Barrier Height Variation in Ni-Based AlGaN/GaN Schottky Diodes

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***Abstract*— In this paper, we have investigated Ni-based AlGaN/GaN Schottky diodes comprising capping layers with silicon-technology-compatible metals such as TiN, TiW, TiWN, and combinations thereof. The observed change in Schottky barrier height of a Ni and Ni/TiW/TiWN/TiW contact can be explained by stress effects induced by the TiW/TiWN/TiW capping layer, rather than by chemical reactions at the metal–semiconductor interface. Secondary-ion mass spectroscopy and transmission electron microscopy techniques, for samples with and without a TiW/TiWN/TiW cap, have been used to show that no chemical reactions take place. In addition, electrical characterization of dedicated samples revealed that the barrier height of Ni/ TiW/TiWN/TiW contacts increases after stepwise selective removal of the TiW/TiWN/TiW cap, thus demonstrating the impact of strain.**

***Index Terms*— AlGaN/GaN, diode, Schottky barrier height (SBH), strain, stress.**

I. Introduction

DEVICES based on AlGaN/GaN are suitable candidates for high-voltage and high-speed electronics due to the GaN material properties such as wide bandgap, large breakdown field, high electron saturation velocity, and good thermal conductivity [1]. The interest in this material system really took off after development of the GaN-on-Si technology, where few-micrometer-thick epitaxial active GaN layers are deposited on silicon (111) wafers by using transition layers that mitigate differences in lattice constants and coefficients of thermal expansion [2], [3]. However, the GaN device technology has by far not reached the same maturity level as Si, and many aspects of the device behavior are still not fully understood. One example is the formation of the Schottky barrier, especially in terms of defining the barrier height [4]. In AlGaN/GaN technology the commonly used Schottky metal is nickel (Ni) [5]–[7] due to its high barrier on GaN and low resistivity. However, Ni by itself suffers from different problems related to the complete device processing flow. For example, when aluminum (Al) is used in the back-end processing to make contacts, it can readily diffuse into Ni and adversely affect the Schottky contact properties [8]. In addition, Ni often suffers from delamination caused by different processing steps and to prevent that, different metal capping layers may be used. In III–V technology, the metal of choice for that protective layer is typically gold [6], [9]. Unfortunately, gold is strictly forbidden in industrial silicon (Si) fabs and it has to be replaced with another Si compatible metal or alloy to allow cost-effective production. These requirements prompted investigation of different metals used in Si fabs, such as titanium–nitride (TiN), titanium–tungsten (TiW), TiW(N), and combinations thereof for the capping layer on Ni.

In this paper, we have observed that Ni contacts with a TiW/TiWN/TiW capping layer, from here referred to as the TiW(N) layer, often have lower Schottky barrier height (SBH) than Ni-only contacts. This is visible in the exemplary set of devices in Fig. 1 where the I–V characteristic for Ni Schottky contact shows lower saturation hence leakage currents.

The thermionic current–voltage relationship of a Schottky barrier diode, neglecting series and shunt resistance, is given by [10]

$$I = AA^*T^2 e^{-\frac{q\Phi_B}{kT}}\left(e^{-\frac{qV}{nkT}} - 1\right) = I_S\left(e^{-\frac{qV}{nkT}} - 1\right) \quad (1)$$

where I_s is the saturation current, A is the diode area, A^* is the Richardson's constant, Φ_B is the SBH, and n is the ideality factor.

The SBH is calculated from the saturation current which is determined by extrapolating the thermionic emission (exponential part) of the forward-biased current–voltage I–V curve to $V = 0$ [as described in (1)]. The ideality factor is determined from the slope of the same plot.

