The role of Al on Ohmic contact formation on $n$-type GaN and AlGaN/GaN

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A standard metallization scheme for the formation of Ohmic contacts on $n$-type GaN does exist. It has the following multilayer structure: Ti/Al/metal/Au. Ti is known to extract N out of the GaN. This leaves a high density of N vacancies (donors) near the interface pinning the Fermi level. The created tunnel junction is responsible for an Ohmic contact behavior. Au is deposited as the final metal layer to exclude oxidation of the contact and the metal should limit the diffusion of Au into the layers below and vice versa. Al in the metallization scheme is known to improve the contact resistance, but the reason why has not been reported yet. We studied Ti and Ti/Al contacts on GaN and AlGaN/GaN as a function of annealing temperature by transmission electron microscopy. The role of Al in the metal multilayer, and of Al in the AlGaN on the Ohmic contact formation, has been determined. The latter result indicates that the standard metallization scheme for GaN cannot be simply transferred to AlGaN/GaN structures. © 2005 American Institute of Physics. [DOI: 10.1063/1.2008361]

For several years, GaN-based devices are receiving a lot of interest. Optimum device performance, however, is still limited by the lack of low-resistance Ohmic contacts, both on light-emitting diode and high electron mobility transistor structures. Contact formation on $n$-type GaN is best understood and a good standard metallization scheme on $n$-type GaN does exist. It typically has a Ti/Al/blocking layer/Au multilayer structure. The blocking layer is often one of the metals Ti, Ni, Mo, or Pt (Refs. 1–5). The basic mechanism responsible for Ohmic contact formation is N extraction by Ti out of the GaN upon thermal annealing. This leaves a high density of N vacancies, which create donor states near the metal interface, pinning the Fermi level and thus creating a tunnel junction. Moreover, the creation of a TiN interfacial layer provides a thermally stable and low-resistive contact to the GaN. The use of a Ti/Al sequence, instead of a single Ti layer, provides a thermally stable and low-resistive contact to the GaN. The use of a TiN interfacial layer provides a thermally stable and low-resistive contact to the GaN. The use of a Ti/Al sequence, instead of a single Ti layer, provides a thermally stable and low-resistive contact to the GaN. The use of a TiN interfacial layer provides a thermally stable and low-resistive contact to the GaN.

For contact formation on AlGaN/GaN structures, one usually transfers the metallization scheme for $n$-type GaN and reoptimizes the metallization scheme parameters. How the electrical coupling occurs between the two-dimensional electron gas in the AlGaN/GaN and the metal is still not well understood. Most reports suggest that the metal penetrates through the AlGaN to get the better contact. It is clear though that the AlGaN should be as thin as possible because electrons need to tunnel through the insulating AlGaN (Ref. 11). However, the exact coupling mechanism is not known, the design of an ideal contact on AlGaN/GaN is still lacking.

In this study, Ti and Ti/Al contacts, both on GaN and AlGaN/GaN, have been systematically studied as a function of the annealing temperature. The samples have been grown with the same multilayer structure. The blocking layer is often one of the metals Ti, Ni, Mo, or Pt (Refs. 1–5). The basic mechanism responsible for Ohmic contact formation is N extraction by Ti out of the GaN upon thermal annealing. This leaves a high density of N vacancies, which create donor states near the metal interface, pinning the Fermi level and thus creating a tunnel junction. Moreover, the creation of a TiN interfacial layer provides a thermally stable and low-resistive contact to the GaN. The use of a Ti/Al sequence, instead of a single Ti layer, provides a thermally stable and low-resistive contact to the GaN. The use of a TiN interfacial layer provides a thermally stable and low-resistive contact to the GaN. The use of a Ti/Al sequence, instead of a single Ti layer, provides a thermally stable and low-resistive contact to the GaN.

