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A new approach to studying the electrical behavior and the inhomogeneities of the Schottky barrier height

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Abstract In this paper, two Schottky structures of Au/n-GaAs (sample A) and Au/0.8 nm-GaN/n-GaAs (sample B) were fabricated and electrically characterized by current–voltage measurements at different temperatures. Two models, a classical one and another previously proposed named Helal model ref (Helal et al. Eur Phys J Plus, 135:1–14, 2020). Both the models show that the ideality factor n grows as the temperature decreases, and the second model shows higher values especially at low temperatures. The barrier height Φ_b calculated using the second model decreases when temperature increases for both structures, according to the temperature-dependent band gap, and in contrast to the results obtained by the classical model. Moreover, the second model gives a homogeneous Schottky barrier height and the best resolution of Richardson constant A^* , for both structures. On the other hand, the classical model shows an inhomogeneity of the barrier height and very far values of A^* from the theoretical one, in both structures. The findings of this study support the validity and dependability of the proposed alternative model. Furthermore, it may give a new insight into the electrical behavior of the Schottky structures.

1 Introduction

Schottky barrier diodes (SBDs) have been widely studied in recent years due to their potential applications [1–9]. Several attempts have been performed to comprehend the electrical behavior and transport mechanisms through SBDs, in order to explain the observed phenomena. The SBDs parameters are extracted using the thermionic emission (TE) model. In this model, the barrier height strongly depends on the composition, inhomogeneity of the metallic layer [6–9], and the defects of the interface contact [10, 11]. These parameters are the main cause of the formation of the barriers height inhomogeneities. This, in turn, leads to significant increase in local current flows through different sub-regions of different resistance [12], causing the current suppressing and self-heating effects, especially at lower temperatures [11], which could lead to the burn out of the junction.

Several authors [13, 14] indicate that using the TE theory, the investigation of the I–V characteristics in GaAs-based SBDs shows nonlinearity of the Richardson characteristics [15] and an abnormal behavior of the barrier height Φ_b , since it decreases when temperature decreases in disagreement with the values of Φ_b extracted from capacitance–voltage characteristics [4–6, 9, 13, 16–20].

Researchers have already attempted to explain this finding, taking into consideration the interface state effect [21, 22], tunneling mechanisms [23–26], and the barrier inhomogeneities [27–31].

A simple common effective contact (CEC) model suggest a method to investigate the variation of the barrier height and the electrical properties with the inhomogeneous interface and the different distribution of the interfacial area [10, 32]. The weakness of the model is that there is a discrepancy between the calculated barrier heights from I–V and C–V characteristics [10].

Helal et al. [1] proposed a new model of thermionic emission mechanism with a calculating method of the electrical characteristics. They obtained a good agreement between the Φ_b derived from both I–V and C–V characteristics for different temperatures in accordance with temperature-dependent band gap. This model was validated by simulation and experimental results.

In this work, we will study the electrical behavior and Schottky barrier height inhomogeneities of two different Schottky structures, by using Helal et al. model and a classical model of TE current.

The tested structures are based on Au/n-GaAs and Au/0.8 nm-GaN/n-GaAs SBDs, where the 0.8 nm nitride layer is used to passivate the GaAs surface and to eliminate the crystallographic interface dislocations, in order to improve the interface quality.

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2 Experimental part

Au/n-GaAs (sample A) and Au/0.8 nm-GaN/n-GaAs (sample B) Schottky diodes were fabricated by two different processes and electrically characterized by I - V measurements. The samples are based on n-GaAs substrate having a doping concentration of $N_d = 4.9 \times 10^{15} \text{ cm}^{-3}$ and a thickness of $400 \mu\text{m}$. The wafers were firstly cleaned chemically by sulfuric acid and methanol. For sample B, the n-GaAs surface were bombarded by an Ar⁺ ion source (ion energy: 1 keV, sample current density: $5 \mu\text{A cm}^{-2}$, time: 1 h) in the ultra-high vacuum UHV chamber. [33, 34]. Then, the wafers were nitrided using a glow discharge nitrogen plasma source, of 5 W for 30 min, and annealed at $620 \text{ }^\circ\text{C}$ for 1 h, in an UHV chamber [3, 35–37]. In-situ, Au dots were deposited by evaporation on the top side with a 0.6 mm diameter and 100 nm of thickness, for the two samples, using a Knudsen cell.