According to the Schottky–Mott rule [10], the SBH of a contact is solely dependent on the metal work function and semiconductor electron affinity in vacuum; therefore, it should be determined by bulk properties of Ni and GaN only. In case of multilayer Schottky metal stacks, ideally the SBH depends on the metal in contact with the semiconductor at the metal–semiconductor (MS) interface. If the metals above the first

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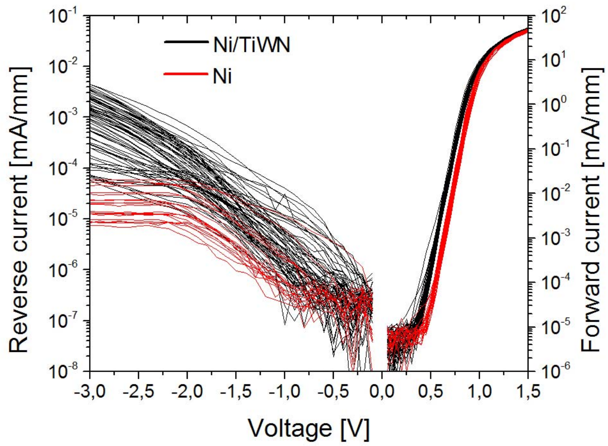

Fig. 1. *I–V* characteristics of two sets of diodes, with and without the TiW(N) cap.

metal (Ni) do not react in close vicinity to the interface, the SBH should not be influenced by them.

MS interface properties, such as the SBH, can also be affected by stress-dependent parameters, for example via polarization-induced charges [11]. One could then expect that the deposition of the metallization layers will affect the stress and therefore the electrical properties of the contacts. Earlier it was shown that the stress induced by the SiN passivation influences the sheet charge density [12]. Some initial work shows the dependence of the sheet carrier concentration of the 2-D electron gas (2-DEG) on Ni thickness [13]. Moreover, strain may affect trap energy levels [14] or the metal work function [15]. However, to our best knowledge the influence of the stress from metal layers in Schottky contacts to AlGaN/GaN has not been studied so far.

In this paper, we show that there are no chemical reactions at the MS interface of different Schottky metal stacks and consequently that the SBH change observed in the experiments can be explained by the stress inside the stack. Subsequently, we conduct an experiment in which we remove the stress source, namely, the TiW(N) layer, and show the extent of SBH change caused by the stress.

II. Methodology

For this paper, we adopted a GaN-on-Si process technology, in a silicon nitride passivation-first integration scheme [16]. The top layers of the wafers used in this experiment consist of 1.5 μm of GaN with 20 nm of $Al_{0.2}Ga_{0.8}N$ and a 3-nm GaN cap, prepared by the metal–organic chemical vapor deposition. The as-grown wafers 2-DEG carrier density obtained from Hall measurements is 5.8×10^{12} cm^{-2} and the electron mobility is equal to 1700 cm^2/Vs.

Devices were patterned by dry etching and isolation was obtained by using argon ion implantation with the energy of 160 keV and dose of 1×10^{14} cm^{-2}.

A Ti/Al-based gold-free metal stack was used for the Ohmic contacts. The Al layer is a few times thicker than the Ti layer, and the Ti/Al ratio and anneal conditions were optimized for a specific contact resistivity (ρ_c) stable at/below 10^{-5} Ωcm^2. More details can be found in [16]. The Ohmic contacts received a rapid thermal annealing treatment at an optimized temperature within a 800–900 °C range, which is typical for contacts to AlGaN/GaN [17], [18]. We investigated two different Schottky contacts, namely, Ni and Ni/TiW(N). In these contacts, the 100-nm thick Ni layer was evaporated in both contact schemes. TiW(N) layers were sputter deposited and their thickness is 10/80/10 nm of, respectively, TiW, TiWN, and again TiW. After the Schottky anode deposition, the wafer was annealed at an optimized temperature between 400 and 600 °C. A schematic cross section of the diode is presented in Fig. 2.

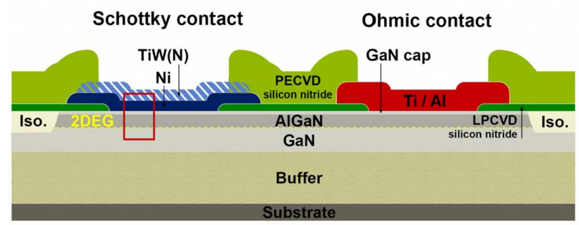

Fig. 2. Schematic cross section of the AlGaN/GaN diode. The red rectangle indicates the area investigated with SIMS.

