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Anti-diffusion barriers for gold-based metallizations to p-GaN

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ABSTRACT

We propose a new metallization scheme to p-GaN, where thin-film transition metal nitrides have been applied to improve thermal stability of gold-based metallization. In this metallization scheme the Pd/Au bilayer was used to form low-resistivity ohmic contact to p-GaN, while Ta-Si-N, Ti-Si-N, and Ti-W-N anti-diffusion barriers were used to protect contact metallization from interaction with Au overlayer. We present the details of optimization of process parameters of barrier layer fabrication and show that $Ta_{0.34}Si_{0.25}N_{0.41}$ and $Ti_{0.26}Si_{0.0.17}N_{0.57}$ thin films fabricated by reactive magnetron sputtering show excellent barrier properties under high temperature stress.

INTRODUCTION

Great interest exists in GaN and related materials since the successful demonstration of optoelectronic devices operating at short wavelengths such as blue and green LEDs and LDs. The formation of stable and reliable ohmic contacts has been a problem in achieving good performance of these devices. This is especially true for p-type ohmic contacts for LDs where high current levels are required and where internal heating still limits their output power and lifetime.

To date, there have been basically two approaches to obtain low resistance ohmic contact to p-type GaN [1]. The first one was to optimise the properties of semiconductor sub-contact region; either by increasing Mg doping during the p-GaN growth or by applying an additional semiconductor structure such as p-AlGaN/p-GaN superlattice [2], p-InGaN/p-GaN superlattice [3], or single-layer low-band-gap p-InGaN [4]. The second one is to optimise contact metallizations itself: choice of material, procedure of semiconductor surface pre-treatment, the parameters of metal deposition and post-deposition heat treatment (temperature, time, atmosphere) [5, 6]. Au and Au-based alloys/multilayers remain the most commonly applied materials for metallization systems in GaN-based device technology. These include making ohmic contacts as well as metal overlayers for bonding and interconnection purposes. In particular, Au-based metallizations such as NiAu or PdAu metallization have been proven to give low resistivity ohmic contact to p-GaN lacking however stability at elevated temperatures [7].

In this work an approach has been undertaken to solve this problem by using anti-diffusion barriers. To be applicable, these thin-film materials must fulfil specific requirements of: high thermal stability, high electrical conductivity, high resistance to corrosion, and compatibility with processes of device fabrication. In search for effective anti-diffusion barrier, conducting amorphous films have been considered as the most promising ones [8]. This is because, owing to the lack of grain boundaries, fast diffusion path are eliminated in such materials. In this respect, transition-metal (TM) nitrides have been taken into consideration including thin films of Ta-Si-N, Ti-Si-N, and Ti-W-N fabricated by reactive magnetron sputtering. The main goal of our work was to evaluate applicability of these materials as anti-diffusion barriers layer in three level metallization system in which they were to protect Pd/Au ohmic contact from thermally activated interaction with Au overlayer.

EXPERIMENTAL PROCEDURE

The p-GaN samples used in these experiments were grown by MOCVD on sapphire substrates. The major part of our experiments involved the use of p-GaN:Mg films with hole concentration of $3x10^{17}$ cm^{-3}. In order to examine the influence of sub-contact semiconductor region on the electrical quality of ohmic contact, samples with additional layer of degenerately doped p^+-GaN or p^+InGaN were used. A number of experiments, especially those concerning development of barrier material were performed using semi-insulating (100) GaAs substrates. (20 nm) Pd/(130 nm) Au bi-layer was chosen as contact metallization to p-GaN. It was prepared by DC magnetron sputtering for elemental targets of 5N purity in Ar^+ plasma. Barrier layers (BL) of Ta-Si-N, Ti-Si-N, and Ti-W-N were fabricated by reactive magnetron sputtering in Ar/N_2 plasma using compound targets, Ta_5Si_3, Ti_5Si_3, Ti(10%)W(90%), respectively. The thickness of Au overlayer was 50 - 100 nm. Heat treatment experiments were carried out at temperatures ranging from 300 to 900^{o}C under Ar or N_2 flow in a RTP unit.

Electrical characterisation of metal/semiconductor contacts involved measurements of I-V characteristics for rectifying contacts and of the specific resistance, by circular transmission line method, for ohmic contacts. The influence of basic process parameters on the composition, crystalline structure, electrical and mechanical properties of barrier layers have been studied by using RBS, XRD, electrical resistivity and stress measurement techniques. Four-point-probe was used to measure electrical resistivity; Tencor FLX-2320 was used to evaluate thin film stress. The effectiveness of TM-nitride layers as anti-diffusion barriers for Au was examined by measuring RBS compositional profiles and electrical resistivity of complex metallization schemes together with XTEM imaging of their microstructure.