The I - V characteristics were investigated at different temperatures in the range of 140 – 380 K , with a Keithley 220, cooled by liquid nitrogen cryostat (Janis VPF 400).

3 Results and discussions

The electrical characteristics I - V of samples A and B are shown in Figs. 1 and 2, respectively.

For both samples, in low bias voltage, the current varies linearly versus bias voltage and shifts gradually toward the higher bias side with decreasing temperature. Then, with the increase in the bias voltage, the linearity is deviated due to the effect of the series resistance.

For ideal Schottky contacts the expression of forward I - V characteristics is

$$I = I_s \left[\exp\left(\frac{qV}{kT}\right) - 1 \right] \quad (1)$$

Fig. 1 I - V - T of sample A (Au/n-GaAs)

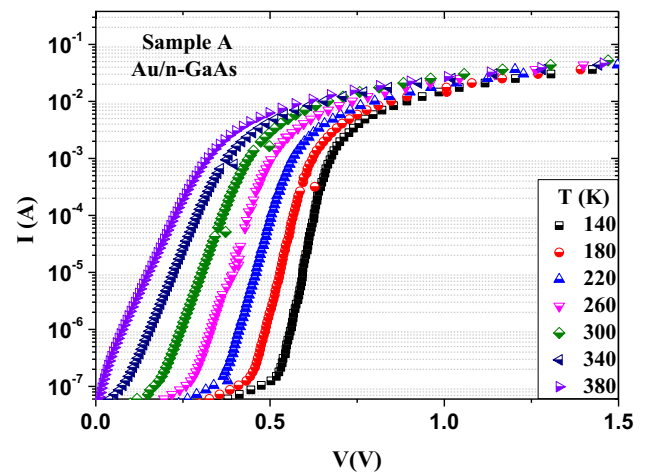
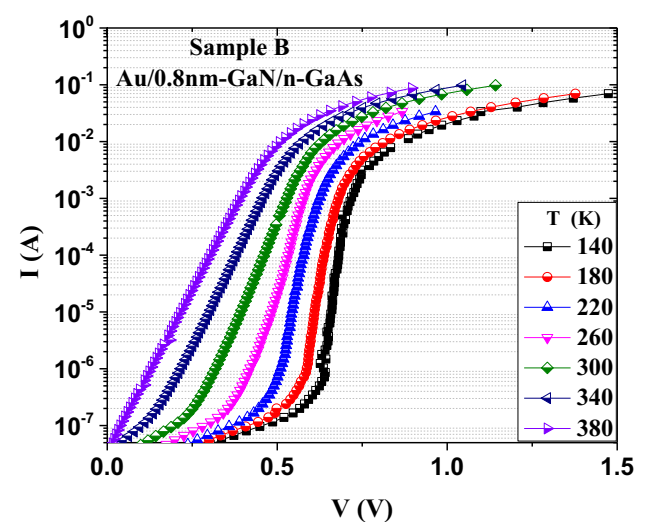


Fig. 2 I - V - T of sample B (Au/0.8 nm-GaN/n-GaAs)



I_s is the saturation current calculated as:

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

k is the Boltzmann constant, A is the effective diode area, and A^* is the effective Richardson constant ($8.16 \text{ A cm}^{-2}\text{K}^2$ for GaAs).

While, for real Schottky contacts the classical model of I - V characteristics is [38–40]:

$$I = I_s \exp\left(\frac{q(V - R_s I)}{nkT}\right) \tag{3}$$

where n and R_s are the ideality factor and series resistance, respectively.