Material analysis has been conducted by using secondary-ion mass spectroscopy (SIMS) and transmission electron microscopy (TEM) with energy dispersive X-ray (EDX) spectrometer. SIMS depth profiles have been measured using a Cameca IMS 6f. Scanning TEM measurements have been performed with an FEI Titan TEM. EDX spectra have been acquired simultaneously with the electron energy loss spectroscopy (EELS) spectra. EELS has been performed with a Gatan Tridiem HR detector.

The extensive material characterization is aimed to show if there are any differences at the MS interface between the two different Schottky metal stacks [i.e., Ni and Ni/TiW(N)]. In case no differences are found, then the difference in SBH between the two contacts cannot be caused by the chemical reactions at the MS interface. Then, the SBH stress dependence could be an explanation. One way to study this is by conducting a deprocessing experiment of Ni/TiW(N) Schottky diodes to remove the possible stress source—the TiW(N) layer.

In the experiment, metal layers were removed in three steps and electrical measurements were conducted in between each process step to obtain the SBH. In the procedure 30% H_2O_2 at 20 °C was used to remove TiW(N) in two steps in which each time 50 nm (±10 nm) of the material was removed. Subsequently, 50 nm of Ni was removed with 1% HNO_3 at 20 °C. The experiment was conducted on one wafer and each time exactly the same devices were measured to avoid wafer-to-wafer and device-to-device variability.

III. Material Analysis

Since the annealing of the Schottky stack was done after the TiW(N) deposition, some interdiffusion and alloying could occur, especially within the metal stack itself, but also at the MS interface. Consequently the interface properties may change, which would affect the SBH. Diffusion of Ni into GaN and outdiffusion of Ga and N from GaN could also affect the barrier [19]. Therefore, SIMS was applied to two different

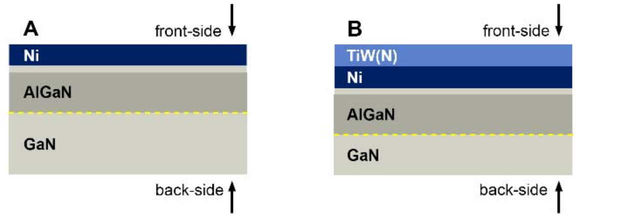

Fig. 3. Cross section of the samples investigated with SIMS: sample A without the TiW(N) cap and sample B with the TiW(N) cap.

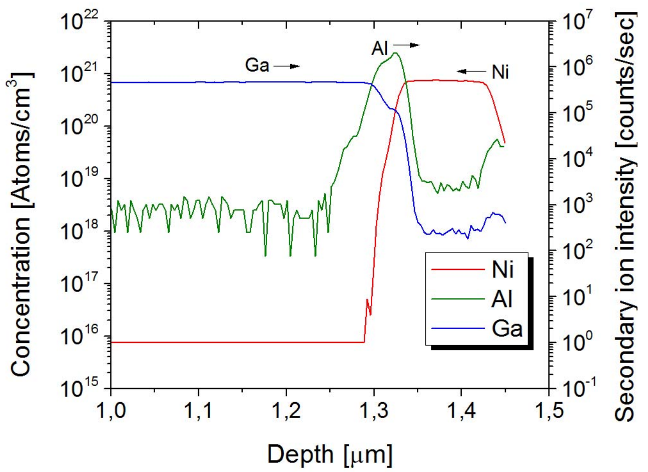

Fig. 4. SIMS profiling from the backside of the wafer for sample A, without the TiW(N) capping layer.

samples, namely, sample A with the Ni metal only, and B with the Ni/TiW(N) stack (Fig. 3).

To avoid artifacts in different areas of the sample caused by roughness or possible differences in metal sputter rate (that can result in an incorrect detection of the MS interface position and composition), we have conducted backside SIMS, by carefully polishing back the substrate up to an appropriate depth below the device region. Results of those measurements are presented in Figs. 4 and 5, indicating that there are no differences between the samples at the interface between Ni and the semiconductor below. The Ni signal is steep in both samples (beyond the instrumental resolution) and the Ga signal is also similar for both. While we see signs of reaction at the AlGaN/GaN interface, the Ni/GaN interface is equally steep in both cases. The W is not present in the close vicinity to the MS interface, hence it was left out from the figures. In other words, based on the SIMS analysis, there is no sign of any reaction at the Ni/GaN interface both in the capped and uncapped version of the anode metal stack.

