structure in sample F.

FIG. 3. (Color online) (a) HAADF STEM image of sample A taken from region without any contact showing that the GaN capping layer is ~ 3 nm thick. (b), (c), and (d) HAADF STEM images of samples A, C, and D, respectively, showing transformation of GaN capping layer (as indicated by circle arrow) into defective TiN layer (as indicated by white arrow) with increasing T_a . An Au-rich layer with bright contrast is present at the interface between GaN capping layer and TiN, as indicated by square arrow.

0.55 to 0.82 when temperatures reach 900 °C. The existence of a liquid phase in some areas would greatly promote the speed of diffusion of metal atoms, so that large Ni–Al intermetallic particles could easily be formed. Moreover, the liquid Al–Au phase would also increase the outdiffusion of Ti atoms toward the contact surface. However, it appears that the outdiffusion of Ti atoms was blocked at the locations of the Ni–Al particles. Thus, the porous ~ 25 -nm-thick Ti-rich layer was only observed in regions of samples E and F where Ni–Al particles were present.

B. Reaction between Au/Ni/Al/Ti contact and GaN capping layer

Figure 3(a) shows a HAADF STEM image taken from a region of sample A without any contact. The AlInN layer is ~ 13 -nm-thick, and a ~ 3 -nm-thick GaN capping layer (as indicated by the round arrow) is clearly visible at the top surface. An unexpected Ga-rich layer was also present between the AlN spacer and the AlInN layer. Analysis of this Ga-rich layer has been reported elsewhere.¹¹ Figures 3(b)–3(d) show further HAADF STEM images of the samples A, C, and D. The thickness of the GaN capping layer has been reduced from its original ~ 3 to ~ 2 nm in this area of sample A to almost 0 nm in sample D. EDXS line profile analysis showed that the disappearance of the GaN capping layer was accompanied by the appearance of a Ti-rich layer (as indicated by triangular arrow). The thickness of the Ti-rich layer increased with decreasing GaN capping layer thickness but remained at ~ 3.5 nm after disappearance of the GaN capping layers in samples D, E, and F. High-resolution TEM imaging showed that the Ti-rich layer was

FIG. 4. (Color online) HAADF STEM images of samples (a) C and (b) D showing that the mushroom-shaped CI penetrates through the AlInN layer into the GaN. The CI is much larger inside the GaN than in the AlInN layer. (c) EDXS line profile across the region indicated in (b) showing that the CI is Ti-rich.

mostly defective cubic TiN. There was also a ~ 0.5 -nm-thick Au-rich layer (indicated by square arrow) between the GaN and Ti-rich layers, as shown in the EDXS line profile. The formation of similar Au-rich layers between TiN and GaN was previously reported in the Au/Ti/Al/Ti/AlGaIn/GaN system.⁸ The Au-rich layer/TiN interface was relatively flat, but the TiN/contact interface was wavy. Figures 3(c) and 3(d) also show that there are some lines of bright contrast inside the defective TiN layer, which may correspond to Au-rich areas at TiN grain boundaries. The AlInN layers for samples A to F had the same thickness, which indicated that the layer was stable in the presence of Ti. However, it should be noted that TiN is chemically more stable, since it has lower enthalpy (TiN: -338 kJ/mol, AlN: -318.4 kJ/mol, GaN: -109.6 kJ/mol, and InN: -138.1 kJ/mol).¹² This is probably because the reaction between Ti and AlInN is nucleation controlled with a very high nucleation barrier and requiring large nucleus size.¹³

C. Contact inclusions and CR

Contact inclusions (CIs) with an inverted mushroom shape were visible in sample C, as shown by the HAADF STEM image in Fig. 4(a). These CIs penetrated through the AlInN layer well into the GaN layer underneath. Both the density and penetration depth of these CIs increased abruptly in sample D [Fig. 4(b)]. The CIs were much wider inside GaN than within the AlInN layer. Most of them had a faceted shape with a surrounding line of bright contrast suggesting a material with high atomic number. EDXS line profile analysis in Fig. 4(c) shows that the CIs were Ti-rich. Moreover,

FIG. 5. Two-beam diffraction contrast TEM images taken from the same specimen area of sample D under diffraction conditions (a) $g=0002$ and (b) $g=1120$, to identify different types of TDs inside the heterostructure. CIs, as indicated by black arrows, penetrate beyond the AlN/GaN interface along mixed-type TDs.

line profiles across the bright shell of the CI (not shown here) confirmed that the bright shell consisted of an Au-rich layer.

Conventional diffraction contrast images taken with diffraction vectors $g=(0002)$ and $g=(1120)$ from the same area under the contact, are shown in Figs. 5(a) and 5(b). Threading dislocations (TDs) with Burgers vectors along the c (screw-type) and $c+a$ (mixed-type) directions are visible in the GaN layers in Fig. 5(a), while Fig. 5(b) shows TDs having Burgers vectors along the a (edge-type) and $c+a$ (mixed-type) directions. By comparing these images taken with different g vectors, it was established that edge- and mixed-type TDs were the most prevalent. The CI density was lower than the TD density. Moreover, most of the CIs were preferentially nucleated along mixed-type TDs. CIs with similar morphology have been reported in the Ti/Al/Mo/Au/AlN/GaN system.¹³ However, the CIs in that system were reported to connect preferentially with edge-type TDs. High-resolution TEM imaging (not shown here) revealed that the CIs were primarily cubic TiN with some internal grain boundaries. The narrow stem of the CI in the AlInN layer was invariably defective. Further increase in T_a led to a slight decrease in density of CIs in samples E and F, where CIs were only observed under Ni–Al particles.