In the Helal et al. [1] model for real Schottky contacts, it is expressed by:

$$I = AA^*T^2 \exp\left(\frac{-q\Phi_b}{kT}\right) \exp\left(\frac{q(V - R_s I)}{kT}\right) \exp\left(-\frac{1}{n}\right) \tag{4}$$

The electrical behavior and the electrical characteristics such as n , I_s , and Φ_b are extracted and studied by the two models described by the Eqs. (3) and (4).

3.1 Extraction of the electrical parameters

3.1.1 Using the classical model

By taking into consideration that at the low bias voltage V , the current I is low, therefore the term IR_s is low compared to V , Eq. (3) becomes:

$$I = I_s \exp\left(\frac{qV}{nkT}\right) \tag{5}$$

and

$$\ln(I) = \frac{q}{nkT} V + \ln(I_s) \tag{6}$$

n and I_s are obtained from the slope and y-axis intercept of $\ln(I)$ vs V plot, respectively. Φ_b is determined using:

$$\Phi_b = \frac{kT}{q} \ln\left(\frac{AA^*T^2}{I_s}\right) \tag{7}$$

3.1.2 Using Helal et al. model

The electrical parameters are extracted by the Helal et al. method [1] using two relationships, $h_1(I)$ and $h_2(I)$, as follows,

$$h_1(I) = \frac{\partial V}{\partial(\ln I)} = \frac{nkT}{q} + R_s I \tag{8}$$

$$h_2(I) = V - \frac{KT}{q} \ln\left(\frac{I}{AA^*T^2}\right) - \frac{KT}{qn} = R_s I + \Phi_b \tag{9}$$

I_s is then calculated using Eq. (2). The two methods are explained in detail in [1].

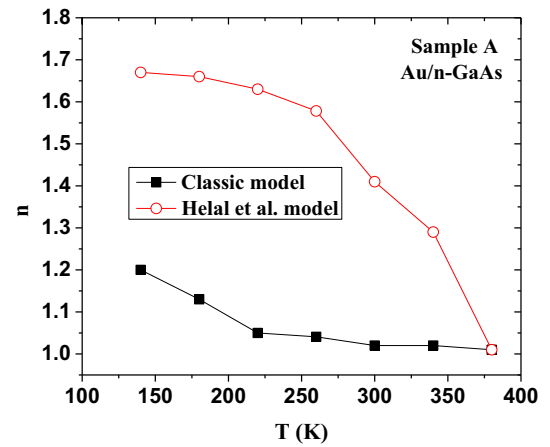
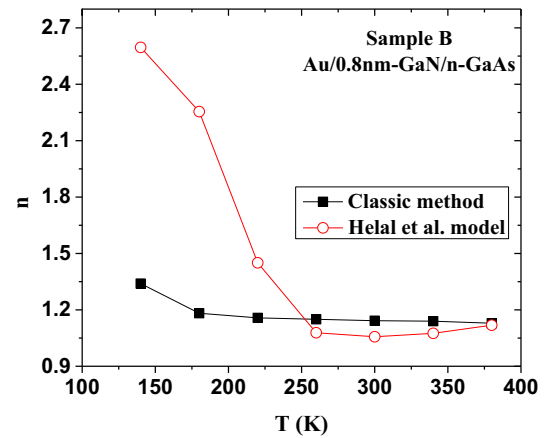
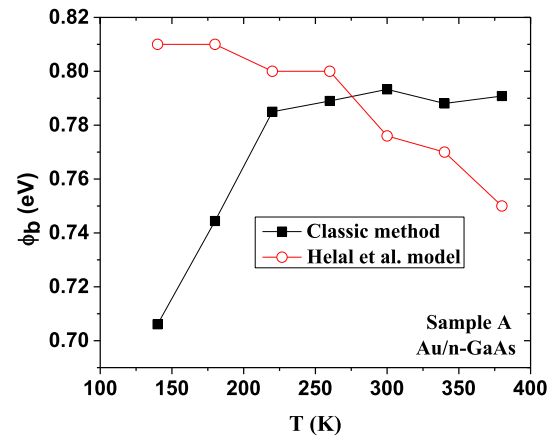
Note that the current range considered in the fit for sample A was from 1.4×10^{-7} A to 1×10^{-3} A, using classical model, and from 1.4×10^{-7} A to 3×10^{-2} A, using Helal model, for all temperatures. For sample B, it was from 4×10^{-7} A to 3×10^{-3} A, using classical model, for all temperatures, while it was from 1.4×10^{-7} A to 3×10^{-2} A for 220 K and 260 K, and from 1.4×10^{-7} A to 3×10^{-2} A for the other temperatures, using Helal model.