In order to confirm the SIMS results, we have also analyzed samples using TEM. In Fig. 6, the TEM cross section and the chemical profile of a contact without TiW(N) cap are shown using EELS and EDX. The amount of Ni in the GaN is below the detection limit, as indicated by the tail shape of the Ni profile in the GaN and the Ga profile in the Ni. EELS and EDX give similar results.

The situation for a contact with the TiW(N) cap (Fig. 7) is similar and the diffusion, if present, is below the detection limit.

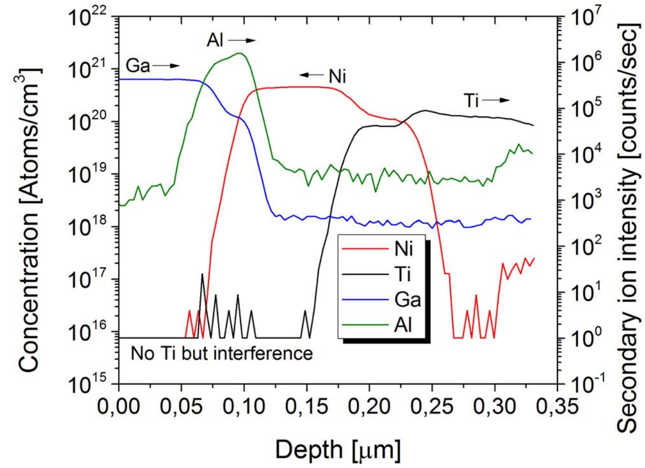

Fig. 5. SIMS profiling from the backside of the wafer for sample B, with the TiW(N) capping layer.

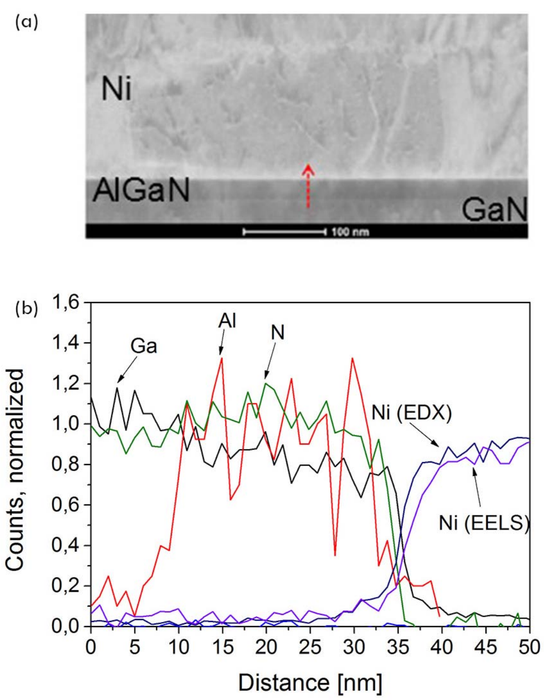

Fig. 6. Contact without TiW(N) cap. (a) TEM cross section of the contact area. (b) Chemical profile along the red line indicated in (a).

Comparing data for the capped and uncapped contact suggests that there is no detectable difference between them at the MS interface. Some diffusion of Ni into GaN cannot be excluded, but it would be very limited. Furthermore, the Ni diffusion should be similar for both metal stacks so it would not explain the observed SBH difference between Ni and Ni/TiW(N) metal stacks.

