TEM STRUCTURE CHARACTERIZATION OF Ti/Al and Ti/Al/Ni/Au OHMIC CONTACTS FOR n-GaN

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ABSTRACT

Transmission electron microscopy has been applied to characterize the structure of Ti/Al and Ti/Al/Ni/Au ohmic contacts on n-type GaN (~10^{17} cm^{-3}) epitaxial layers. A thin polycrystalline cubic TiN layer epitaxially matched to the (0001) GaN surface was detected at the interface with the GaN substrate. This layer was studied in detail by electron diffraction and high resolution electron microscopy. The orientation relationship between the cubic TiN and the GaN was found to be: $\{111\}_{TiN}//\{00.1\}_{GaN}$, $[110]_{TiN}//[11.0]_{GaN}$, $[112]_{TiN}//[10.0]_{GaN}$. The formation of this cubic TiN layer results in an excess of N vacancies in the GaN close to the interface which is considered to be the reason for the low resistance of the contact.

INTRODUCTION

Nitride-based electronics and optoelectronics requires high reliability of metal contacts for n- and p-GaN because the performance of devices strongly depends on contact resistance. Recent success in fabrication of such devices as visible light-emitting diodes (LEDs)[1-3] and metal-semiconductor field-effect transistors (MESFETs)[4] evidences that GaN and related compounds are very promising for optoelactronics applications and, in particular, for high temperature applications. Nitrides are known to have an excellent thermal conductivity, high saturation velocity and large breakdown field.[5] Thus, a development of a low resistance ohmic contact for GaN is of great practical importance. A few attempts to achieve good ohmic contacts on GaN epilayers have been reported recently.[5-8] Most of these metallization schemes include Ti as a first metal layer and reactive ion etching (RIE) of the GaN surface prior to the metal deposition. Low resistance contacts to GaN were formed as a result of these processes, even without annealing (e.g. 6.5×10^{-5} Ω cm^2 in the case of a Ti/Ag contact[6]). Similar results were reported for W and WSi_x contacts.[8] The reason for the low resistivity of these contacts is still under discussion. It is resonable to assume that the low resistivity might be related to the interaction of Ti or W with the GaN. As a result, the formation of TiN or WN layers on the GaN surface and, associated with them, an excess of N vacancies near the interface is a possible cause for the low contact resistivity. However, until the present study no direct evidence of the formation of such a layer or its structure has yet been reported.

The structure and morphology of the Ti/Al and Ti/Al/Ni/Au thin composite layers which provide ohmic contacts on n-type GaN (~10^{17} cm^{-3}) epitaxial layers are the focus for the present study. Here, we report results on the metallurgy of GaN/Ti/Al and GaN/Ti/Al/Ni/Au contacts which form a thin cubic TiN layer on the GaN surface.

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EXPERIMENTAL

3 μm-thick n-GaN layers were grown by molecular beam epitaxy (MBE) on c-plane Al_2O_3.[7] The GaN layers contained two sublayers, a 2 μm thick Si-doped layer with a carrier concentration of about $5x10^{18}$ cm^{-3} and a 1μm thick undoped n-GaN layer on top with a carrier concentration of about 10^{17} cm^{-3}. Before the metal deposition, the GaN surface was exposed to reactive ion etching (RIE). The composite metal layers were either Ti/Al (20 nm/100nm) or Ti/Al/Ni/Au (15nm/220nm/40nm/50nm). Details of metallization schemes are reported elsewhere.[5,7] A rapid thermal anneal (RTA) at 900 °C for 30 s in an N_2 environment provides the lowest resistance contact of about $8x10^{-6}$ Ω cm^2 and $8.9x10^{-8}$ Ω cm^2 for the Ti/Al and Ti/Al/Ni/Au contacts, respectively.

Transmission electron microscopy (TEM), high resolution electron microscopy (HREM) and electron diffraction have been applied to study the structure of the contacts. Cross-sections were prepared for the TEM study by dimpling followed by ion milling. TEM studies were carried out on Topcon 002B and JEOL 200CX microscopes operated at 200 kV. Energy dispersive X-ray (EDX) spectra were taken from different metal sublayers to study the metal interdiffusion after thermal annealing.

RESULTS AND DISCUSSION

Ti/Al contact

Typical cross-sectional TEM images of a Ti/Al contact are shown in Figs. 1 before (a) and after (b) thermal annealing at 900 °C for 30 s.

