Study of Scandium Based Ohmic Contacts to AlGaN/GaN Heterostructures

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Abstract. Development of semiconductor devices based on AlGaN/GaN heterostructure requires study and improvement of ohmic contacts, whose necessary improvement lies in process of checking new metallic compositions and thermal formation process parameters. Usually, in metallic ohmic annealed contacts of AlGaN/GaN heterostructures, titanium is applied as the first layer, but scandium may be an alternative. It was proved to be useful to obtain both ohmic and Schottky characteristics, depending on annealing temperature of the contact. In the presented research, contacts including scandium (Sc/Al/Mo/Au) were fabricated, and, as reference sample, contacts with titanium including metallization (Ti/Al/Mo/Au). Reference sample was annealed at 825°C, and forming temperatures for scandium contacts were 825°C, 625°C, and 425°C. All samples after thermal formation process were additionally thickened with Ru/Au bilayer. To quickly compare level of metals in metallization mixing during formation process and to check applicability of EDS (Energy-Dispersive X-ray Spectroscopy), the simulations of electrons trajectories and EDS point scans were performed.

Keywords

AlGaN/GaN, ohmic contact, scandium.

1. Introduction

Fabrication of ohmic contacts has few purposes. One of them is to obtain as low contact resistivity as possible. The other is to simplify preparation process keeping contact’s parameters repeatability. One solution is to look for contact’s multilayer metallic scheme and its preparation conditions resulting in the best electrical and physical parameters. Usually, contact’s composition consists of few metals chosen according to their properties. Probably annealed ohmic contacts gain ohmic characteristics due to two processes. One of them is formation of nitrogen vacancies during annealing process. Nitrogen is absorbed by the first contact’s layer - titanium that also absorbs oxygen from heterostructure’s surface and improves adhesion of contacts to semiconductor. Another process resulting in ohmic characteristics is probably diffusion of aluminium through AlGaN/GaN heterostructure, which allows to generate metallic connection between 2DEG (Two Dimensional Electron Gas) and contact’s metallization. The role of other layers in contact’s composition is to protect the mentioned Ti and Al layers, simultaneously allowing to get low-resistance electrical connection with devices outside contact’s structure (Au), and to protect the rest of the contact from gold diffusion during formation process (Mo). Although Ti plays its role well, its work functions suggest obtaining slightly rectifying contacts with n-dopped AlGaN/GaN heterostructure.

There are few metals that have lower work function and should also allow to fabricate ohmic contacts to used semiconductor. One of them is scandium. Although its parameters suggest possibility of good effect on ohmic contacts parameters, there are not many studies made on scandium applicability to ohmic contacts to AlGaN/GaN heterostructures production [2]. More, but still only few works, present
research on scandium usage in ohmic contacts production to n-GaN \cite{2} and \cite{3}. These suggest various behaviour of scandium contacts depending on formation temperature. In the mentioned works, scandium in metallizations is used as monolayered contact or covered only with gold. Only characteristics of contacts are checked. Electrical parameters are not presented. To use this metal in ohmic contacts, finding proper metallization scheme and formation conditions is necessary. According to this research, metallization scheme used in samples’ preparation was the same as in the case of titanium-including devices: Sc/Al/Mo/Au. As reference samples, Ti/Al/Mo/Au metallization scheme contacts were prepared \cite{4} and \cite{5}.

In process of HEMT (High Electron Mobility Transistor) fabrication, or other devices based on AlGaN/GaN heterostructure including ohmic contacts, process of deposition of additional gold layer is important. Role of additional layer is to reduce sheet resistance. Because of heating process of metallic multilayer composed of thin layers, the metallization ingredients melt partially, although their melting temperature is usually higher than RTP (Rapid Thermal Processing) temperature; except aluminium with melting point of 660 °C. For other metals, melting points are: 1066 °C for gold, 1651 °C for scandium, and 1541 °C for molybdenum. In different RTP conditions and using different thicknesses of layers, metallization remelts differently. Remelting and alloy formation in metallization have negative effect on sheet resistance, surface condition and, in extreme cases, contact may be damaged. Contact destruction occurs when gold atoms diffuse into heterostructure. To protect contact from this negative effect, stopping layer is used. In this case, it is Mo layer. As it was mentioned, Mo has melting point equal to 2623 °C, almost 1000 °C higher than the highest melting point of other used metals. But in melting process, aluminium dissolves other metals - titanium or scandium and molybdenum. Highly diffusive gold mixes partially with Mo layer. In effect, agglomerates of metals occur. Gold layer mixed with molybdenum layer does not protect contact as well as pure gold. Electrical parameters of metallization change. Usually, sheet resistance increases. Reduction of sheet resistance may be obtained by deposition of additional gold layer. However, adhesion of gold to contact metallization, despite the last gold layer, is weak. Adhesion improving the layer should be used. In this work, ruthenium was used as adhesion layer.

