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Temperature Dependence of the Ideality Factor of GaAs and Si Schottky Diodes

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Current–voltage–temperature (I–V–T) measurements of different metal–semiconductor diodes are carried out and the temperature dependence of the ideality factor and the Schottky barrier height of these diodes are studied using different approaches. Based on certain assumptions and previously proposed models, different diode parameters are extracted and their correlations show that the interface imperfection of a metal–semiconductor contact can contribute to these temperature dependences. Moreover, in this work, the Au/n-Si and Al/n-GaAs diodes are shown to have the most imperfect contact interface amongst the sample diodes.

1. Introduction

For a perfect metal–semiconductor interface, provided the current flow is only due to thermionic emission, the ideality factor (n-factor) should be equal to unity [1, 2]. However, due to various reasons, the ideality factor usually deviates from the ideal case of n ($n = 1$). Moreover, previous studies observed that n may become temperature dependent and in some cases this temperature dependence can be expressed by the relation [3 to 7]

$$n = 1 + \frac{T_0}{T}, \tag{1}$$

where T_0 is a constant independent of the temperature (T).

This dependence has sometimes been referred to as the "T_0 effect" or the "T_0 anomaly" [4]. More generally, the temperature dependence of n can be given by [8, 9]

$$n = a + \frac{b}{T}, \tag{2}$$

where a and b are two temperature independent parameters.

Associated with the above-mentioned temperature dependence of n, the temperature dependence of the barrier height Φ_{I-V} obtained from the current–voltage (I–V) characteristics shows a trend to decrease with decreasing temperature (positive temperature dependence). As pointed out by previous studies, this decreasing trend conflicts with the results obtained from capacitance–voltage (C–V) and internal photoemission measurements (IPE) [10 to 12].

With a view to taking into account the effect of these anomalies of the I–V characteristics, different methods have been suggested for dealing with the activation and Richardson plots

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[7, 8, 13, 14]. In addition, modified $I-V$ expressions are introduced by putting the ideality factor n into the saturation current term I_s and the expression can be written as [3, 7, 13]

$$I = A^* A_e T^2 \exp\left(\frac{-q\Phi_B}{nkT}\right)\left[\exp\left(\frac{qV}{nkT}\right) - 1\right] \tag{3}$$

or more generally as [6, 15]

$$I = A^* A_e T^2 \exp\left(\frac{-q\Phi_B}{mkT}\right)\left[\exp\left(\frac{qV}{nkT}\right) - 1\right], \tag{4}$$

where n and m are diode factors.

Since the ideality factor n indicates how well the current transport of a diode obeys the thermionic emission theory and the Schottky barrier height is an important parameter in device physics, factors that cause these anomalies have stimulated many studies and much research. In an attempt to investigate the possible reasons for n to depart from unity and to exhibit a positive temperature dependence, recent studies on the recombination current effect and interfacial imperfection have shed some light on these problems. As far as recombination current effect and interfacial imperfection are concerned, it has been shown that the imperfection at the interface can enhance the recombination current effect and consequently causes the n-factor to increase with increasing temperature and Φ_{I-V} to decrease with decreasing temperature [2, 10, 11].

On the other hand, in recent years, these puzzling problems were also addressed by other workers from quite another point of view. The central point of their models adopted for explaining these anomalies is the barrier inhomogeneity at the Schottky contact [16 to 18]. According to these barrier inhomogeneity models, the barrier height of the contact will be affected by the uniformity of the interfacial layer and will form a distribution over the contact. As a result, this fluctuation of the built-in potential or barrier height over a Schottky contact may lead to non-ideal $I-V$ characteristics and may account for the differences between the barrier heights obtained from $I-V$ measurements and from other methods.

As the barrier inhomogeneity model is also a reasonable approach for explaining the metal–semiconductor interface imperfection and its effect on the current–voltage characteristics of the MS junctions, it is reasonable and worthwhile for us to incorporate this model in our experimental studies and compare the results so obtained with the conventional $1/T$ anomalies. In this study, different GaAs and Si Schottky diodes are fabricated and their $I-V-T$ characteristics are studied. In order to investigate the effect of interface imperfection on the performance of Schottky diodes, the temperature dependences of the n-factor and the barrier height Φ_{I-V} of the diodes are analysed in the light of the inhomogeneity model. The correlation between the conventional anomaly expression and the one from the barrier inhomogeneity model is also studied.