IV. Electrical Characterization

A. Deprocessing to Release Stress

Since it appears that there are no chemical reactions at the MS interface which could cause the SBH shift, we conducted a deprocessing experiment in order to show whether

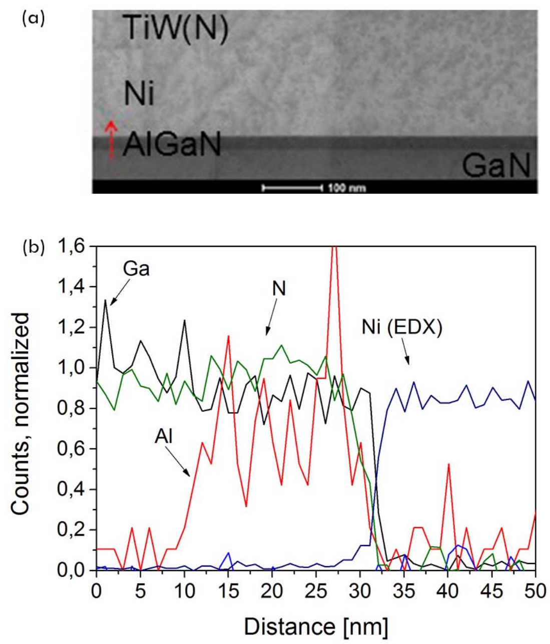

Fig. 7. Contact with TiW(N) cap. (a) TEM cross section of the contact area. (b) Chemical profile along the red line indicated in (a).

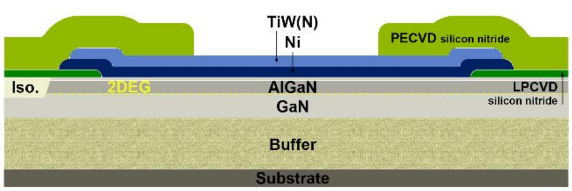

Fig. 8. Schematic cross section of the deprocessed diode design.

or not a partial removal of the cap would result in a change in SBH possibly caused by a partial removal of the stress. We removed the TiW(N) capping layer in steps that is expected to be the source of the stress affecting the SBH [13]–[15], [20]. The Ni/TiW(N) anode metal stack was etched in steps on a wafer which was removed from processing after opening the contact windows in the second insulating layer (plasma-enchanced chemical vapor deposition (PECVD) silicon nitride). As illustrated in Fig. 8, due to a partial covering of the anode area with PECVD nitride, only half of the area could be etched away.

The etchants used to remove TiW(N) and Ni (H_2O_2 and HNO_3, respectively) have a high selectivity to silicon nitride and have some influence on the Ohmic contact parameters. On average the contact resistance, extracted using transfer length method test structures, increases from 0.35 to 0.60 $\Omega \cdot$ mm, but is of minor importance to this paper as it does not influence SBH extraction. Moreover, the H_2O_2 etch is highly selective toward Ni, therefore we were able to completely remove TiW(N) without any detrimental effects to other materials.

The etching had only a small influence on the Schottky contact surface roughness as observed in the atomic force miscroscopy (AFM) topography 3-D scans presented in Fig. 9. After the first etch step, the arithmetic average of the roughness

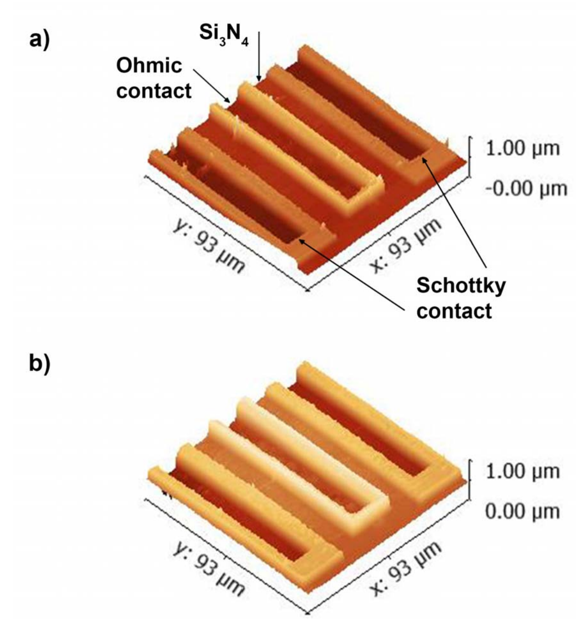

Fig. 9. 3-D AFM topography image of the contacts (a) before the etch and (b) after the first etch. The central contact is the Ohmic contact and the outer ones are Schottky contacts.