2. Sample Preparation

All steps in contacts’ fabrication were the same for all samples, except formation temperatures and first metal deposited in contacts’ multilayer. Studied samples were AlGaN/GaN heterostructures grown by MOVPE (Metalorganic Vapor Phase Epitaxy) process. Mesa structures were etched by RIE (Reactive Ion Etching) process using Cl2/BCl3/Ar plasma to the fabricated TLM (Transfer Length Method) test structures. Then, in PVD (Physical Vapor Deposition) process, the following metallization multilayers were deposited:

- Ti (23 nm)/Al (100 nm)/Mo (45 nm)/Au (190 nm),
- Sc (23 nm)/Al (100 nm)/Mo (45 nm)/Au (190 nm).

Then, samples were annealed in RTP process. Annealing time for all samples was 60 s. Temperatures were 825 °C for Ti/Al/Mo/Au metallizations and 825 °C, 625 °C and 425 °C for Sc/Al/Mo/Au metallizations. Then, after formation process, a Ru (30 nm)/Au (190 nm) bilayer was deposited.

3. Measurements and Results

For photolithography process during samples’ preparation, as flat metallization surface as possible is important. Agglomerates and remelting in contact’s metallization, affecting contact’s electric parameters, influence also lift-off process used to produce thickening layer in the specific areas. Insufficiently flat surface prevents proper coverage sample with resist and thus, problems with necessary resist thickness, coverage and finally with shape of thickening layer may occur. To check samples’ surfaces after RTP process, samples were examined by SEM (Scanning Electron Microscope) microscope (Fig. 2). Samples containing titanium have the lowest sheet resistance (Tab. 1)
Table 1: Electrical parameters of contacts.

<table>
<thead>
<tr>
<th>Metallization</th>
<th>RTP temp. (°C)</th>
<th>Deposited $R_s$ ($\Omega \cdot \square^{-1}$)</th>
<th>Annealed $R_s$ ($\Omega \cdot \square^{-1}$)</th>
<th>$\rho_c$ ($\Omega \cdot \text{cm}^2$)</th>
<th>Thickened $R_s$ ($\Omega \cdot \square^{-1}$)</th>
<th>$\rho_c$ ($\Omega \cdot \text{cm}^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ti/Al/Mo/Au</td>
<td>825</td>
<td>0.66</td>
<td>1.54</td>
<td>1.39 $\cdot 10^{-4}$</td>
<td>0.44</td>
<td>1.21 $\cdot 10^{-4}$</td>
</tr>
<tr>
<td>Sc/Al/Mo/Au</td>
<td>825</td>
<td>0.68</td>
<td>1.92</td>
<td>3.52 $\cdot 10^{-3}$</td>
<td>0.44</td>
<td>3.50 $\cdot 10^{-3}$</td>
</tr>
<tr>
<td>Sc/Al/Mo/Au</td>
<td>625</td>
<td>0.78</td>
<td>2.19</td>
<td>6.40 $\cdot 10^{-3}$</td>
<td>0.98</td>
<td>4.40 $\cdot 10^{-3}$</td>
</tr>
<tr>
<td>Sc/Al/Mo/Au</td>
<td>425</td>
<td>0.79</td>
<td>1.68</td>
<td>non-ohmic</td>
<td>0.96</td>
<td>non-ohmic</td>
</tr>
</tbody>
</table>

Fig. 2: Samples after RTP process (upper) and after thickening (bottom): a) Ti/Al/Mo/Au (RTP: T=825 °C), b) Sc/Al/Mo/Au (RTP: T=825 °C), c) Sc/Al/Mo/Au (RTP: T=625 °C), and d) Sc/Al/Mo/Au (RTP: T=425 °C).

and their surface is characterized by specific remelting on metallization’s edges (Fig. 2(a), upper). All samples including scandium look similar. All of them show metallic agglomerates. Differences are in agglomerates’ size and amount. Metallization of sample annealed at 825 °C seems to be flatter than others. On SEM images, it is visible that decrease in RTP temperature increases the number of metallic agglomerates.

New metallization adhesion to AlGaN/GaN heterostructure turned out to be good. During contact’s preparation process, metallization didn’t detach from semiconductor and edges are not folded up. To compare scandium and titanium adhesion, additional research should be conducted.

Sheet resistance of Sc including samples is the lowest in the case of samples heated to 425 °C (Tab. 1). Increase to 200 °C causes sheet resistance to increase. Further increase of 200 °C allows to reduce sheet resistance but not so much as at 425 °C. The lowest sheet resistance of all prepared samples occurred in the case of reference samples. In the case of contact’s resistivity, the lowest one was obtained for reference sample (Ti/Al/Mo/Au, RTP: T=825 °C, see Tab. 1).