2. Experimental

All the wafers used in this experiment were first degreased in CH_4, acetone, and alcohol. For the etching processes, GaAs wafers were etched in $NH_4OH:H_2O_2:H_2O$ (3:1:120) for 1 min and in $H_2SO_4:H_2O_2:H_2O$ (10:1:1) for another 1 min. Si wafers were put into $H_2SO_4:H_2O_2:H_2O$ (10:1:1) solution for a few minutes and then etched in $HF:HNO_3$:

Table 1
Summary of the fabrication details of experimental diodes

sample	film thickness (Å)	doping conc. (10^{15} cm^{-3})	ohmic contact	orientation
Ni/n-Si	500	2 to 5	Au–Sb alloy	⟨100⟩
Ag/n-Si	1000	2 to 5	Au–Sb alloy	⟨100⟩
Au/n-Si	1000	2 to 5	Au–Sb alloy	⟨100⟩
Sn/n-Si	1000	2 to 5	Au–Sb alloy	⟨100⟩
Au/n-GaAs	1000	21	tin alloy	⟨100⟩
Al/n-GaAs	600	21	tin alloy	⟨100⟩
Ag/n-GaAs	1200	21	tin alloy	⟨100⟩

H_2O (3 : 1 : 10) solution for 1 min. Metal deposition and ohmic contact formation are carried out through standard procedures described elsewhere [9,19]. Other fabrication details of the experimental diodes are summarized in Table 1.

In $I-V$ measurements, the voltage applied to the Schottky diodes was supplied by a programmable voltage generator (HP3245A) and the current through the diodes was measured with a pico-ammeter (Keithley 485). All the $I-V$ measurements were carried out inside a well regulated cryostat (Oxford Instruments). The values of Φ_{I-V} and n were extracted from the $I-V$ characteristics by a modified method described previously [20].

3. Results and Discussion

In the conventional approach, an n versus $1/T$ plot of a diode is usually used to infer the diode performance at different temperatures and the value of b (the slope of the plot) is an important parameter which indicates the degree of diode performance degradation at low temperatures. The plot of n versus $1/T$ of the Si diodes is shown in Fig. 1a, all four metal/Si systems appear to have the $1/T$ or T_0 anomaly. The temperature dependence of n is most significant in the Au/n-Si diode, while this dependence for the Sn, Ag, and Ni/n-Si systems is more gentle. The corresponding n versus $1/T$ plot for the metal/n-GaAs systems is shown in Fig. 1b. The ideality factor n of the Ag and Au/n-GaAs system is not very sensitive to the change of temperature. However, the n-values of the Al/n-GaAs system show a more significant change with temperature.

As discussed briefly in the introduction section, the barrier inhomogeneity approach mainly assumes that there is a distribution of barrier heights over the Schottky contact. As far as the Schottky barrier height distribution is concerned, different functions, including exponential and Gaussian distributions, have been proposed by different workers. Amongst these functions, the Gaussian distribution is most widely adopted and it leads to useful expressions for the $I-V$ characteristics. We are following now the potential fluctuation model of Werner and Güttler [17]. Generally speaking, the adopted Gaussian distribution can be given by

$$dn = B \exp\left[-\frac{(\Phi(V,T) - \Phi_a(V,T))^2}{2\sigma^2(V)}\right] d\Phi\,, \tag{5}$$

where Φ is the barrier height of the sub-area, Φ_a the mean value of the Gaussian barrier height distribution, B the normalization constant of the Gaussian barrier height distribution, and σ the standard deviation of the Gaussian barrier height distribution.