Figures 3 and 4 show the ideality factor n versus temperature for samples A and B, respectively, extracted by the two models.

As can be seen in these plots, for sample A (Au/n-GaAs), n increases with decreasing the temperature for both models. For sample B (Au/0.8 nm-GaN/n-GaAs), the same behavior is observed at low temperatures, while n remains almost constant and low at high temperatures (250–380 K) for the two models.

The increasing of n at low temperatures is due to the thermionic field emission TFE and field emission FE currents which became dominant instead of TE current [9, 13, 41]. This deviation of the transports mechanisms is more clearly defined in the Helal et al. model. This is due to the fact that in the classical model, the electrical parameters are extracted only from the linear part of the semi-logarithmic scale of the current–voltage (I - V), in the low base voltage range. In the other hand, in the Helal model, the electrical parameters are extracted from all the bias voltage for $V > 3kt/q$, and it is well known, that the ideality factor increases with increasing of the bias voltage due to the increase in the tunnel currents and the series resistance [42].

Also, the two models show low ideality factor in $T > 250$ K for the sample B, due to the nitridation of the GaAs surface which enhance the interface properties and improve the characteristics of the Schottky structure.

Fig. 3 n versus T for sample A**Fig. 4** n versus T for sample B**Fig. 5** Φ_b versus T for sample A

Figures 5 and 6 show the barrier height Φ_b variation versus temperature for samples A and B, respectively.

From these two figures, Φ_b extracted from the Helal et al. model decreases when temperature increases for both structures. These results confirm those previously obtained by Helal et al. [1]. As it is well known, with lowering temperature, Φ_b should grow according to the temperature-dependent band gap [13, 41, 43, 44]. On the other hand, the classical model shows the contrary, the Φ_b increases when temperature increase for sample A and it remains almost constant in the whole temperature range for sample B.

The discordance of the Φ_b obtained using the classical model and Helal model is due to the fact that classical model describe partially the current flow through the diode, and the real electrical parameters values. It is evidence by abnormal behavior of the barrier height obtained with the classical model, where it increases with increasing temperature in discordance with the band gap variation with temperature. As it is well known, with lowering temperature, Φ_b should increase according to the temperature-dependent band gap [13, 41, 43, 44]. The two models differ in the position of the ideality factor parameter in the equations. Also, in the Helal method, a wide range of current and voltage is used in the fit compared to the classical model, as mentioned before.