The samples with scandium including metallization formed at 425 °C turned out to have non-ohmic characteristics. Samples formed at 625 °C had resistivity of contacts equal to 5.40 $\cdot 10^{-3}$ ($\Omega \cdot \text{cm}^2$). Increase in RTP temperature of next 200 °C reduced resistivity 1.6 times (3.52 $\cdot 10^{-3}$ $\Omega \cdot \text{cm}^2$) but characteristics of contacts obtained at lower temperature had lower deviation from linear characteristics than in the case of sample heated to higher temperature.

Despite the different contact’s resistivities, the characteristics of scandium-including samples annealed at 825 °C and 625 °C were similar. To check if there were differences in characteristics not evident on I-V plot, the differential graph for examined samples was drawn (Fig. 3(c)). It was observed that deviation from linear characteristics is higher in the case of scandium-including sample formed at 825 °C than in the case of the sample with the same type of metallization annealed at 625 °C. The same measurements were taken for samples after deposition of Ru/Au bilayer (thickened). In Tab. 1, sheet resistance results for samples after Ti/Al/Mo/Au and Sc/Al/Mo/Au deposition before RTP process were also included.

Nonohmic characteristics of deposited contacts were not included to be presented in Tab. 1 results. To check metallization surface difference between annealed samples and thickened samples, SEM photos of samples after Ru/Au deposition were included (Fig. 2). Deposition of the Ru/Au thickening layer resulted in decreased sheet resistance for all samples. Similar sheet resistance was obtained for both, Ti and Sc in-
Fig. 3: I-V characteristic for annealed samples (a), I-V characteristics for thickened metallization samples (b) and differentials for annealed samples (c).

Tab. 2: EDS measurements of composition of formed (F) and thickened (T) metallizations. Quantities in % of atoms.

<table>
<thead>
<tr>
<th>Element</th>
<th>F 825 °C</th>
<th>T 825 °C</th>
<th>F 625 °C</th>
<th>T 625 °C</th>
<th>F 425 °C</th>
<th>T 425 °C</th>
</tr>
</thead>
<tbody>
<tr>
<td>O</td>
<td>14.5</td>
<td>2.5</td>
<td>24.6</td>
<td>3.7</td>
<td>15.3</td>
<td>4.2</td>
</tr>
<tr>
<td>N</td>
<td>9.4</td>
<td>9.6</td>
<td>11</td>
<td>15.5</td>
<td>13.5</td>
<td>17.8</td>
</tr>
<tr>
<td>Ga</td>
<td>5.1</td>
<td>1.4</td>
<td>6.5</td>
<td>1.7</td>
<td>1.3</td>
<td>1.2</td>
</tr>
<tr>
<td>Ti</td>
<td>8.3</td>
<td>0.2</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>Sc</td>
<td>–</td>
<td>–</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
</tr>
<tr>
<td>Al</td>
<td>18.8</td>
<td>2.2</td>
<td>14.4</td>
<td>1.5</td>
<td>21.6</td>
<td>2.2</td>
</tr>
<tr>
<td>Mo</td>
<td>13.2</td>
<td>3.9</td>
<td>9.3</td>
<td>3.1</td>
<td>12.6</td>
<td>3.4</td>
</tr>
<tr>
<td>Au</td>
<td>30.7</td>
<td>78.8</td>
<td>33</td>
<td>72.4</td>
<td>35.5</td>
<td>68.7</td>
</tr>
<tr>
<td>Ru</td>
<td>–</td>
<td>1.4</td>
<td>–</td>
<td>1.9</td>
<td>–</td>
<td>2.3</td>
</tr>
</tbody>
</table>

Fig. 4: Monte Carlo simulations of electron traces in metallic compositions: a) Sc/Al/Mo/Au, b) Ti/Al/Mo/Au, c) thickened Ti/Al/Mo/Au, and d) thickened Sc/Al/Mo/Au. Simulations are for not thermally formed compositions.

Inclucing samples formed at 825 °C and it was equal to 0.44 (Ω·□⁻¹).

Additionally, to test EDS point scan applicability to compare the atoms’ diffusion and metallization remelting level in contacts, the EDS scans were performed and compared to simulations of electrons trajectories in metallic contact multilayer composed of pure metals. The elements and their contents in metallizations of examined contacts are presented in Tab. 2. It is difficult to define the depth of EDS scan, which is different for each metal and varies in metallic composition due to formation process. However, depth of EDS scan for annealed metallization should be similar to pure metal composition. To check possible EDS scan depth and possible trajectories of electrons in metallic contact composed of pure metals, the simulations were performed in CASINO software. An electron beam with energy 15 keV was simulated, i.e., the same as in the case of EDS scan of samples. Results of electrons’ trajectories are presented in Fig. 4. The sample formed in 425 °C is the most similar to not annealed sample, and to simulated compositions, because and during RTP process none of metallization metals is a fluid.