An AlGaN/GaN structure, with 30% Al and 21 nm thick, has been grown on (0001) sapphire in a 3 $\times$ 2" close-coupled showerhead MOVPE reactor. Ammonia (NH$_3$), trimethylgallium (TMGa), and trimethylaluminium (TMAI) were used as precursors; N$_2$ was used as carrier gas. To exclude possible microstructural differences, all contacts have been deposited on the same AlGaN/GaN wafer. The AlGaN samples (nominally undoped) have been prepared by selectively removing the AlGaN cap layer using inductively coupled plasma etching. Ti contacts were made by sputtering 20 nm and evaporating 180 nm Ti contacts are formed by sputtering 10 nm Ti and evaporating 190 nm Al. The policy was adopted to deposit the contacts without Au cap layer, in order to reduce possible metal-metal interactions. In this way, it was possible to circumvent unwanted reactions (between Au and Al, ...) induced, e.g., by a nonoptimized metal thickness. All samples have been thermally annealed for 90 s in an N$_2$ ambient in a rapid thermal anneal furnace, operating at constant power dissipation. End temperatures have been calibrated to be 805 and 991 °C for a low-temperature anneal and a high-temperature anneal, respectively. These anneal conditions, applied to a standard Ti/Al/Ti/Au metal scheme on AlGaN/GaN, produce, respectively, Schottky and Ohmic contact behavior. The contacts on AlGaN/GaN have been electrically characterized by the transmission line method. All samples have been investigated structurally and chemically using conventional, high-
than the TiN that above the TiN a Ga-Ti alloy has formed, slightly thicker large voids below the TiN. The re-action would be that aggressive, resulting in the formation of some small voids have been observed, similar to the voids observed in the Ti/GaN samples. TiN has been observed on top of this TiN. Al in the AlGaN thus strongly gained—reaction is a substitutional replacement of Ga by Ti below are highly oxidized, as evidenced by EELS measurements. The found crystal structures are those of TiO and Al2O3 respectively, −110.9, −265.5, and −318.1 kJ/mol. As energy is gained by the extraction of N out of GaN by Ti, this reaction can easily take place. However, because the Al-N bond is stronger than the Ti-N bond, the Al in AlGaN keeps the N atoms at its place. The only possible—energy gaining—reaction is a substitutional replacement of Ga by Ti. Once the slow substitutional process has completely transformed the AlGaN, the GaN below is affected in the classical way: high amounts of N are extracted out of the GaN leading to a decomposition of the GaN.

In Ti/Al contacts on GaN, annealed at low temperature, the well-known N extraction by Ti, triggered by a higher enthalpy of formation of TiN with respect to GaN (Ref. 13), has been observed. It was, however, unexpected that the reaction would be that aggressive, resulting in the formation of large voids below the TiN (Fig. 1). Chemical analysis shows that above the TiN a Ga-Ti alloy has formed, slightly thicker than the TiN (Fig. 1). Annealing at high temperatures enhanced the reaction, resulting in even larger voids and thicker TiN and TiGa layers on top (Fig. 2). This indicates that the strong reaction of the Ti with GaN is able to extract enough N atoms to destabilize GaN and to trigger its decomposition. The liquid Ga evidently alloys with the Ti. The reproducibility of the void size in different TEM specimens of these two wafers and the absence of voids in other TEM specimens of contacts on GaN, indicates that the void formation is inherent and not due to TEM specimen preparation.

Ti contacts on AlGaN/GaN, annealed at low temperature, show a very limited reaction. Only the top 5 nm of the AlGaN has reacted with the Ti (Fig. 3). Detailed TEM shows that this top part of the AlGaN has turned into a highly defected phase where locally the cubic stacking, typical for the TiN fcc lattice, can be observed. Chemical analysis, however, indicates that this layer still contains Al; the concentration is more or less equal to that in AlGaN. The fact that the interface layer is highly defected does not allow us to identify the phase formed (or a mixture of phases) as in the case of the formation of an epitaxial AlTi2N layer observed by Ref. 14. Therefore, the phase formed will be denoted by Al +Ti+N. Again, some Ga is found on top of this defected layer. Basically, the reaction can be seen as Ti substituting for the Ga in the AlGaN. Annealing at high temperature results in a complete transformation of the AlGaN into the highly defected Al+Ti+N phase. Below the former AlGaN, some small voids have been observed, similar to the voids observed in the Ti/GaN samples. TiN has been observed on top of the highly defected phase, N most likely originating from the GaN voids below the AlGaN. A Ga-Ti alloy is found on top of this TiN. Al in the AlGaN thus strongly limits the reaction of Ti. This can simply be explained by considering the enthalpies of formation of GaN, TiN, and AlN (respectively, −110.9, −265.5, and −318.1 kJ/mol). As energy is gained by the extraction of N out of GaN by Ti, this reaction can easily take place. However, because the Al-N bond is stronger than the Ti-N bond, the Al in AlGaN keeps the N atoms at its place. The only possible—energy gaining—reaction is a substitutional replacement of Ga by Ti. Once the slow substitutional process has completely transformed the AlGaN, the GaN below is affected in the classical way: high amounts of N are extracted out of the GaN leading to a decomposition of the GaN.