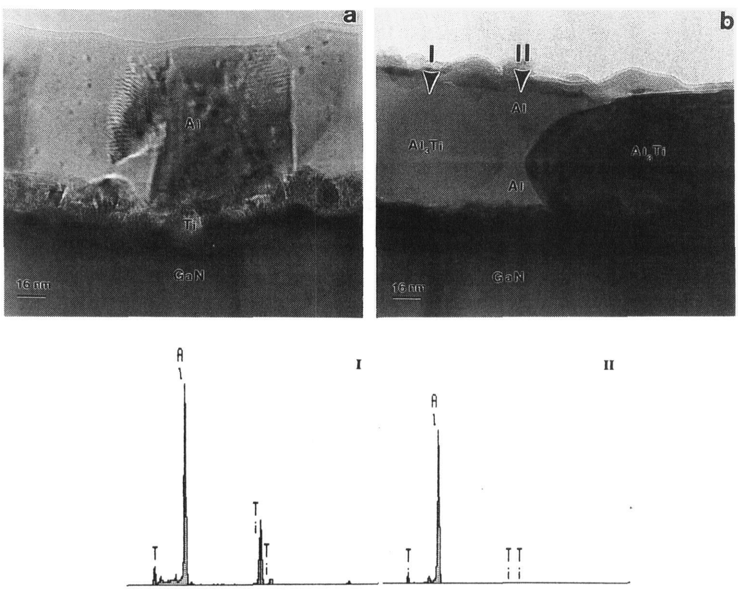

Fig. 1, a-b. Bright field TEM micrographs of Ti/Al contact in cross-section before (a) and after (b) annealing. EDX spectra from regions I and II of micrograph (b) are shown on the bottom.

Both as-deposited layers are textured polycrystalline material with c-planes of the metal grains mostly parallel to the c-plane of GaN.The Al-Ti and Ti-GaN interfaces are very rough as a result of a rough surface morphology of the GaN due to the reactive ion etching prior to metal deposition. Annealing does not change the surface morphology of the GaN significantly, but leads to metal interdiffusion and alloying. The thickness of the metal composite layer decreases after annealing due to the interdiffusion and formation of alloys with higher densities than that of pure Al. In the case of the Ti/Al composite layer, RTA results in the formation of one polycrystalline layer which consists of large $Al_{3+x}Ti$ ($x<1$) and Al grains with the c-plane almost parallel to that of GaN.

Ti/Al/Ni/Au contact

Similar results were obtained for the Ti/Al/Ni/Au contact (see Fig.2). TEM bright-field micrographs (a) and (b) of Fig.2 represent structure of the metal composite before and after thermal annealing. All of the as-deposited layers are also textured polycrystalline with rough interfaces. In contrast with the Ti/Al contact where no significant interdiffusion was detected by EDX between the Ti and Al in the as-deposited sample, the formation of a Al-Ni alloy was observed in the Ti/Al/Ni/Au metal composite just after Au deposition.

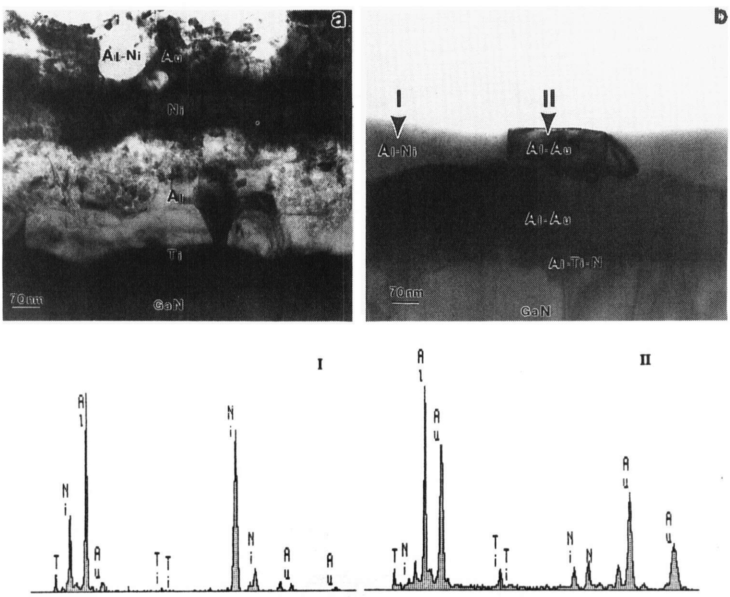

Fig. 2, a-b. Bright field TEM micrographs of Ti/Al/Ni/Au contact in cross-section before (a) and after (b) annealing. EDX spectra from grains I and II of Fig. (b) are shown on the bottom.

