Realization of improved metallization-Ti/Al/Ti/W/Au ohmic contacts to n-GaN for high temperature application

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Received 1 August 2004, accepted 12 October 2004
Published online 8 February 2005

PACS 68.37.Hk, 68.37.Lp, 73.40.Cg, 73.61.Ey

Tungsten metal layer was used for the first time as an effective diffusion barrier for the standard Ti/Al/Ti/Au ohmic metallization scheme to obtain thermally stable ohmic contact suitable for high temperature applications. Comparative studies were performed on three distinct metallization schemes: 1) standard GaN/Ti/Al/Ti/Au, 2) GaN/Ti/Al/W/Au, and 3) GaN/Ti/Al/Ti/W/Au. For the GaN with doping level of 5 × 10^{17} cm^{-3}, the lowest specific contact resistance for the Ti/Al/Ti/W/Au metallization scheme annealed in argon at 750 °C for 30 sec was 5 × 10^{-6} Ω cm^2, which is comparable to the standard Ti/Al/Ti/Au scheme. X-ray diffractions (XRD), auger electron spectroscopy (AES) depth profiling, field-emission scanning electron microscopy (FE-SEM), atomic force microscopy (AFM), and cross-sectional transmission electron microscopy (TEM) revealed that the Ti/Al/Ti/W/Au metallization has superior morphology and microstructural properties compared to standard Ti/Al/Ti/Au metallizations. Remarkably, this metallization was able to withstand thermal aging at 500 °C for 50 hrs with only marginal morphological and electrical deterioration. These studies revealed that the utilization of a compound diffusion barrier stack, as in the Ti/Al/Ti/W/Au metallization, yields electrically, structurally, and morphologically superior metallizations with exceptional thermal stability.

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1 Introduction
Success of III-Nitride devices depends largely on the realization of metal-semiconductor ohmic contacts, capable of reliable performance at high temperatures and/or high power levels. Various schemes have been studied for ohmic contact to n-GaN [1–5], the most common being the Ti/Al/Ti/Au (with Au being the top metal) contacts [3, 4]. Despite providing low contact resistances, Ti-Al based ohmic metallizations suffer from severe problems of intermetallic diffusions, oxide formation, rough surface morphologies, and poor thermal stability. Although the inter-diffusion and alloying of Ti and Al layers has been proven to be beneficial [4], in all cases it has been found that during annealing Ti and Al diffuse out towards the contact surface, where they form oxides, and also Au diffuses through the entire stack of metal layers towards the GaN interface. Both of these effects compromise long term thermal stability of these contacts. This article presents a novel metallization scheme that utilizes tungsten as a diffusion barrier layer. The rationale for using W as a barrier is based on the fact that binary phase diagrams of W with Au and Ti show that it has practically no solid solubility with Au at any temperature and limited solid solubility with Ti below ~740 °C and does not form intermetallics with both metals [6].

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cate that we have been able to realize an ohmic metallization scheme (Ti/Al/Ti/W/Au) for n-GaN with superior electrical, morphological and microstructural properties, which can provide a reliable solution for high temperature nitride electronics.

2 Experimental details The GaN samples were obtained commercially from Technologies and Devices International, Inc. The 7 µm thick GaN epilayer was grown by hydride-vapor-phase epitaxy on a 2 inch sapphire (0001) substrate. Hall measurement was carried out on the sample to extract the mobility and sheet carrier concentration. The mobility obtained at 296.2 K was 197 cm²/V·s. The sheet resistance and carrier concentration was about 50 Ω / square and 9.2 × 10¹⁷ cm⁻³. Prior to processing, the samples were cleaned using standard procedure [4]. Samples were then photolithographically patterned for circular TLM pads. Metal evaporation was done using an electron beam evaporator, with a base pressure of 2 × 10⁻⁸ Torr. Three different metallization schemes were prepared for comparison: Sample 1 (standard) had Ti/Al/Ti/Au (300Å/1000Å/300Å/300Å), sample 2 had Ti/Al/W/Au (300Å/1000Å/300Å/300Å) and sample 3 had Ti/Al/Ti/W/Au (300Å/1000Å/300Å/300Å/300Å) respectively with Au being the top metal layer for all cases. Metal lift-off produced circles with TLM spacings of 2, 5, 10, 15, 20, 25 and 30 µm.

Rapid thermal annealing (RTA) of the samples was then performed in UHP argon additionally gettered from oxygen. Four probe current-voltage (I-V) characteristics of the contact layers were measured before and after annealing using a KEITHLEY 238 Source-Measure Unit. The TLM analysis of contact resistance was performed for those contacts that had linear I-V characteristics. Auger electron spectroscopic depth profiles (AES) of the metallizations were obtained commercially. Phase analysis in the metallized samples was done using X-ray diffraction (XRD). The 0-2θ scans were collected on a standard diffractometer with CuKα radiation. Surface morphology was examined using a scanning electron microscopy (SEM) and atomic force microscopy (AFM). Microstructure of the contacts was studied using cross-sectional transmission electron microscopy (TEM).