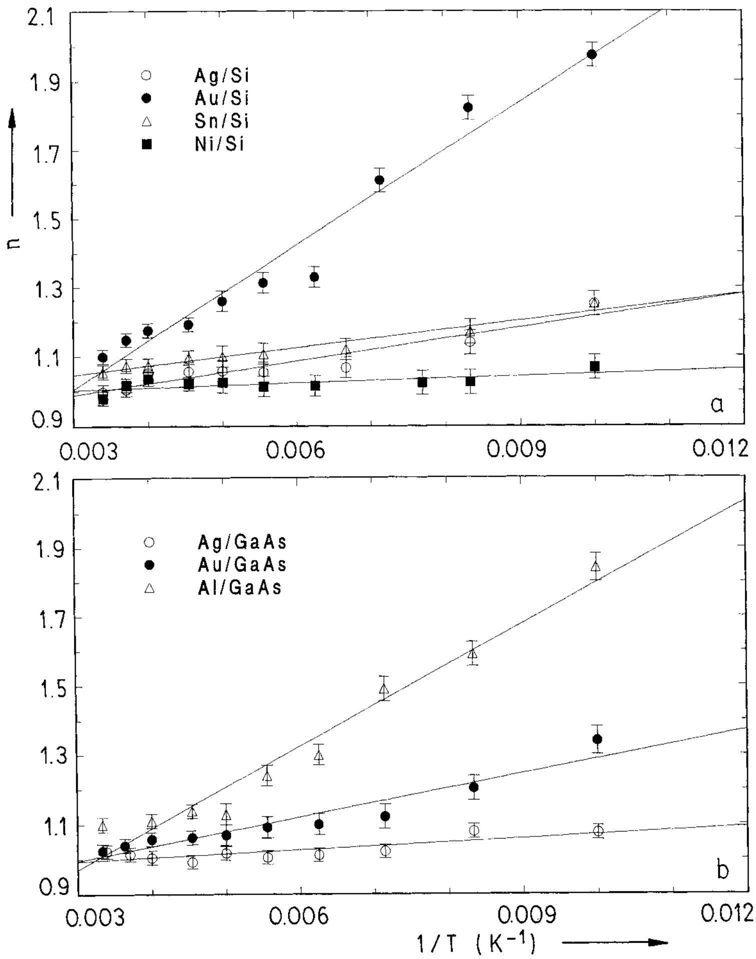

Fig. 1. The plot of n against $1/T$ for a) Si diodes and b) GaAs diodes

The subsequent expression of the $I-V$ characteristics can be written as

$$I_f = A_e A^* T^2 \exp\left(-\frac{q\Phi_{I-V}(V,T)}{kT}\right)\exp\left(\frac{qV}{n_0 kT}\right), \tag{6}$$

where

$$\Phi_{I-V}(V,T) = \Phi_a(V,T) - \frac{q\sigma^2(V)}{2kT} \tag{7}$$

and n_0 can be regarded as the ideality factor caused by other factors except the inhomogeneity effect.

When we compare (6) with the general $I-V$ characteristics,

$$I_f = A^* A_e T^2 \exp\left(\frac{-q\Phi_{B0}}{kT}\right)\exp\left(\frac{qV}{nkT}\right), \tag{8}$$

where Φ_{B0} is the zero bias Schottky barrier height. Therefore, in our case, $\Phi_{B0} = \Phi_{I-V}(0, T)$. If we assume (7) also true for $V = 0$,

$$\Phi_{I-V}(0, T) = \Phi_a(0, T) - \frac{q\sigma^2(0)}{2kT}.$$

Assuming $n_0 = 1$ (the ideal case), we obtain the expression as suggested by Werner and Güttler [17],

$$n^{-1}(T) - 1 = -\left(\frac{\Phi_{I-V}(V, T) - \Phi_{I-V}(0, T)}{V}\right) \tag{9}$$

