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Conduction mechanisms in Au/0.8nm-GaN/n-GaAs Schottky contacts in a wide temperature range

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Abstract

Au/0.8nm-GaN/n-GaAs Schottky diodes were manufactured and electrically characterized over a wide temperature range. As a result, the reverse current I_{inv} increments from 1×10^{-7} A at 80 K to about 1×10^{-5} A at 420 K. The ideality factor n shows low values, it decreases from 2 at 80 K to 1.01 at 420 K. The barrier height $q\phi_b$ grows abnormally from 0.46 eV at 80 K to 0.83 eV at 420 K. The tunnel mechanism TFE effect is the responsible for the $q\phi_b$ behavior. The series resistance R_s is very low, it decreases from 13.80 Ω at 80 K to 4.26 Ω at 420 K. These good results are due to the good quality of the interface treated by the nitridation process. However, the disadvantage of the nitridation treatment is the fact that the GaN thin layer causes an inhomogeneous barrier height.

Keywords: nitridation; GaN/n-GaAs; Schottky diode; I-V-T; conduction mechanisms; barrier height;

Introduction

Metal-semiconductor (MS) contacts are very important in microelectronics [1-4]. They are used in optoelectronic devices, bipolar integrated circuits, high-temperature, and high-frequency applications [5, 6]. The thermionic emission (TE) theory is the principal theory used to determine the parameters of the Schottky contact.

However, the experimental current-voltage (I-V) characteristics present some anomalies at low temperatures and that both Schottky barrier height and ideality factor are temperature-dependent [5, 7-10].

This deviation of the thermionic emission theory is corrected by introducing other mechanisms, operating at the Schottky barrier such as the thermionic field emission TFE and the emission field FE currents [5, 11].

The origin of these currents is explained by considering several phenomena. First, the Schottky barrier is typically not homogeneous in space [7, 12-15], as measured using ballistic electron emission microscopy [16, 17]. The most widely accepted approach for interpreting experimental data considers that the spatial barrier inhomogeneity can be modeled with a Gaussian distribution function [12, 18-24].

Secondly, the existence of interface states [7, 25], act as recombination centers and generate local electric fields, causing random metallic paths, reducing carrier lifetime, and inducing large leakage current [26-29]. These interface states come from surface dislocations and surface contaminations incorporated during the elaboration process [27, 30, 31]. In addition, the Schottky metallization step can cause interfacial modifications [31-34].

Therefore, the interface quality has an essential impact on device behavior and performance. In this context, surface passivation is the best method to control the defective states [27, 30, 31, 35-39]. Particularly, many studies have carried out to improve the interface properties by nitridation of the GaAs surface [27, 30, 37, 38, 40-43], in order to improve the behavior and the electrical properties of the Schottky contacts such as ideality factor, barrier height, saturation current, series resistance and reverse current. Also, the nitride layers have good stability against the formation of amorphous surface oxides, high electronegativity, and thermal stability [27, 44].

In this work, we measure experimentally the electrical characteristics of Au/0.8 nm-GaN/n-GaAs Schottky contacts fabricated using a glow discharge plasma source (GDS) for nitridation. Moreover, we analyze the current transport mechanisms and several electrical parameters are characterized in a wide range of temperatures (80–420 K).

Experimental part

The Schottky contacts were elaborated using commercially available Si-doped n-GaAs (100) substrates, of a thickness of 400 μm and electron concentration $N_d=4.9\times 10^{15}\text{cm}^{-3}$. The samples were cleaned chemically using H_2SO_4 , deionized water, cold and hot methanol sequentially, and dried with N_2 . Then, the surfaces were bombarded with Ar^+ ions (ion energy of about 1 keV, sample current equal to 5 $\mu\text{A cm}^{-2}$, during 1 h) in UHV conditions [30, 40]. After surface cleaning, the substrates were heated at 500 $^\circ\text{C}$ and nitrided using a glow discharge nitrogen plasma source, running at 5 W for 30 min in an UHV chamber. This nitridation process led to the growth of a 0.8 nm-thick of undoped GaN layer. Following the nitridation step, the samples were annealed at 620 $^\circ\text{C}$ for 1 hour in view to crystallize the GaN layer [39, 45, 46].