In Ti/Al on GaN and AlGaN/GaN samples, annealed at low temperature, hardly any reaction between the Ti and the nitride has been observed. Only a very thin layer (0.5 nm) of TiN is retrieved, both on GaN and AlGaN/GaN. The Ti/Al bilayer transformed to large AlTi precipitates in an Al matrix (Fig. 4), a reaction predicted by the Ti-Al bulk phase diagram. In samples annealed at high temperature, the original Ti/Al bilayer can be retrieved, although some diffusion of Al into Ti is observed. At the metal-nitride interface no reaction occurs. The reason for the difference is related to the O content of the samples. At high temperature, the Al and the Ti below are highly oxidized, as evidenced by EELS measurements. The found crystal structures are those of TiO and a strongly oxidized Al (not yet Al2O3). Although the samples...
annealed at high temperature obviously do not produce good contacts, this failure provides a number of clues. Al in the metal scheme is able to decrease the reactivity of Ti towards GaN, as evidenced in the low-temperature annealed samples. The mechanism, however, is different compared to the situation where the Al is only in the AlGaN. Which reaction takes place is related to the dominant diffusion process at the anneal temperature. At low anneal temperature, the Al-Ti intermixing process probably has a much lower-temperature onset and, once mixed, the Ti loses its reactivity towards AlGaN. The same mechanism explains the oxidation of the samples annealed at high temperature. At that specific temperature, oxidation has been the dominant process blocking all other reactions. Very likely the high annealing temperature is able to make the oxide layer, present on the surface of the nonannealed sample, oxygen transparent.

Electrical measurements are only given for the nonoxidized samples. Ti and Ti/Al on AlGaN/GaN, annealed at low temperature, have a specific contact resistance of 16.7 and 54.5 Ω mm, respectively (at 1 V). Current-voltage characteristics, however, are not linear. In the case of the Ti/Al contact, the AlGaN has been retrieved intact. Because of the insulating nature of AlGaN, this evidently leads to a bad non-Ohmic contact. The Ti contact annealed at high temperatures shows Ohmic behavior and has a specific contact resistance of 9.4 Ω mm. Current results thus indicate that an intermixed AlGaN layer is necessary to obtain Ohmic behavior. The rather bad contact resistance is thus attributed to some oxygen contamination. Electrical characteristics on GaN have not been measured because the GaN was nominally undoped. However, the Ti contacts will be inferior to the Ti/Al contacts: the presence of voids below the Ti contacts decreases the contact surface. This definitely increases the contact resistance.

In summary, it has been shown that Al, in all cases, reduces the reaction between Ti and GaN. The important points are: (i) Which metal preferentially forms (or keeps) a bond to the N atoms? (ii) Which process is dominant at the applied annealing temperature? Al in the AlGaN is able to maintain its bond with N and therefore N extraction by Ti becomes more difficult. Instead, Ti substitutionally replaces Ga, which is a much slower process. Al in the metallization scheme alloys with the Ti layer below. Alloyed Ti loses its reactivity towards GaN. The mechanisms revealed explain why an optimum Ti/Al relative thickness exists in the standard metallization scheme on GaN (for a certain annealing condition). Al should be present to decrease the aggressive Ti-GaN reaction. However, there should be enough Ti left to form the TiN layer at the interface. Too much Ti, on the other hand, leads to the formation of voids below the TiN. Regarding the contacts on AlGaN/GaN, it has been shown that the interfacial reaction, resulting in the formation of an Al-rich layer, is clearly different from the interfacial reaction on GaN. However, a proposal of guidelines for good contact formation on AlGaN/GaN will depend on how the electrical coupling between the metal and the two-dimensional electron gas occurs. A high Ti/Al relative thickness is required to penetrate through the AlGaN; a low Ti/Al relative thickness is needed for a reduced interface reaction.

The high oxidation in some samples is due to the fact that nonstandard contacts, without Au cap layer, have been used in this study. It may, however, be expected that the addition of Au will complicate the reaction mechanism because much more possible reaction pathways have to be considered.

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