RESULTS AND DISCUSSION

Contact metallization to p-GaN for low-resistivity ohmic contacts

Our preliminary studies on ohmic contacts to p-GaN suggested that Pd/Au metallization is the most promising one as far as low resistivity of metal/semiconductor contact is concerned [9]. In this work we show (Table 1) that the resistivity of p-GaN/Pd/Au contacts strongly depends on both, the properties of semiconductor sub-contact region and the parameters of post-deposition heat treatment. As-deposited contacts are nonlinear when formed on lightly doped p-GaN and become ohmic after heat treatment at 300^{o}C for 3 min. Pd/Au contacts to highly doped p^+-GaN or p^+-GaInN are ohmic in as-deposited state and their specific resistance reaches a minimum when annealed in N_2 at 300^{o}C for 3 min. Heat treatment at higher temperature, $\geq$ 400^{o}C causes an increase of the specific resistance of all Pd/Au contacts under investigation.

Table.I. The effect of the composition of semiconductor sub-contact region and of the post-deposition heat treatment on the specific resistance of p-GaN/(20 nm) Pd/(130 nm) Au contacts.

Structure	Subcontact layer	Metallization	Heat treatment	r_c [Ωcm^2]
GaN : Mg Substrate	without subcontact layer $p = 3x10^{17} at/cm^3$	Pd/Au 20/130 nm	as deposited	nonohmic
			300ºC / 3 min. / N_2	$\sim 1{\cdot}10^{-3}$
			400ºC / 3 min. / N_2	$1 - 2{\cdot}10^{-3}$
GaN : Mg GaN : Mg Substrate	p^+-GaN N_{Mg} >$2x10^{19} at/cm^3$ d = 15 nm	Pd/Au 20/130 nm	as deposited	$4{\cdot}10^{-5} - 1{\cdot}10^{-4}$
			300ºC / 3 min. / N_2	$7x10^{-6} – 5x10^{-5}$
			400ºC / 3 min. / N_2	$4 – 9x10^{-5}$
InGaN GaN : Mg GaN : Mg Substrate	p^+-InGaN/p^+-GaN X_{In} = 0.2, d = 2 nm	Pd/Au 20/130 nm	as deposited	$1x10^{-5}$
			300ºC / 3 min. / N_2	$4x10^{-5}$
			400ºC / 3 min. / N_2	$5x10^{-5}$

The results of RBS profiling (Fig. 1) indicate that Pd and Au form separate layers in as-deposited contact. Under mild annealing intermixing of Pd and Au is observed without however visible interaction with semiconductor sub-contact region. Further increase of the temperature of heat treatment activates metal/semiconductor reaction and leads to pronounced penetration of fully reacted metallization into semiconductor sub-contact region.

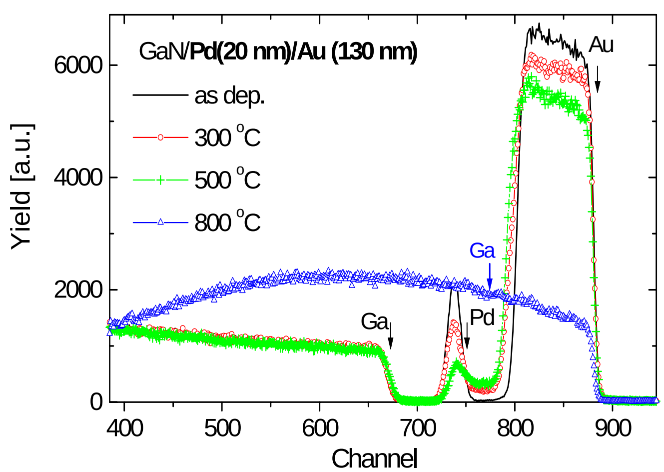

Figure 1. 2 MeV He^+ RBS spectra of p-GaN/(20 nm) Pd/(130 nm) Au contact under heat treatment in Ar flow.

These results as a whole prove that Pd/Au metallization enables fabrication of low resistance ohmic contacts to p-GaN but possesses only limited thermal stability. This may have detrimental effect on long-term device performance, especially when thick Au overlayers are to be applied.

Amorphous thin-film TM-nitrides for anti-diffusion barriers

Plasma composition and RF power have been found to be the main parameters of sputter deposition process affecting chemical composition and crystalline structure of TM-nitride films with direct impact on their electrical, mechanical, and barrier properties. While an increase of N_2 flow (or N_2 partial pressure) during nitride deposition enables obtaining thin film materials with higher nitrogen content, an increase of RF power has opposite effect. These relationships are shown on Fig. 2 for Ta-Si-N films. Similar dependencies have been obtained for Ti-Si-N and Ti-W-N films. Due to these interplays, a compromise was necessary when optimizing process parameters in order to obtain highly conducting amorphous nitrides. The influence of plasma composition on the electrical resistivity and stress is illustrated in Fig. 3. It should be noted that TM nitride films exhibit relatively high compressive stress, characteristic for high melting point materials. Thus stress minimizing has been taken into consideration when setting the final process parameters.