Fig. 6 Φ_b versus T for sample B

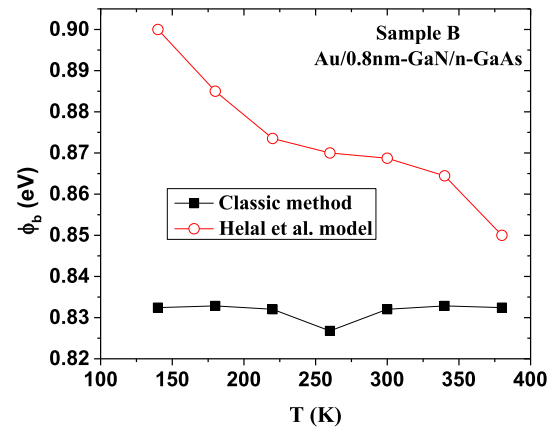


Fig. 7 I_s versus T for sample A

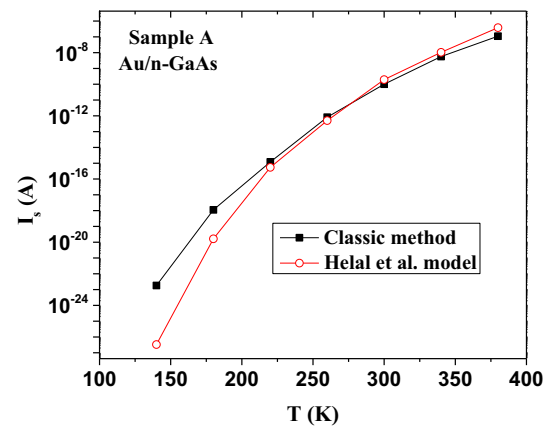
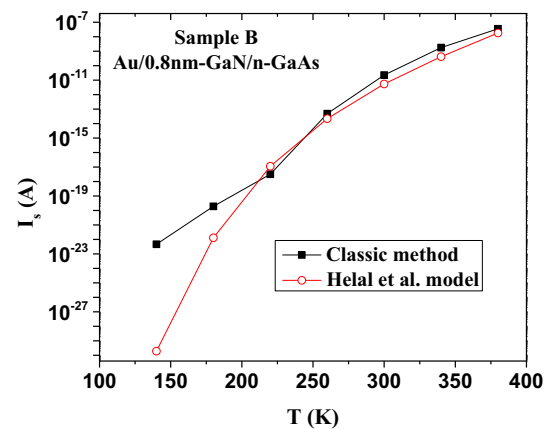


Fig. 8 I_s versus T for sample A



In addition, the Φ_b extracted from the sample B is higher than of sample A. This is due to the presence of the thin GaN layer [45].

The saturation current I_s is presented in Figs. 7 and 8 for samples A and B, respectively.

As shown in Figs. 7 and 8, the values of I_s obtained from the two models increases with increasing temperature for both samples. However, for low temperatures, the values of I_s obtained from the classical model diverges from that obtained with the model of Helal et al., and show two different forms of variation versus temperature.

Using the two models, Richardson characteristic ($\ln(I_s/T^2)$ Vs q/kT) is used to analyze the inhomogeneity of barrier height, and is illustrated in Figs. 9 and 10 for sample A and B, respectively. Here, the following equation is used:

$$\ln\left(\frac{I_s}{T^2}\right) = \ln(AA^*) - q \frac{\Phi_{bn}}{kT} \tag{10}$$

Fig. 9 $\ln(I_s/T^2)$ versus q/kT for sample A

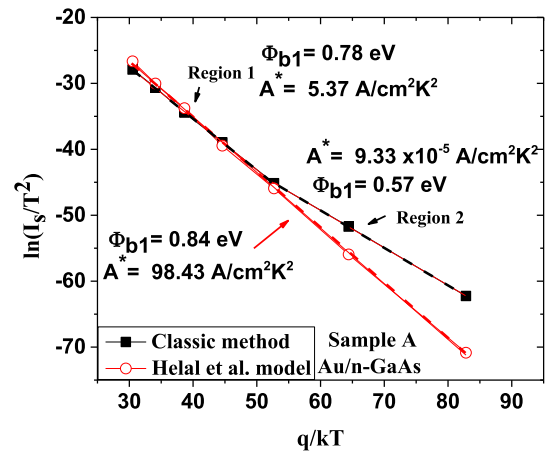
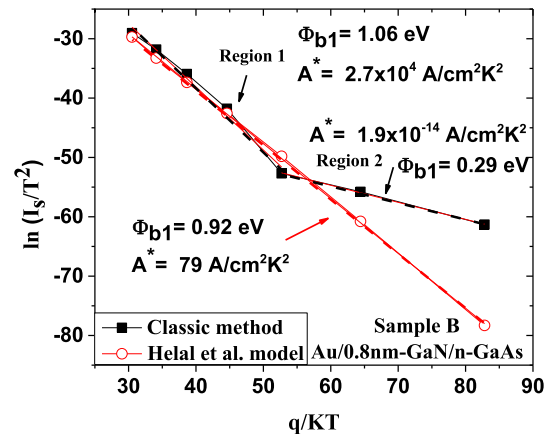