A XPS system characterized by dual anode Al–Mg X-ray source and hemispherical electron energy analyzer were used for in-situ measurement of the chemical composition and crystal structure. The GaN thickness was calculated by comparing the experimental spectra data to the theoretical XPS peak intensities and positions [38]. The Au dots were deposited with area of $4.41 \times 10^{-3} \text{ cm}^2$ and thickened up to 100 nm. A Bruker Dimension Icon atomic force microscope (AFM) equipped by ScanAsyst and Nanoscope software 9.7 was used to investigate the film surface roughness. Using the PeakForce tapping mode, the AFM topography measurements were taken in the air. In order to accomplish this, a silicon tip on nitride cantilever (ScanAsyst Air model), with a 0.4 N m^{-1} spring constant and a nominal tip radius of 2 nm, were utilized to examine regions of $1 \times 1 \mu\text{m}^2$ with a resolution of $256 \text{ pixels} \times 256 \text{ pixels}$. The current-voltage measurements were investigated under different temperatures (80–420 K), utilizing a current source Keithely 220.

Results part

Figure 1 presents the PeakForce tapping AFM topography images for (a) GaN surface and (b) Au electrode within a scan size area a $1 \times 1 \mu\text{m}^2$ represented at the same height scale. The Au texture is formed by interconnected grain channels while that of GaN is almost flat. The obtained root mean square (RMS) surface roughness values indicate a difference of almost one order of magnitude between Au and GaN smoothness, i.e., 0.3 nm for GaN and 4.6 nm for Au. The value of the RMS surface roughness for GaN was calculated neglecting the areas occupied by the contamination features that clearly stand out in the image of Fig. 1(a). This value of roughness (0.3 nm) is less than half the nominal GaN layer thickness (0.8 nm).

The roughness difference is better shown in (c) where the frontier between the Au electrode and the GaN surface is shown as a rendered illuminated 3D AFM image, and the different topographies of Au and GaN are clearly shown. To bring out this difference in roughness more clearly, the height distribution histograms shown in Figure 1(d) were obtained from the topography images. GaN exhibits a narrow peak showing that in comparison to Au, which has a larger peak, the surface layer is more homogeneous. To clarify the difference between the peaks, they have been fitted to a single Gaussian distribution with a peak centered at 2.15, and 21.3 nm, and a full width at half maximum (FWHM) of 1.3 nm, and 9.5 nm for GaN and Au, respectively.