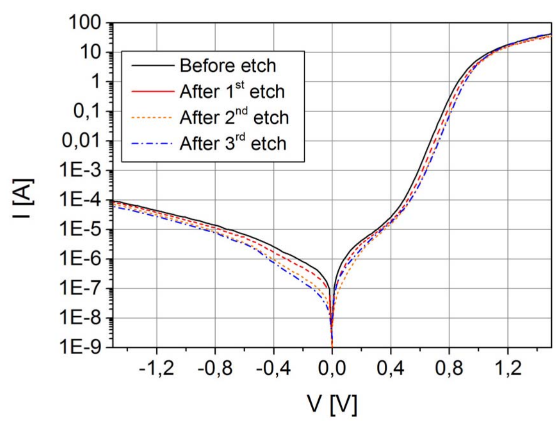

Fig. 10. *I*–*V* characteristics of an example diode at different deprocessing stages.

profile (R_a) increased from 7.35 to 8.10 nm and the root-mean-square average of the profile height deviations (R_{rms}) increased from 9.20 to 11.02 nm.

The diodes were probed directly on the contacts, as there were no bond pads yet present at this processing stage. At each step, the same devices were measured to assure one-to-one comparison and to avoid effects due to variability over the wafer. Forward I–V characteristics of 200 diodes were measured at each stage and the shift in SBH was determined. A Keysight B1505A semiconductor parameter analyzer has been used for the electrical characterization. Automated measurements were conducted using a Tesla system from Cascade Microtech.

B. Results

In Fig. 10, the I–V characteristic of an exemplary device is shown at different deprocessing stages. It can be seen that the

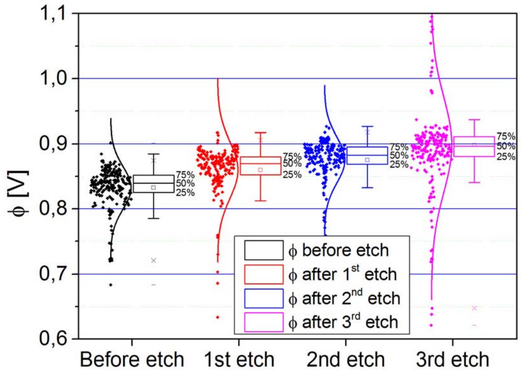

Fig. 11. Measured SBHs of devices before and after each etch step.

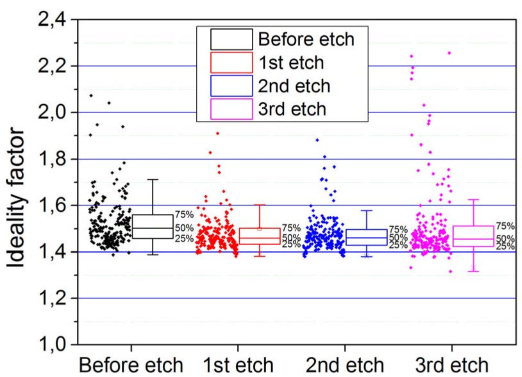

Fig. 12. Measured ideality factor at each processing stage.

removal of the TiW(N) layer leads to a shift in the I–V toward higher voltages (i.e., lower saturation current) and hence to an increase in the effective SBH.

The SBH after the first, second and third etch step as well as the initial values were acquired on over 200 Schottky diodes and compared 1 to 1, meaning that the observed shifts are not a result of the variability over the wafer.

In Fig. 11, we present the statistical distribution of the SBH shift for all etch steps. For each TiW(N) etch step of the same depth (about 50 nm for each step) the change in SBH is similar. In total an SBH reduction of around 50 mV is observed because of the metal stack. The SBH ~10 mV shift due to Ni removal is relatively low compared to the total ~50 mV shift. Consequently, we can say the effect of Ni exposure to H_2O_2 after TiW(N) removal, and subsequent etching in HNO_3 is of less importance.

As can be seen in Fig. 12, there is no significant change in the devices' ideality factors between the processing steps.