EDXS elemental mapping from a region of sample D with a CI is shown in Fig. 6. A Ga signal is observed in the Ni–Al layer immediately above the CI and also in the TiN CI within the AlInN layer, which suggests that the CI stem in the AlInN layer is acting as a channel for outdiffusion of Ga atoms and indiffusion of Ti atoms during GaN decomposition and TiN formation. Outdiffusion of Ti to the Au–Al intermetallic surface is clearly visible in Fig. 6(c). However, no Ti signal is observed inside the Ni–Al intermetallic phase. The formation of Ni–Al and Au–Al intermetallic regions is confirmed in Figs. 6(d)–6(f), but no obvious diffusion of Au or Ni into the AlInN layer is observed.

Figures 7(a) and 7(b) show plan-view TEM images of the contact/AlInN interface areas of samples C and D. The hexagonal-shaped patches are top-views of the CIs. The CI densities are measured to be $\sim 2 \times 10^6$ and $\sim 7 \times 10^7$ cm⁻²

FIG. 6. (Color online) HAADF STEM image (a) and elemental mapping [(b)–(f)] of sample D. (b) Ga has diffused into the Ni–Al alloy right above the CI through the mushroom stem. (c) Ti is visible in the CI, AlInN/contact interface, as well as on the contact surface.

for samples C and D, respectively. Figures 7(c) and 7(d) show bright-field TEM and HAADF STEM images of hexagonal CI in sample D. TDs are invariably visible near the middle of these patches, confirming the preferential nucle-

FIG. 7. Plan-view TEM images of samples C (a) and D (b) showing abrupt increase in hexagonal-shaped CIs in sample D. (c) Bright-field TEM image showing hexagonal-shaped CI in sample D. The black dot in the middle is a TD. (d) HAADF plan-view STEM image showing the Au-rich layer (bright layer) around the CI.

FIG. 8. Schematic illustration of CI formed by Ti diffusion into GaN along mixed-type TDs. The inverted mushroom-shaped TiN inclusions serve as direct conducting paths between metal contacts and the 2DEG.

ation of these CIs at TDs. The dark lines [Fig. 7(c)] or bright lines [Fig. 7(d)] correspond to the Au-rich shells observed in the cross-sectional STEM imaging. Plan-view TEM sample preparations for sample E and F were not successful because of the rough metal surface. Estimates of the CI density in samples E and F based on cross-sectional TEM images indicated that the CI density was $\sim 2 \times 10^7 \text{ cm}^{-2}$.

The decrease in CI density for annealing above 850°C could be explained by the following mechanism. The formation of TiN CIs depends on the diffusion of Ti atoms into the AlInN/AlN/GaN heterostructure along TDs. Simultaneously, Ti atoms also tend to diffuse outwards toward the contact surface, as shown by the EDX line profile and mapping in Figs. 4 and 6. At temperatures below 850°C , the outdiffusion of Ti is insufficient to reduce the amount of Ti available for indiffusion. Thus, the indiffusion of Ti increases with higher T_a and an increase in CI density is observed. Further increase in T_a would be accompanied by the occurrence of larger and larger areas of liquid phase in the Al–Au metal alloy. The Ti outdiffusion speed will thus increase abruptly and the amount of Ti available for indiffusion is greatly reduced. As a result, TiN CI would only be formed under Ni–Al particles where the Ti outdiffusion is partly blocked. The formation of these CI might also be affected by the thicknesses of the different metal layers and the [In] concentration inside the AlInN layer. A previous microstructural study showed an increase in CI density with increasing T_a for samples with different metal layer thickness.¹¹

Table I summarizes CR and microstructural characterization results for samples A to F. The minimum CR was measured from sample D, which also had the maximum CI density. Moreover, all samples showing CI had lower CR. Thus, it can be concluded that CI density has a major impact on the performance of Ohmic contacts in the AlInN/GaN system. Similar to the spike mechanism for carrier injection proposed for the AlGaIn/GaN system, those CI in the AlInN/AlN/GaN system that penetrate through the AlInN layer are likely to act as channels along which carriers flow between the 2DEG and the contact electrodes.⁹

Figure 8 is a schematic illustration of CIs formed by Ti diffusion into GaN along TDs. The inverted mushroom-shaped TiN CIs with Au-rich shell will serve as direct conducting paths between the metal contact and the 2DEG. An increase in TiN CI density would thus promote electron transport efficiency. However, the CIs will also destroy part

of the 2DEG interface and possibly degrade overall device quality. As a result, an optimum CI density is required. For the Au(50 nm)/Ni(40 nm)/Al(100 nm)/Ti(30 nm)/AlInN/GaN system, our present and former studies have shown that contacts annealed at 800°C with CI density of $\sim 10^8 \text{ cm}^{-2}$ give the best performance.¹¹

IV. CONCLUSIONS

The microstructure of AuNiAlTi/AlInN/AlN/GaN devices, with Ohmic contacts subject to rapid thermal annealing from 700 to 900°C , has been analyzed using a variety of electron microscopy techniques. With increasing T_a , the contact metals start to intermix. Large Ni–Al particles are formed embedded inside an Au–Al intermetallic phase, and Ti diffuses outwards to the Au–Al intermetallic surface. The intermixing and phase separation of these different contact metal layers has direct impact on the metal surface roughness. The GaN capping layer is transformed completely into TiN, after annealing at 800°C . TiN CIs penetrating through the AlInN layer into GaN are formed along mixed-type TDs after annealing at 780°C . The CI density is highest ($\sim 10^{-8} \text{ cm}^{-2}$) in samples annealed at 800°C , which also show the lowest CR. The TiN CIs are likely to act as conducting paths between the metal contacts and the 2DEG.

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