The lowest melting point is for aluminium (660 °C). As presented in Fig. 4(a) and Fig. 4(b), electron trajectories are mainly in gold layer, partially in molybdenum and aluminium layers. Scandium layer is thin and small number of electrons reaches this layer. Contrary, heterostructure layer is thick, so probability of obtaining signals from heterostructure is high. Metal’s atoms diffusion increases with the increasing temperature. Scandium, not detected in sample formed at 425 °C, is detected in the same level in samples formed at higher temperatures and in samples after thickening process. This does not mean diffusion of scandium atoms during thickening process. It is a result of different shape of elements’ signals obtaining.
volume. Gold quantity difference between all formed metallizations suggests increase of gold diffusion and metals mixing with RTP temperature growth. Also, during formation process, metals from heterostructure diffuses into mettallization, which is reason for gallium and nitrogen presence in metallization. High presence of titanium in Ti/Al/Mo/Au metallization after formation, its low presence after thickening, and low scandium quantity in all measurements suggest the higher titanium than scandium diffusion in thermal formation process.

4. Conclusion

Results of research on metallization composition of ohmic contacts to AlGaN/GaN heterostructure including scandium showed possibility of obtaining good ohmic contacts formed at lower temperature, than in the case of Ti/Al/Mo/Au metallization scheme. However, nonohmic characteristics make Sc/Al/Mo/Au metallization annealed at 425 °C unusable to produce ohmic contacts. It is possible that modification of metallic layers’ thickness would allow using low temperature in ohmic contacts to AlGaN/GaN heterostructures’ fabrication process. Both resistivity of contacts and sheet resistances suggest the best parameters for Sc including samples possible to be obtained in contacts formation at temperatures between 625 °C and 825 °C. In future research, these samples should be fabricated and examined.

Surface’s look suggests that to obtain surface of metallization as flat as possible, the temperatures of annealing should be closer to 825 °C than 625 °C. With RTP process temperature reduction, the final sheet resistance raised after additional layer deposition. It means that additional bilayer does not change sheet resistance to the specific value but interacts with previously fabricated contact and its mettallization. The same sheet resistances compared to sheet resistances of contact’s metallizations before thermal formation process show that although every metallic composition has specific sheet resistance (Ti/Al/Mo/Au - 0.66 (Ω · □^{-1}), Sc/Al/Mo/Au - 0.78 (Ω · □^{-1})), the final sheet resistance (after thickening of contact’s mettallization) is dependent on the previous thermal formation conditions and its dependence on metallic scheme may be negligible. Contact resistivity reduction after Ru/Au deposition seems to be interesting. Additional layer should not influence the formed contact’s resistivity, because contact’s parameters are set due to reactions between metallization and AlGaN/GaN heterostructure in formation process. Additional layers do not react with previously prepared contact and its mettallization. However, measures show differences in resistivity of contacts in 19 % in the case of Sc/Al/Mo/Au mettallization formed at 625 °C. Samples formed at 825 °C for both Ti and Sc metals have small difference in contact’s resistivity before and after thickening, which may be negligible. However, because no mettallization schemes, especially using scandium, produce ohmic contacts to AlGaN/GaN heterostructures, more research should be made to find the best metallic composition and formation conditions. Experiment shows a possibility of reduction of formation temperature to 625 °C. However, not only temperatures between 625 °C and 825 °C are proper to produce ohmic contacts using scandium as the first metallic layer. Different mettallization composition formed at lower temperature like 425 °C, for example with thin scandium layer, may be useful.

Diffusion raises with temperature growth, so lower temperature allows to obtain similar diffusion level between heterostructure, Sc and Al layers. Therefore, the thin scandium layer would allow atoms between all three layers to diffuse faster and allows to reduce temperature needed to fabricate ohmic contacts using scandium. Effects of temperature influence on diffusion level are presented in Tab. 2. Titanium turned out to be more diffusive than scandium, and its amount in proper metallization is 8.3 % before thickening, and 0.2 % after thickening process. It may suggest using scandium, whose diffusion rate and presence in other layers may be more predictable than of titanium. Ruthenium quantity increases with decrease in temperature of RTP, but these layer parameters are the same for all samples deposited in one process. Differences include different shape of volume, from which EDS scan gets specific for atoms signals. The EDS scan is good method for homogenous metallic alloys. Contrary, when forming the multilayer alloy at high temperature, the result may be useful for fast comparison of similar samples, but not to check depth of presence of elements’ atoms.

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Author Contributions

G.I. and W.M. carried out the experiment, G.I. wrote the manuscript with the assistance of W.M. and R.P. G.I., W.M., J.P.-C. and A.S. conducted device processes for test structures fabrication. G.I. and W.M. formulate the original idea. R.P. supervised the project.

References


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