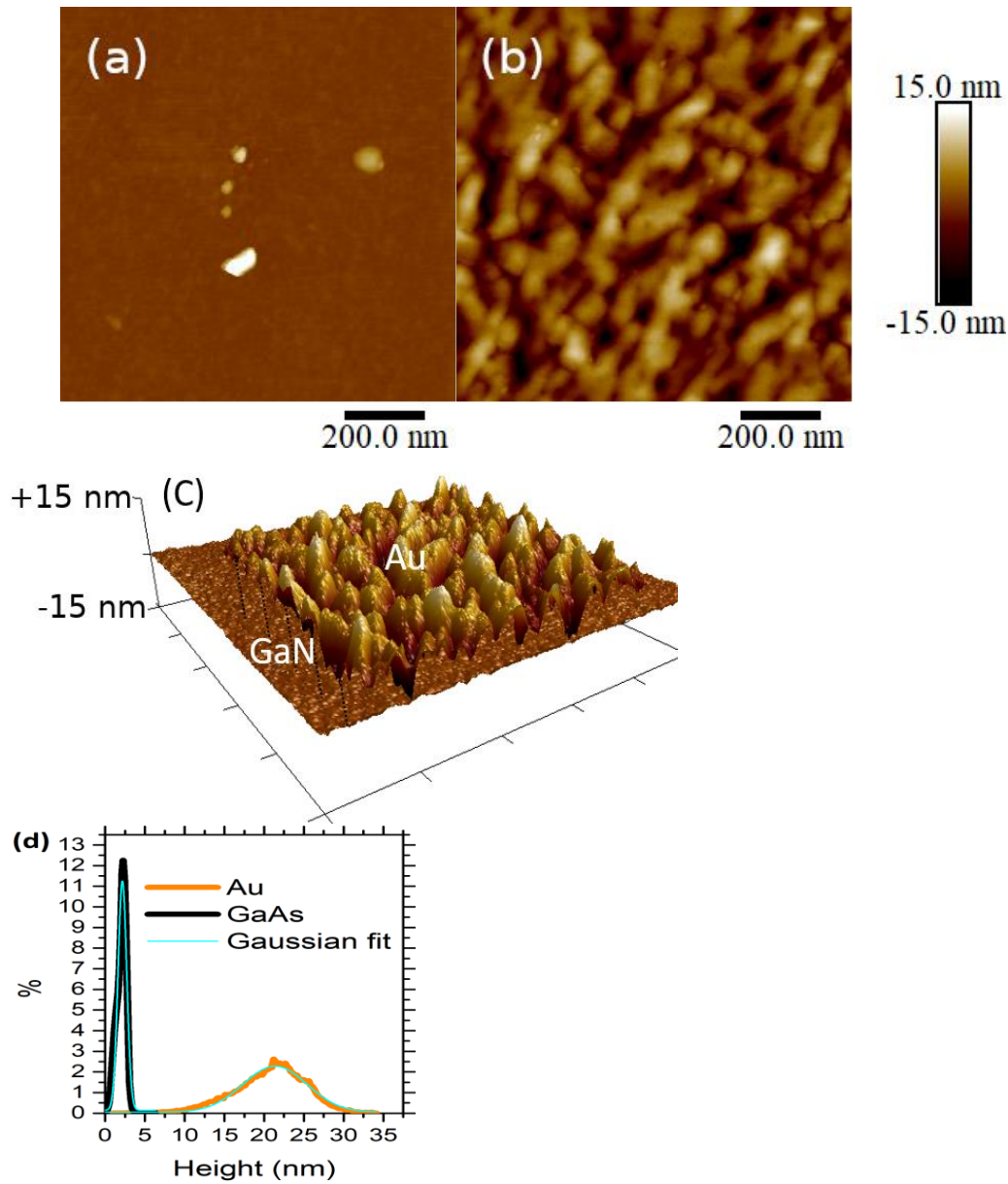


Figure 1: PeakForce tapping AFM topography for (a) GaN, and (b) Au surfaces. (c) Rendered illuminated 3D AFM image of GaN/Au frontier. (d) Height distribution functions obtained from the topography images.

Surface roughness induces a non-uniformity of the thickness, a distribution of interfacial charges, and a local variation of the Fermi level. These phenomena yield to the inhomogeneity of the Schottky barrier height and affect the transport mechanism [47].

Figure 2 depicts the I-V characteristics of the Au/0.8nm-GaN/n-GaAs structure, at temperatures ranging from 80 to 420 K.

The values of the reverse current I_{Rev} at -1 V and the threshold voltage V_{Th} are extracted and illustrated in figure 3. Where, with increasing temperature, I_{Rev} increases exponentially from 1×10^{-7} A at 80 K to 1×10^{-5} A at 420 K, and V_{Th} decreases from 0.65 V at 80 K to 0.2 V at 420 K.