Fig. 10 $\ln(I_s/T^2)$ versus q/kT for sample B



As can be seen, the Helal et al. model shows a homogeneous Schottky barrier height for both structures, since the $\ln(I_s/T^2)$ versus q/kT results in a linear dependence. Parameters Φ_b and A^* were estimated at 0.84 eV and $98.43 \text{ A cm}^{-2}\text{K}^{-2}$, respectively for sample A and at 0.92 eV and $79 \text{ A cm}^{-2}\text{K}^{-2}$ respectively for sample B.

On the other hand, the classical model shows an inhomogeneity of the barrier height for both structures with two distinct regimes. For sample A, Φ_b and A^* are estimated at 0.78 eV and $5.37 \text{ A cm}^{-2}\text{K}^{-2}$ in region 1 (high temperature range), and at 0.57 eV and $9.33 \times 10^{-5} \text{ A cm}^{-2}\text{K}^{-2}$ in region 2 (low temperature range), respectively. For sample B, Φ_b and A^* are estimated at 1.06 eV and $2.7 \times 10^4 \text{ A cm}^{-2}\text{K}^{-2}$ in region 1 and at 0.29 eV and $1.9 \times 10^{-14} \text{ A cm}^{-2}\text{K}^{-2}$ in region 2, respectively.

Considering the theoretical value $8.16 \text{ A cm}^{-2}\text{K}^{-2}$ of A^* for n-GaAs material and comparing the two models, it is clear that the Helal et al. model gives the best resolution and agreement, whilst the classical model shows a different behavior in two regions with some values that are very far from the expected theoretical one, and a good approximation is only shown in one region (high temperature, region 1, in sample A).

Several authors [4, 9, 18, 19, 46, 47] have found effective Richardson constant A^* values that are also very far from the theoretical one by using the classical model. This is due to the fact that the classic model is not accurate enough.

These findings support and confirm the validation and the dependability of Helal et al. model, in a wide temperature range, and show that it provides the best description of the variation of the electrical characteristics with temperature. And it gives the best approximation of the Richardson constant, which allow to the good description of the barrier height homogeneity. Also, it may give a new insight into the electrical behavior and characteristics of the Schottky structures. On the other hand, it has been shown that the classical model shows an abnormal behavior of the barrier height and gives values of the Richardson constant very far from the theoretical one, which leads to wrong description of inhomogeneity of the barrier height.

4 Conclusions

Au/n-GaAs (sample A) and Au/0.8 nm-GaN/n-GaAs (sample B) are studied in temperature range (140–380 K). The electrical parameters such as n , I_s , and Φ_b are extracted using the Helal et al. model and the classical model. The values of n obtained by the two models increases when temperature decreases in both samples, but the Helal et al. model shows higher values, especially at

low temperatures. The values of the barrier height Φ_b extracted from the Helal et al. model decreases when temperature increases for both structures, according to the variation of the band gap with temperature, in contrast to the results obtained by the classical model. Helal et al. model provides a homogeneous Schottky barrier height and the best agreement of A^* with its theoretical value, in both structures. On the other hand, the classical model shows an inhomogeneity of the barrier height and values of A^* that are far from its theoretical value in both structures. The results obtained in this work confirm the validation and the dependability of the Helal et al. model. Such model can be applied to extract real parameter values in other material junctions.

Data Availability Statements The authors declare that all other data supporting the findings of this study are available within the article.

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