3 Results and discussions As-deposited contacts for all three metallizations exhibited non-linear I-V characteristics, whereas annealing at 750 °C for 30 sec in Argon resulted in ohmic behavior for all. Table 1 summarizes the effect of annealing on the specific contact resistance, morphology and microstructure of the different metallizations. It is evident that both sample 1 (Ti/Al/Ti/Au) and sample 3 (Ti/Al/Ti/W/Au) had similar contact resistivity with the lowest value of 5.0 × 10⁻⁶ Ω·cm² for sample 3. It is worth mentioning that sample 2 (Ti/Al/W/Au), had irreproducible I-V curves after annealing, due to severe surface degradation. Hence, the design of sample 3 produced electrically superior ohmic contact properties compared to samples 1 and 2. All three as-deposited samples had smooth surface morphology with surface roughness in the range of 7-10 nm (5 µm × 5µm scale), which is the typical roughness of HVPE grown GaN. After annealing, sample 3 (Ti/Al/Ti/W/Au) had the lowest surface roughness of about 18 nm as compared to 22 nm for standard Ti/Al/Ti/Au metallization. The AES depth profile of sample 1 (Fig. 1a) revealed that significant intermetallic diffusion have occurred, notably indiffusion of Au towards GaN interface and outdiffusion of Al and Ti towards the contact surface, which is the possible cause of the severe degradation of the contact characteristics that occurred after additional thermal annealing at 500 °C for 50 hrs in vacuum. On the contrary, after annealing, sample 3 with the W-interlayer had much less metal interdiffusion as compared to sample 1 as seen from the AES depth profile in Fig. 1b. The elemental profile of the W layer remained practically unchanged as compared to the as-deposited sample. In addition, very limited indiffusion of Au and outdiffusion of Ti and Al occurred through the W-barrier. When thermally aged at 500 °C for 50 hrs in vacuum, sample 3 showed exceptional stability with marginal electrical and morphological deterioration. XRD confirmed the presence of unreacted Au in the annealed samples 2 and 3 by detecting Au 111 peak. However, while W interlayer fulfilled its role as a diffusion barrier in both samples 2 and 3, these samples were different in morphology and phases formed after annealing (see Table 1 and Fig. 1(b)-2(b)).

* Certain commercial equipments, instruments, or materials supplier are identified in this paper in order to specify the experimental procedure adequately and do not imply endorsement by NIST.
Table 1 Summary of contact characteristics after annealing at 750 °C for 30 sec.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Contact resistivity ($\Omega\cdot\text{cm}^2$)</th>
<th>RMS roughness (nm)</th>
<th>Phases detected in XRD</th>
<th>Phases and corresponding lattice parameters (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Au</td>
</tr>
<tr>
<td>#1 (Ti/Al/Ti/Au)</td>
<td>300Å/1000Å/300Å/300Å</td>
<td>5.8×10$^{-6}$</td>
<td>22</td>
<td>No</td>
</tr>
<tr>
<td>#2 (Ti/Al/W/Au)</td>
<td>300Å/1000Å/300Å/300Å</td>
<td>**</td>
<td>**</td>
<td>Yes (0.4081)</td>
</tr>
<tr>
<td>#3 (Ti/Al/Ti/W/Au)</td>
<td>300Å/1000Å/300Å/300Å/300Å</td>
<td>5.0×10$^{-6}$</td>
<td>18</td>
<td>Yes (*)</td>
</tr>
</tbody>
</table>

* The 111 Au peak is broad, therefore the parameter was not calculated
** The contact resistance was not measured due to the irreproducible nature of the I-V characteristics of the contacts; rms roughness was not measured due inhomogeneous surface with large “donut” -like formations with up to 20 µm in diameter
*** m indicates metastable cubic (Pm3m) structure of Al,Ti [PDF#49-1446]

Therefore it can be inferred that in the Ti/Al/W/Au metallization, part of the Al reacted with Ti and formed Al,Ti phase, while the remaining Al diffused through the W barrier into the Au and formed the Al,Au phase that developed into the “donut” -like features (not shown here). Interestingly enough, these “donut” formations in the Ti/Al/W/Au metallization are very similar to those observed in Ti/Al/Mo/Au metallization [5]. Thus the scheme, Ti/Al/W/Au, of sample 2 was disadvantageous in terms of both morphological and electrical properties, while the scheme 3, Ti/Al/Ti/W/Au, demonstrated smooth surface and superior contact resistance.

Fig. 1 (a) AES depth profile of Ti/Al/Ti/Au metallization annealed at 750 °C for 30 sec.

Cross-section TEM analysis of the annealed sample 1 revealed rough interfaces with voids formed both at the GaN/metal interface and inside of metal layers (not shown), while cross-section of sample 3 in Fig. 3 had planar interfaces with no voids. Planar interfaces in sample 3 correlate well with the smooth contact surface as determined from AFM and SEM. Analysis of interfacial layers in samples 1-3 with SAD and EDS in HRTEM is currently in progress. Based on preliminary SAD and EDS in combination with the XRD and AES data, the layers in sample 3 were identified (Fig. 3, from bottom up) as GaN, TiN, Al,Ti(m), W and Au-rich cap layer.
4 Conclusion A novel metallization (Ti/Al/Ti/W/Au) for n-GaN has been successfully realized to yield improved contact characteristics, which are superior to standard Ti/Al/Ti/Au Ohmic metallization for n-GaN. Newly developed contacts not only performed equally well electrically, also had smoother morphology and favourable microstructure (less metal intermixing) for high temperature reliable operation.

Acknowledgements Authors would like to acknowledge Sandy A. Claggett of NIST for TEM sample preparation.

References