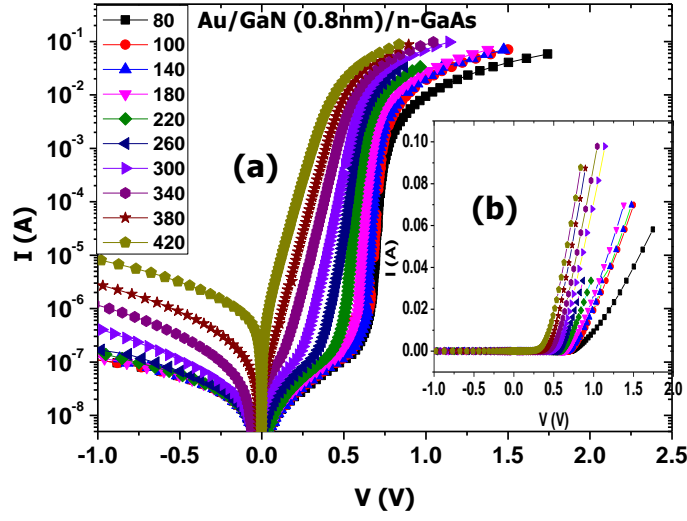


Figure 2: I-V measurements of Au/0.8nm-GaN/n-GaAs structure, (a) semi-logarithmic scale and (b) linear scale.

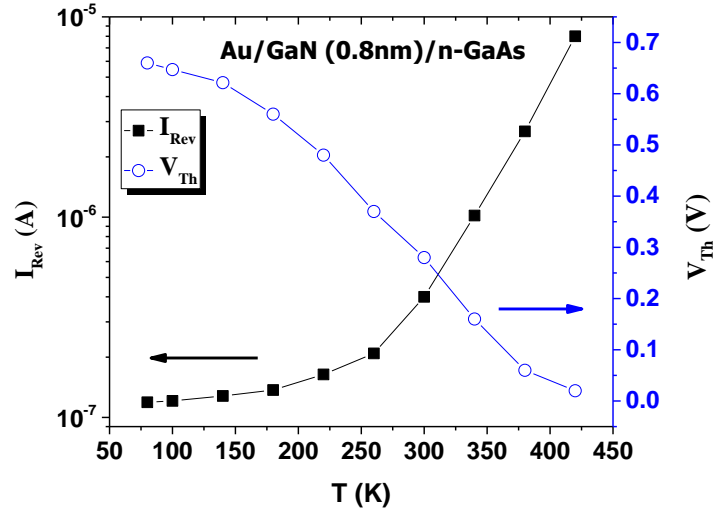


Figure 3: Variation of reverse leakage current and threshold voltage versus temperature.

The expression of the current for non-ideal Schottky diodes is [48]:

$$I = I_s \left(\exp \left(\frac{q(V - IR_s)}{nkT} \right) - 1 \right) \quad (1)$$

and

$$I_s = AA^* T^2 \exp \left(- \frac{q\phi_b}{kT} \right) \quad (2)$$

Where,

I_s is the saturation current,

R_s is the series resistance,

$q\phi_b$ is the barrier height,

n is the ideality factor,

k is the Boltzmann constant,

A is the effective diode area,

A^* is the effective Richardson constant equal to $8.16 Acm^{-2}K^2$ for GaAs,

At the low bias voltage V , the current I is low, therefore the term IR_s is low compared to V , and (eq.1) becomes as:

$$I = I_s \exp\left(\frac{qV}{nkT}\right) \quad (3)$$

and

$$\ln(I) = \frac{q}{nkT}V + \ln(I_s) \quad (16)$$

n and I_s values are calculated from the slope and y-axis intercept of $\ln(I)$ - V , respectively. The ϕ_b value is determined as follows:

$$\phi_b = \frac{kT}{q} \ln\left(\frac{AA^*T^2}{I_s}\right) \quad (4)$$

The R_s values are extracted using Cheung and Cheung method [48] which is based on:

$$G(I) = \frac{\partial V}{\partial(\ln I)} = R_s I + \frac{nkT}{q} \quad (5)$$

The extracted values of n and $q\phi_b$ are plotted in figure 4.