Annealing leads to further metal interdiffusion and alloying. The thickness of the metal composite layer decreases after annealing due to the interdiffusion and formation of alloys with higher densities than that of pure Al. For the Ti/Al/Ni/Au composite, annealing leads to the formation of at least three polycrystalline layers. The top layer consists mostly of an Al-Ni alloy with some grains of an Al-Au alloy. The middle layer is formed mostly by an Al-Au alloy with some Al-Ni grains. This is consistent with the high diffusivity of Au and shows a strong interaction between Al and the other species (Au, Ni, Ti). The bottom layer contains mostly Al-Ti and Ti-N alloys, but other species are also present in the layer. An EDX of the GaN interface indicates the presence of 61.5 at.% Ti, 26.2 at.% Al, 6.8 at.% Ga, 3.8 at.% Au, and 1.6 at.% Ni. In fact all of these species are present in various proportions over the metal composite after annealing.

Structure of Ti-GaN interfacial region

The interfacial region between the metal composite layers and the GaN is very complex and also polycrystalline. Both HREM and electron diffraction establish the presence of a textured polycrystalline layer of cubic TiN on the GaN surface. A thin TiN layer was detected by electron diffraction at the Ti-GaN interface even for as-deposited samples. The thickness of this TiN layer increases to 5 nm (Fig.3a) after annealing of the Ti/Al contact and to 10-15 nm (Fig.3b) for the Ti/Al/Ni/Au contact.

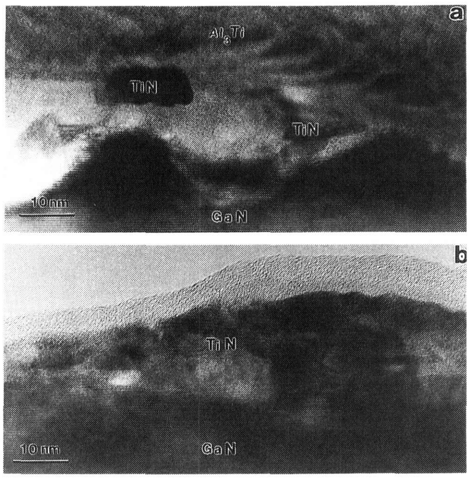

Fig.3, a-b. Low magnification HREM images of the interfacial area near the GaN surface of Ti/Al (a) and Ti/Al/Ni/Au (b) metal composites in cross-section after RTA.

The high resolution electron micrographs in Figs.3b and 4 show the interfacial region between the metal Ti/Al/Ni/Au composite and the GaN after annealing at 900 °C for 30 s. The orientation relationship between the TiN layer and the GaN was determined from the electron diffraction pattern as: $\{111\}_{TiN}//\{00.1\}_{GaN}$, $[110]_{TiN}//[11.0]_{GaN}$, $[112]_{TiN}//[10.0]_{GaN}$.

The TiN grains are often in a twinned orientation. The mismatch in the lattice parameters of TiN and GaN is about 5.6-6.0%. This leads to the formation of relatively small grains of about 5-20 nm in lateral size which are slightly misoriented to each other and with respect to the GaN. The interface between the TiN grains and the GaN in Fig.4 is quite abrupt, but the GaN region near the interface contains many structural defects which are possibly N vacancy complexes. The accumulation of N vacancies may lead to the formation of voids or protrusions at the TiN-GaN interface (see Fig.4).