and

$$n^{-1}(T) - 1 = -\varrho_a + \frac{q\varrho_b}{2kT}, \tag{10}$$

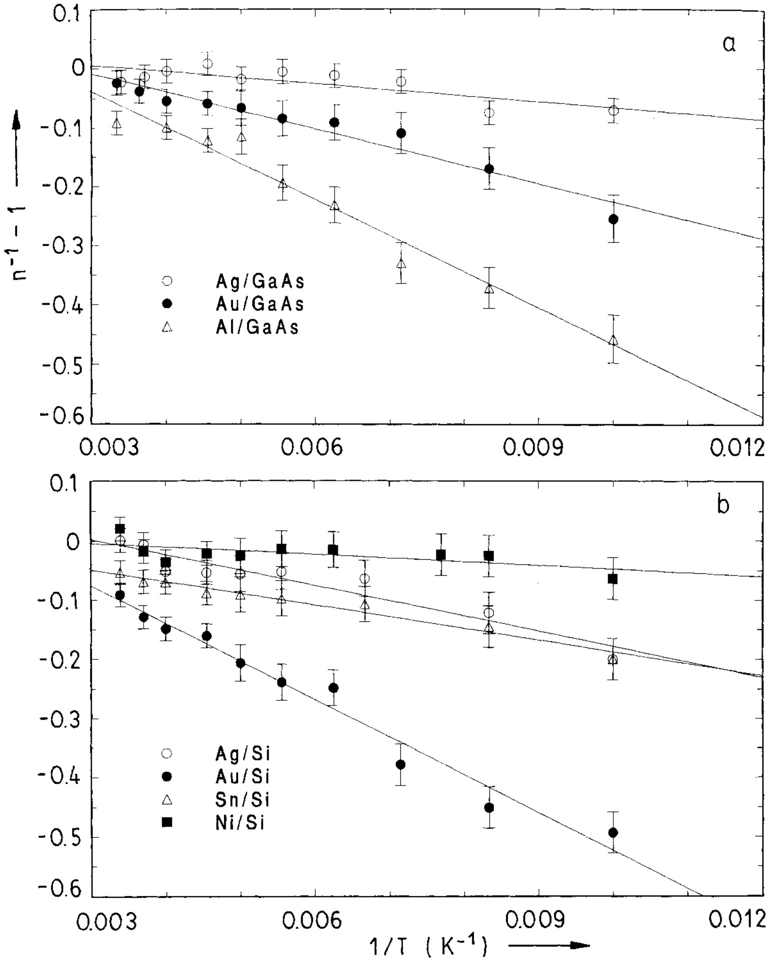

Fig. 2. The plot of $(n^{-1} - 1)$ against $1/T$ for a) GaAs diodes and b) Si diodes

where

$$\varrho_a V = \Phi_a(V, T) - \Phi_a(0, T)$$

and

$$\varrho_b V = \sigma^2(V) - \sigma^2(0) .$$

According to (10), a plot of $(n^{-1}(T) - 1)$ against $1/T$ should give a straight line with the slope and the y-axis intercept related to the voltage coefficient ϱ_b and ϱ_a, respectively. Fig. 2a and b show these plots for GaAs and Si diodes, respectively. All plots give a negative value for the slope which indicates that $\sigma^2(V) < \sigma^2(0)$ (for $V > 0$) as $\varrho_b V = \sigma^2(V) - \sigma^2(0)$. These values of ϱ_b indicate that the distribution of the barrier height becomes more homogeneous with voltage increase when the barrier maximum recedes to the semiconductor direction due to the image force lowering effect as suggested by Werner and Güttler [17]. As both b and ϱ_b can, to a certain extent, be viewed as parameters which indicate how well a Schottky diode will perform at different temperatures, the correlation between ϱ_b and the corresponding b-values for all diodes is investigated and plotted in Fig. 3. Since ϱ_b represents the sensitivity of $\sigma^2(V) - \sigma^2(0)$ to a voltage change (i.e. $\varrho_b = (\sigma^2(V) - \sigma^2(0))/V$), a large value of ϱ_b indicates that the barrier distribution at the interface is broader than that inside the semiconductor. In other words, it implies that the interface structure has more imperfections than the semiconductor bulk. As we can see from Fig. 3 ϱ_b becomes more negative as the value of b increases. This indicates that a large value of b signifies a deterioration of the contact uniformity.

Another important parameter that we are interested in is σ. Although ϱ_b can be used to estimate the difference between the values of σ^2 at the interface and in the inhomogeneous region, the rough order or the value of σ is not available from this approach. In order to estimate the value of σ at the interface, namely $\sigma(0)$, we can use equation (7) by putting $V = 0$ and obtain