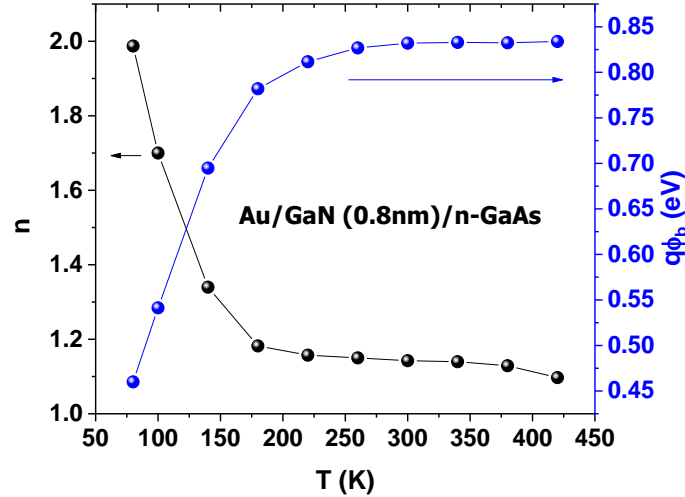


Figure 4: n and ϕ_b extracted at each temperature.

As can be seen from figure 4, with the rising temperature, n drops from 2 for 80 K to 1.1 for 420 K. The decrease is very slow from 250 K to 450 K and such behavior is in accordance with the literature [5-7, 11, 26]. The low values of n may be due to the effect of the nitridation process which improves the quality of the interface. $q\phi_b$ rises abnormally as temperature rises, from 0.46 eV for 80 K to 0.83 eV for 420 K. These

results are similar to several studies [7, 12, 20, 49-51]. For Schottky contacts, the $q\phi_b$ value should decrease as the temperature rises, due to the bandgap's temperature variation [1, 2, 7, 48, 50, 52-54]. The $q\phi_b$ behavior may be explained by the tunnel effect mechanisms, such as thermionic field emission (TFE) [5, 11].

The tunneling current can be expressed as following [1, 12, 55, 56]:

$$I = I_{tun} \left[\exp\left(\frac{q(V-IR_s)}{E_0}\right) - 1 \right] \quad (6)$$

$$\frac{E_0}{kT} = \frac{E_{00}}{kT} \cot h\left(\frac{E_{00}}{kT}\right) \quad (7)$$

$$E_{00} = \frac{h}{4\pi} \left(\frac{N_D}{m_e^* \epsilon_s}\right)^{\frac{1}{2}} \quad (8)$$

where

E_{00} is the characteristic tunneling energy,

h is the Planck constant,

m_e^* is the effective mass of electron,

ϵ_s is the dielectric constant of GaAs.

Figure 5 shows the variation of $(E_0 = nkT/q)$ versus kT/q .

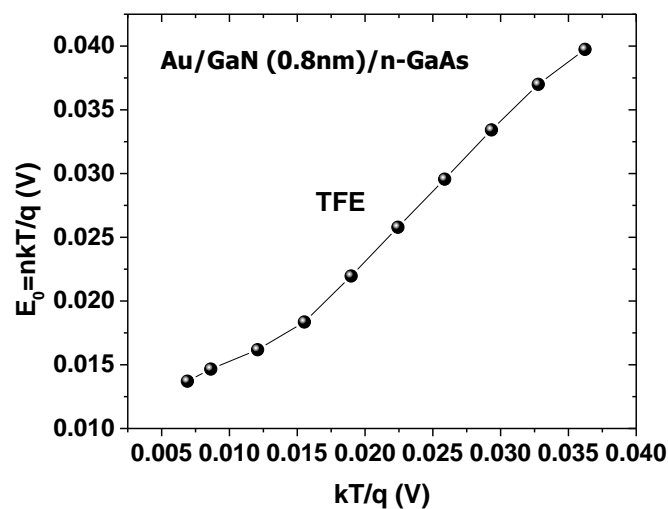


Figure 5: Variation of E_0 (nkT/q) versus kT/q .

From figure 5, E_0 is about kT/q , this confirms that the TFE mechanism is the dominant one [26], instead of the theoretical mechanism TE of the Schottky contacts, which explains the abnormal behavior of the barrier height and the deviation of the ideality factor from the unity. This is maybe due to the interface states which behave as recombination-generation centers at the interface that affect the conduction mechanism [57].