V. Discussion

Both SIMS and TEM results have shown that there are no significant differences at the MS interface of the Ni and Ni/TiW(N) contacts. Neither Ti nor W appears to diffuse toward the interface and there is also no Ni diffusion into the semiconductor.

The electrical measurements clearly indicate that the TiW(N) capping layer is responsible for SBH differences between diodes with Ni and Ni/TiW(N) metal stacks.

So far our experimental analysis points out that the nature of SBH change is physical (stress), rather than chemical (reactions at MS interface). The presence of the stress may influence the Schottky contact to AlGaN/GaN in several ways.

First of all, the piezoelectric polarization is expected to change in both (piezoelectric) materials. This would result in change of the electron concentration in the 2-DEG [21]. Since the spontaneous polarization is an intrinsic material property, stress can only affect the piezoelectric polarization. We could further assume that the amount of additional stress in both AlGaN and GaN layers caused by the anode metal is similar. Subsequently, since the piezoelectric coefficients of AlGaN and GaN are within the same range [22] (parameters for AlGaN are taken from linear interpolation between GaN and AlN), the difference in the strain-induced piezoelectric polarization is negligible, therefore the 2-DEG sheet carrier density should not be affected much [23]. However, small changes in the effective SBH would appear because of the presence of additional piezoelectric polarization-induced charge.

Second, another parameter that directly defines the SBH is the position of the conduction band in AlGaN and GaN. In the experiments, we observed an increase in the SBH of +50 mV. Hence, there is a $\Delta E_c = -50$ meV induced by the metal stack. According to the work of Fonoberov and Balandin [20] for the Wurtzite GaN conduction band shift holds

$$\Delta E_C = a_c^{\parallel} \cdot \varepsilon_{zz} + a_c^{\perp} \cdot (\varepsilon_{xx} + \varepsilon_{yy}) \tag{2}$$

where $a_c^{\parallel} = -9.5$ eV, $a_c^{\perp} = -8.2$ eV ($a_c^{\parallel} = -12.0$ eV, $a_c^{\perp} = -5.4$ eV), and the strain tensor ε_{ij} with x, y is the in-plane GaN (AlN) surface and z is out-of-plane (c-axis).

Also here, for obtaining values for AlGaN as a first estimate linearly interpolated values from AlN and GaN can be taken. So, for $Al_{0.20}Ga_{0.80}N$, present at the surface of our contacts $a_c^{\parallel} = -10.0$ eV, $a_c^{\perp} = -7.9$ eV,

This implies that for the electron affinity of (Al) GaN holds

$$\chi = \chi_0 - \Delta E_C = \chi_0 - a_c^{\parallel} \cdot \varepsilon_{zz} - a_c^{\perp} \cdot (\varepsilon_{xx} + \varepsilon_{yy}). \tag{3}$$

Since the strain is attributed to differences in the lattice constant and thermal expansion coefficients between different materials [i.e., Ni, TiW(N), (Al)GaN], it is expected that the strain in the layers is a biaxial (in-plane) strain. In this case, we can say that $\varepsilon_{xx} = \varepsilon_{yy}$ and for the out-of plane component [24]

$$\varepsilon_{zz} = \frac{-\upsilon}{1-\upsilon} \cdot \varepsilon_{xx} \tag{4}$$

with υ is the Poisson ratio (≈0.23). Hence, $\varepsilon_{zz} \approx -0.3 \cdot \varepsilon_{xx}$.

Based on the Poisson ratio and (2) for a reduction in the SBH (or increase in work function) of 50 mV, as observed in our experiments, we estimate a biaxial tensile strain of around 0.27% in our $Al_{0.20}Ga_{0.80}N$ layer induced by the metal stack.

VI. Conclusion

We have shown that there is no indication of any chemical reactions at the MS interface in AlGaN/GaN Schottky with

Ni/TiW(N) metallization. This indicates that the barrier height difference has to be of physical, rather than chemical, origin. This barrier height change can be attributed to the stress induced by the TiW(N) capping layer on top of the Ni. We have outlined possible stress-related mechanisms that can affect the effective SBH and further experiments should be conducted to explain exact stress mechanisms.

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