$$\Phi_{I-V}(0, T) = \Phi_a(0, T) - \frac{q\sigma^2(0)}{2kT} . \tag{11}$$

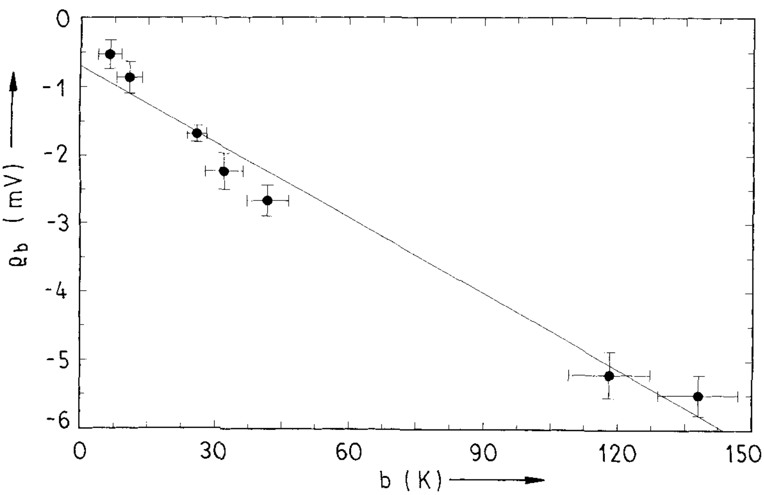

Fig. 3. The plot of ϱ_b against b for the experimental diodes

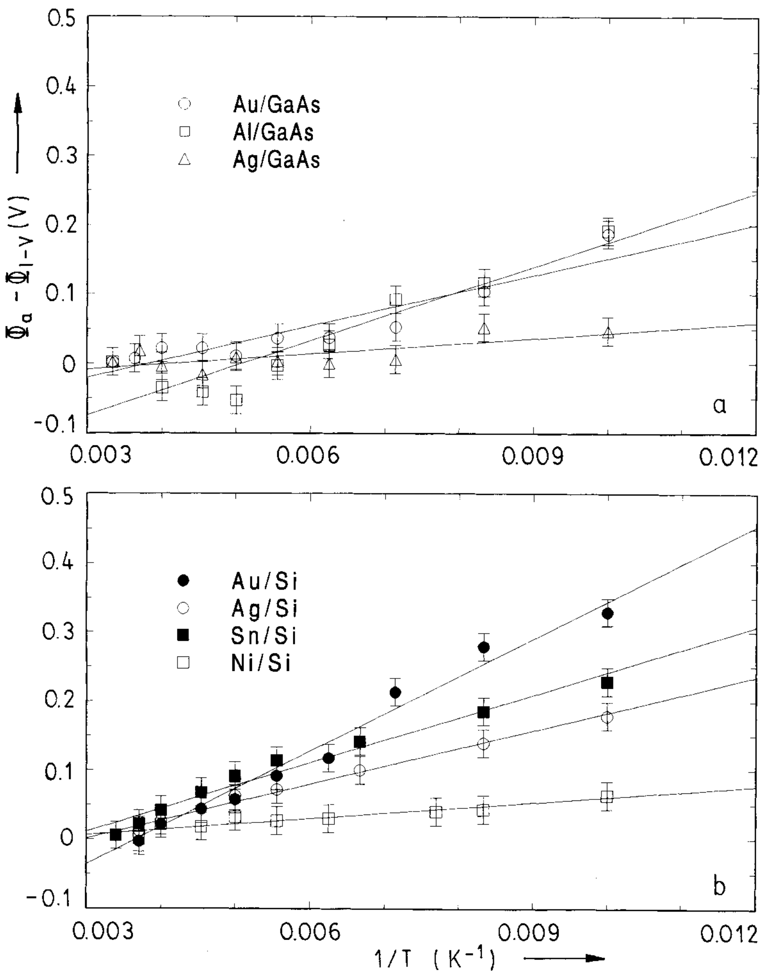

Fig. 4. The plot of $\Phi_a(0, T) - \Phi_{I-V}(0, T)$ against $1/T$ for a) GaAs diodes and b) Si diodes

From previous experiments concerning the temperature dependence of the barrier height measured by different methods, the value of $\Phi_{I-V}(0, T)$ at 300 K is very close to the corresponding barrier height obtained by $C-V$ and internal photoemission measurements [10, 11]. If we also assume $n(T)$ to be close to unity at room temperature, we can approximate the mean barrier height $\Phi_a(0, T)$ at room temperature by the value of $\Phi_{I-V}(0, T)$ with $T = 300$ K, i.e. Φ_{I-V} (0, 300 K). For the change of $\Phi_a(0, T)$ with temperature, according to previous studies [12], we can assume that $\Phi_a(0, T)$ follows the expression

$$\Phi_a(0, T) = \Phi_a(0, 300\ \mathrm{K}) + \Delta\Phi(T) \tag{12}$$

with

$$\Delta\Phi(T) = \begin{cases} \Delta E_g(T) & \text{for metal/Si contacts}\,, \\ 0 & \text{for metal/GaAs contacts}\,, \end{cases}$$