The resistivity of both the Ti/Al and Ti/Al/Ni/Au contacts decreases drastically after annealing, but their lowest values differ by two orders of magnitude. A thin TiN layer was found at the interface between the metal composite and the GaN in both cases but the TiN is twice as thick in the case of the four metal contact. This may be the result of the specific structure of the composite layer formed after annealing. In the Ti/Al/Ni/Au contact, Au diffuses through the Ni layer and forms an Au-Al alloy while an Al-Ni alloy layer resides at the surface. The Au-Al layer underneath may prevent further diffusion of Ni toward the GaN surface. On the other hand, formation of the Au-Al alloy might prevent outdiffusion of Ti into the Al layer to form an Al-Ti alloy.[7]

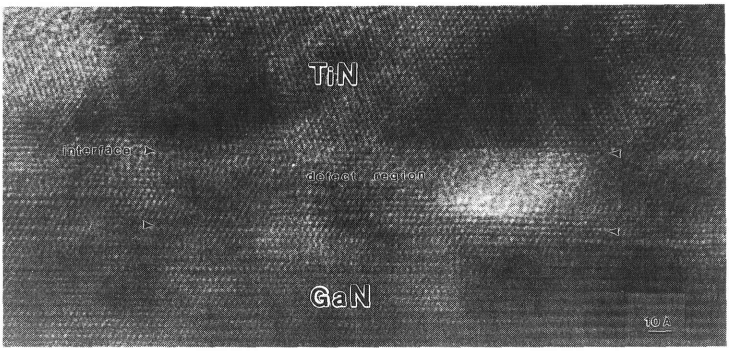

Fig.4. HREM micrograph of the interfacial area near the GaN surface of Ti/Al/Ni/Au contacts in cross-section after RTA.

Role of RIE

There are several possible explanations for the reduction of contact resistivity by RIE. First, it provides a method to clean the surface and remove any oxide layer.[7] Second, it increases the GaN surface roughness due to the preferential etching of dislocated material and, hence, increases the contact area. Third, RIE causes radiation damage near the GaN surface and, hence, increases the point defect density in a thin GaN region near the surface. As a result, it makes diffusion of Ti into the GaN more rapid, even during the metal deposition. Thus, the formation of a good contact is expected even before annealing. Indeed, a low resistance contact to GaN of $6.5x10^{-5}\ \Omega\ cm^2$ was reported for the Ti/Ag metallization[6] without annealing. The role of dislocations in GaN in the formation of a good contact is beyond the scope of this paper, but this role appears to be considerable. Indeed, diffusion is enhanced along dislocation cores so that dislocations might be considered as pipes for metal atom migration.

The dislocation density at the top of the GaN layer is as high as $5x10^9$. This high dislocation density is associated with the formation of small angle grain boundaries. Preferential etching of GaN at end points of dislocations leads to the formation of grooves on the GaN surface during RIE. The defect distribution over the thickness of the GaN layer is the following: rather high at the interface of the GaN with the AlN buffer, but sharply decreasing over a distance of 0.2 μm toward the layer surface.

Low resistivity metal contacts for n-GaN

Both RIE-induced damage of the GaN and formation of the TiN phase can lead to a supersaturation of N vacancies within the near interface area.[5] For example, formation of a donor-rich surface layer has been detected by Fonash et al.[9] after ion irradiation of the surface. Jenkins & Dow[10] have shown that N vacancies in GaN act as donors. This led Z. Fan et al.[7] to suggest that a heavily doped TiN-GaN interfacial area causes bending of the GaN conduction band sufficient for tunneling. Another type of low resistance ohmic contact is the low barrier Schottky contact[11,12] which might be associated with intermediate or graded band-gap interface material. Because the band gap of AlN is larger than that of GaN, ternary Al-Ti-N compounds or their mixture might have a band gap which is close to that of GaN and, hence, provide such a low-barrier Schottky contact.[5] EDX shows the presence of a certain amount of Al in the interfacial area near the GaN surface. However, the formation of ternary or quaternary Ga-Ti-Al-N compounds has not been detected by TEM in this study. This may be because of the small amount of such material. On the other hand, success in the development of a low resistance contact using the Ti/Ag[6] or W[8] metallization schemes suggests that TiN and WN formation and, associated with it, an excess of N vacancies in the GaN under the contact is the most important factor for achieving low contact resistivity.

CONCLUSIONS

In conclusion, TEM shows the formation of a thin polycrystalline cubic TiN layer at the metal composite-GaN interface. The orientation relationship between the cubic TiN layer and the GaN was found to be: $\{111\}_{TiN}//\{00.1\}_{GaN}$, $[110]_{TiN}//[11.0]_{GaN}$, $[112]_{TiN}//[10.0]_{GaN}$. The formation of this TiN layer and, associated with it, an excess of N vacancies in the GaN under the contact is the most likely explanation for the low resistance of the Ti/Al and Ti/Al/Ni/Au contacts.

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