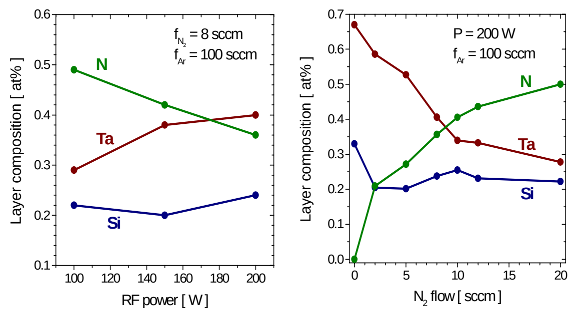

Figure 2. Influence of RF power and N_2 flow on the composition of Ta-Si-N films.

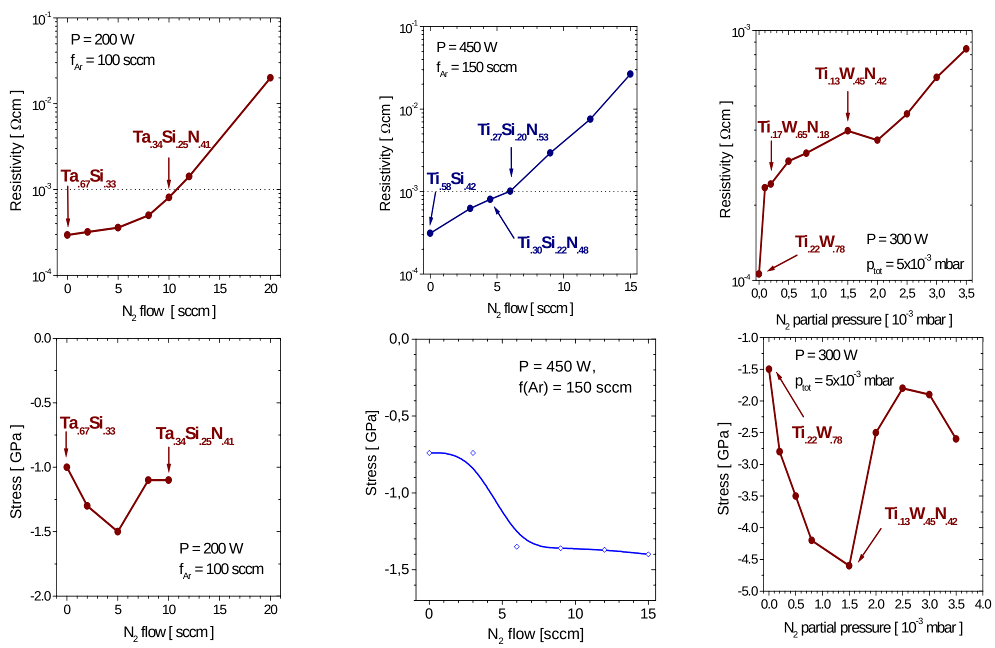

Figure 3. Influence of plasma composition (N_2 flow/N_2 partial pressure) on the resistivity and stress in Ta-Si-N, Ti-Si-N, and Ti-W-N films.

XRD analyses have shown that as-deposited Ta-Si-N and Ti-Si-N films incorporating approx. 2 at.% of silicon and at least 50 at.% of nitrogen are amorphous and keep such structure after heat treatment at temperature up to 800^{o}C and 750^{o}C, respectively. As for Ti-W-N films, homogeneous amorphous structure has been obtained for material having 14-17 at. % of Ti and at 18-30 at.% of nitrogen, and are being preserved after heat treatment at temperature up to 700^{o}C.

Taking into account these results two barrier materials has been chosen for further investigation. These were $Ta_{0.34}Si_{0.25}N_{0.41}$ and $Ti_{0.26}Si_{0.0.17}N_{0.57}$ applied in multilayer metallization scheme Pd/Au/BL/Au on p-type GaN.

Multilayer metallization Pd/Au/BL/Au to p-GaN

Fig. 4 shows the influence of heat treatment on RBS compositional profiles of p-GaN/Pd/Au/$Ta_{0.34}Si_{0.25}N_{0.41}$/Au and p-GaN/Pd/Au/$Ti_{0.26}Si_{0.0.17}N_{0.57}$/Au contacts. The most important feature to be pointed out is that high temperature annealing weakly influences the height of the RBS signal from top Au metallization and the position of high-energy edge of Ga signal. These give evidence that thermally activated interfacial reaction is restricted to the contact metallization Pd/Au and indicate that both barrier materials effectively suppress gold diffusion from top over-layer into the metal/semiconductor contact region.