To further study the abnormal behavior of the barrier height, the Richardson characteristic $\ln(I_s/T^2)$ versus q/kT is presented in figure 6 using the equation,

$$\ln\left(\frac{I_s}{T^2}\right) = \ln(AA^*) - q\frac{\phi_{b1}}{kT} \quad (9)$$

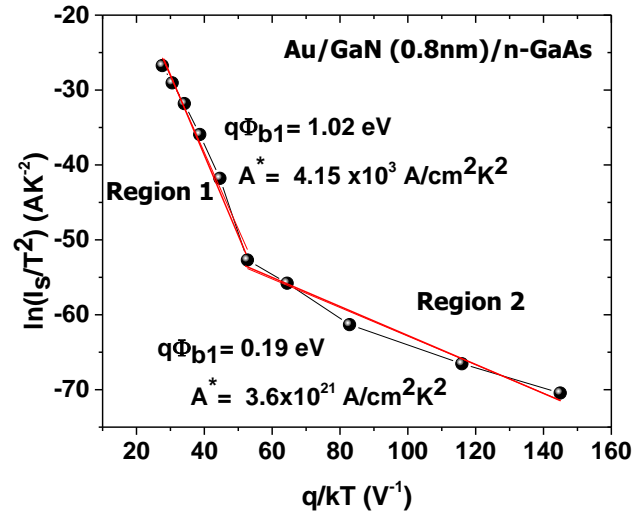


Figure 6: variation of Richardson characteristic $\ln(I_s/T^2)$ versus q/kT . Red lines are linear fits of experimental data according to the root mean square method.

Figure 6 gives two linear regions which are due to the inhomogeneity of the barrier height [12]. $q\phi_b$ and A^* values are $1.02 eV$ and $4.15 \times 10^3 Acm^{-2}K^{-2}$ respectively in region 1 and equal to $0.19 eV$ and $3.6 \times 10^{21} Acm^{-2}K^{-2}$ respectively in region 2. These values of A^* are significantly far from the theoretical value $8.16 Acm^{-2}K^{-2}$ for n-GaAs [52].

Figure 7 presents the variation of ϕ_b versus n .

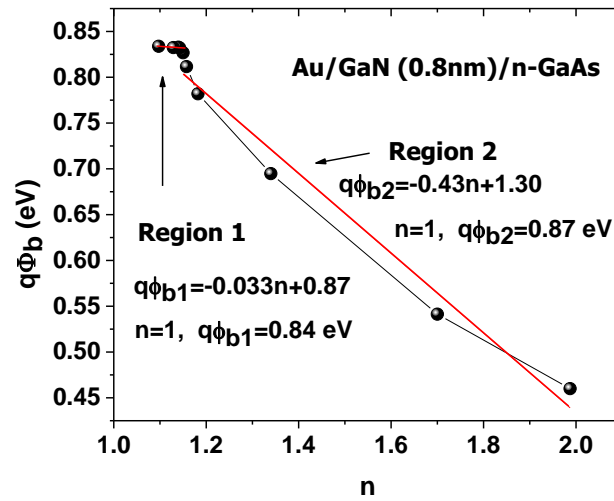
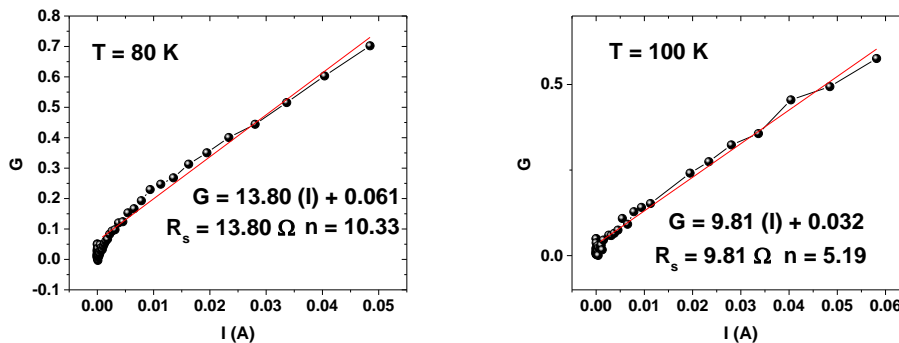


Figure 7: ϕ_b versus n .