The results of TEM analysis are consistent with those of RBS. XTEM micrographs of annealed p-GaN/Pd/Au/$Ta_{0.34}Si_{0.25}N_{0.41}$/Au contacts (Fig. 5) prove that the presence of barrier layer slows down the interaction between Pd and Au in the contact metallization when annealed at 400^{o}C and protects the contact region form interaction with the Au over-layer during annealing at 800^{0}C.

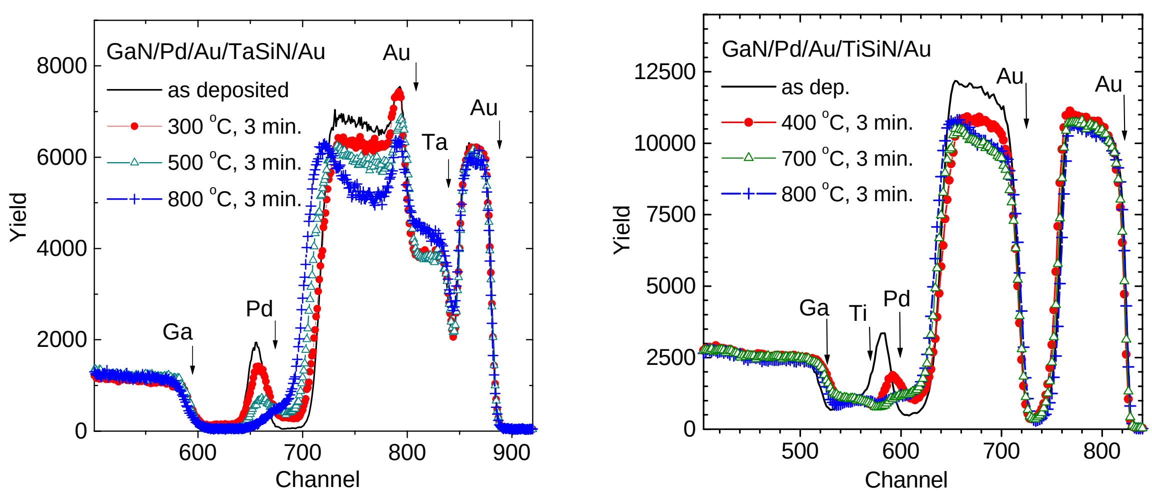

Figure 4. 2 MeV He^{+} RBS spectra of (20nm)Pd/(130nm)Au/(100nm)$Ta_{0.34}Si_{0.25}N_{0.41}$/(50nm)Au and (20nm)Pd/(130nm)Au/(100nm)$Ti_{0.26}Si_{0.0.17}N_{0.57}$/(100nm)Au contacts to p-GaN under heat treatment for 3 min. in Ar ambient at temperatures up to 800^{o}C.

a) b)

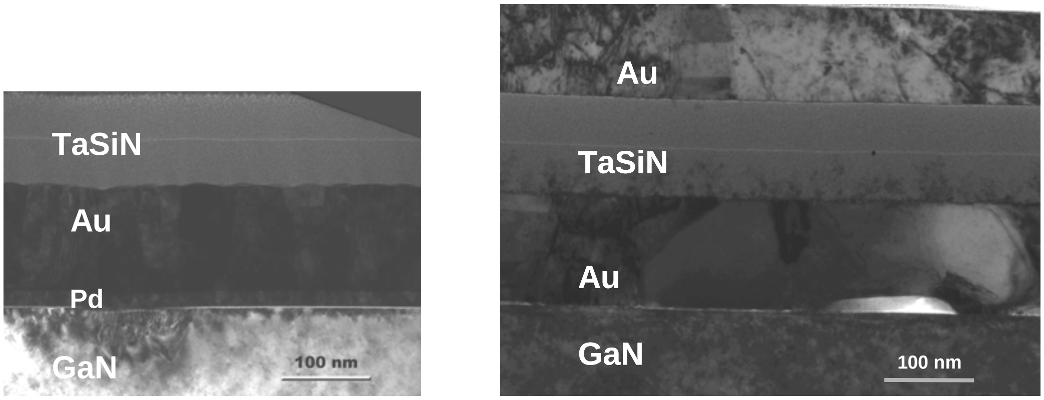

Figure 5. XTEM micrographs of (20nm)Pd/(130nm)Au/(100nm)$Ta_{0.34}Si_{0.25}N_{0.41}$/(100nm)Au contact to p-GaN heat treated in Ar ambient for 5 min. at temperature 400^{o}C (a) and 700^{o}C (b).

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