The structure has two linear characteristics, this is due to barrier height inhomogeneity [58, 59]. By extrapolation, the estimated values of $q\phi_b$ for $n=1$ are 0.87 eV for region 1, and 0.84 eV for region 2. The obtained values are closer than those extracted from the Richardson characteristics.

The authors of this work [5] have previously performed simulations of Au/n-GaAs Schottky at temperatures ranging from 80 K to 400 K, with and without thin GaN (1 nm) interfacial layer. They found that Au/n-GaAs shows a homogeneous barrier height while Au/1nm-GaN/n-GaAs structure shows an inhomogeneous one. Therefore, the experimental results shown here, that it is the inhomogeneity of the barrier height shown in the Richardson characteristics, and in the plot of $q\phi_b$ versus n , are most likely because of 0.8 nm GaN layer.

Figure 8 illustrates $G(I)$ plots of Cheung and Cheung method at different temperatures (80 K-420 K).



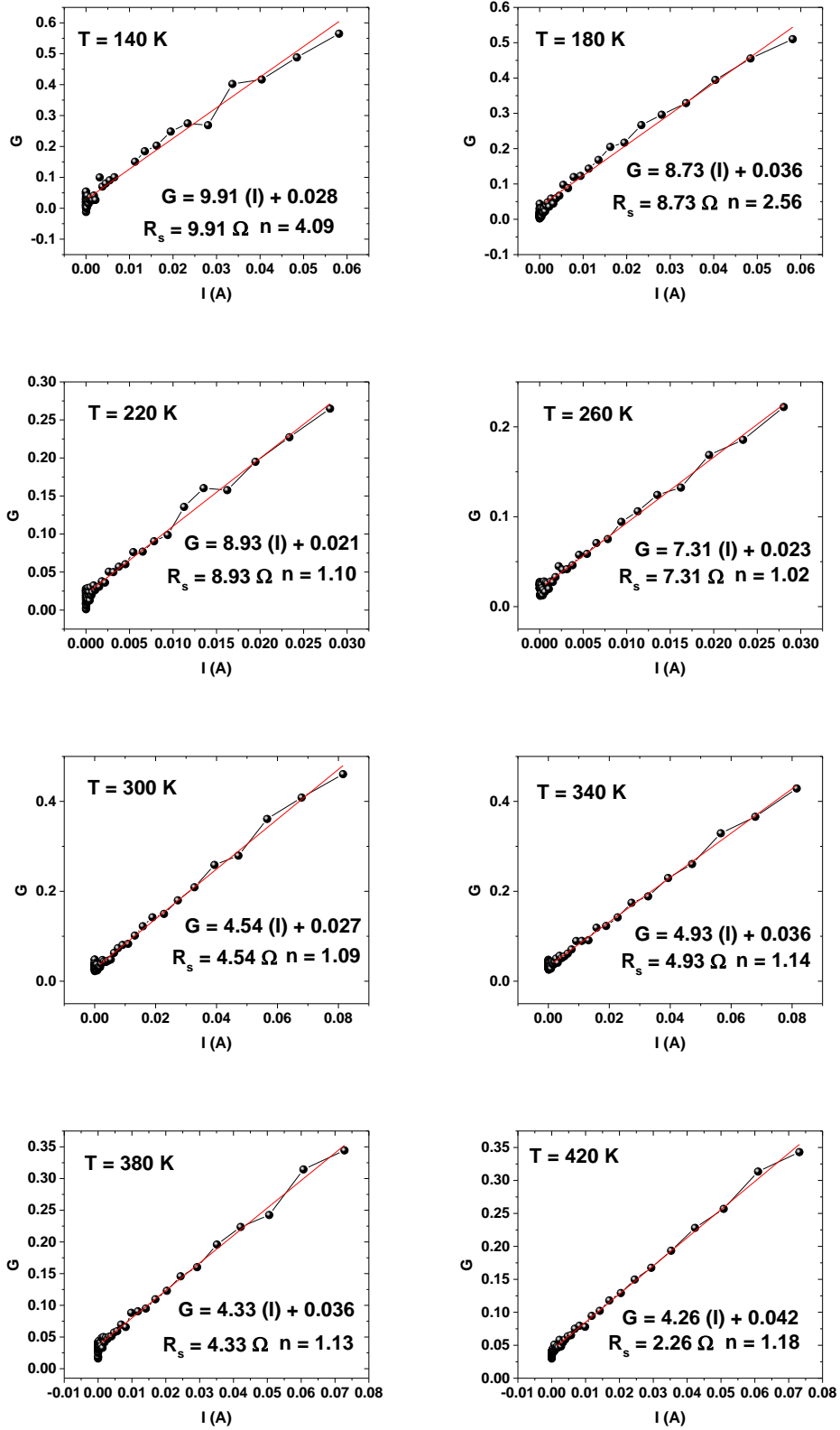


Figure 8: $dV/d(\ln I)$ plots at different temperatures.

R_s and n are extracted by Cheung and Cheung method for each temperature and presented in figure 9 and 10, respectively.

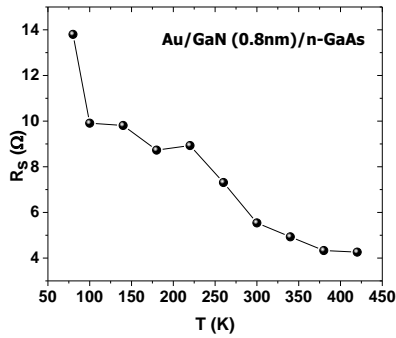


Figure 9: R_s (Cheung and Cheung method) versus temperature.

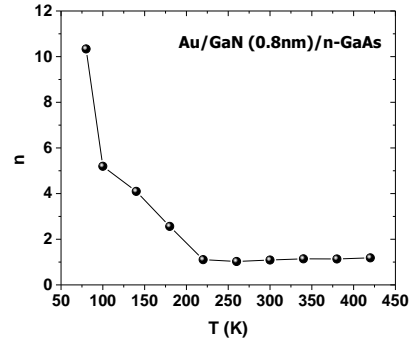


Figure 10: n (Cheung and Cheung method) versus temperature.

As can be seen, the structure gives low resistance series R_s which decreases from 13.80Ω at 80 K to 4.26Ω at 420 K, showing the good quality of the interface, improved by the nitridation and the annealing processes [28].

The n values obtained by Cheung and Cheung method are very high at low temperatures compared to those extracted from the first method. This discrepancy is because n values obtained by the first method were extracted from the low bias voltage range, where the series resistance is very low. On the other hand, the n values extracted using Cheung and Cheung method were extracted from all bias voltage range, where the series resistance in high bias voltages affects the calculation of the ideality factor.

Finally, the growth of 0.8 nm of GaN layer on n-GaAs surfaces with an annealing process leads to improving the electrical parameters of the Schottky contacts, such as the series resistance and the ideality factor. However, it can cause the inhomogeneity of the barrier height at the structure.

Conclusion

Au/0.8nm-GaN/n-GaAs structures were fabricated using a glow discharge plasma source (GDS), and their current-voltage characteristics were investigated for different temperatures. The samples showed good electrical parameters where, n decreases from 2 for 80 K to 1.01 for 420 K. The barrier height $q\phi_b$ grows abnormally from 0.46 eV at 80 K to 0.83 eV at 420 K, due to the tunnel mechanism TFE effect. Also, the samples show low R_s which drops from 13.80Ω at 80 K to 4.26Ω at 420 K. Finally, the results strongly suggest that the GaN thin layer causes an inhomogeneous barrier height that is also in agreement with our previous simulations [5].

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