Table 2
Summary of the ϱ_b, b, and $\sigma(0)$ values of the experimental diodes

sample	b (K)	ϱ_b (mV)	$\sigma(0)$ (V)
Au/n-Si	138.0 ± 9.0	-5.50 ± 0.3	0.097 ± 0.005
Ni/n-Si	6.6 ± 2.0	-0.53 ± 0.2	0.037 ± 0.005
Sn/n-Si	26.0 ± 2.2	-1.68 ± 0.2	0.075 ± 0.004
Ag/n-Si	32.1 ± 4.2	-2.20 ± 0.3	0.067 ± 0.002
Au/n-GaAs	41.7 ± 5.0	-2.70 ± 0.3	0.065 ± 0.009
Al/n-GaAs	118.0 ± 9.0	-5.20 ± 0.3	0.078 ± 0.012
Ag/n-GaAs	11.0 ± 3.0	-0.87 ± 0.3	0.036 ± 0.01

where $\Delta E_g(T) = E_g(T) - E_g(300\text{ K})$ and $E_g(T) = E_g(0) - \alpha T^2/(T + \beta)$. For Si, $\alpha = 4.73 \times 10^{-4}$ eV K^{-1}, $\beta = 636$ K, and $E_g(300\text{ K}) = 1.17$ eV. From our assumption, (12) can further be approximated as

$$\Phi_a(0, T) = \Phi_{I-V}(0, 300\text{ K}) + \Delta\Phi(T)\,. \tag{13}$$

With this simple picture in mind, the value of σ can be estimated by plotting $\Phi_a(0, T) - \Phi_{I-V}(0, T)$ versus $1/T$, this plot should be a straight line with the slope equal to $\sigma^2 q/k$ (assuming that $\sigma(0)$ does not change significantly with temperature). Fig. 4a and b show the plots of $\Phi_a(0, T) - \Phi_{I-V}(0, T)$ versus $1/T$ for GaAs and Si diodes, respectively. It can be seen that all plots show well fitted straight lines among relevant points. The values of $\sigma(0)$ estimated from these plots and the corresponding values of b and ϱ_b are summarized in Table 2. Au/n-Si and Al/n-GaAs diodes have the largest values of $\sigma(0)$, ϱ_b, and b compared to the other diodes in their series. This indicates that the interface structure of Au/Si and Al/GaAs is more imperfect than that of other diodes.

In general, interface imperfections or disorder can be related to native oxide, contamination, intermixing of metal with semiconductors, and other surface defects at the interface. Since Au atoms can intermix with Si and are very effective recombination centres in Si [2], it is not surprising that the Au/Si diode has the largest values of ϱ_b, $\sigma(0)$, and b. Similarly, for the Al/GaAs diode, we envisage that the largest values of these parameters might be caused by the intermixing of Al with GaAs and other imperfections at the interface.

4. Conclusion

In this paper, the temperature dependence of n of the metal/Si and the metal/GaAs diodes has been investigated by different approaches. Both the n versus $1/T$ and $(n^{-1} - 1)$ versus $1/T$ plots have been used to estimate the effect of interface imperfection on the I–V characteristics of Schottky diodes. Important parameters such as ϱ_b and b have also been extracted for making comparisons. Further, using the inhomogeneity model and a number of assumptions, the values of $\sigma(0)$ for different sample diodes have been estimated.

The correlations between ϱ_b, $\sigma(0)$, and b show that the values of these parameters reflect the uniformity of the contact and the performance of a diode at low temperatures. However, some of the theories and assumptions adopted in describing the contact interface and estimating these parameters may be too simple to describe the complex current transport mechanism at the interface. Other factors such as thermionic field emission and the recombination current effect may not be negligible and may complicate the situation. These factors will affect the validity of the Gaussian distribution assumed in the inhomogeneity model and cause n_0 in (6) to depart from unity. Consequently, the accuracy of ϱ_b and $\sigma(0)$ may be affected. In spite of the above-mentioned shortcomings caused by the simple assumptions, we have shown in this work that the interface imperfection should be one of the possible causes which results in the temperature dependence of n and the barrier height. Moreover, the values of ϱ_b, $\sigma(0)$, and b obtained indicate consistently that the Au/Si and Al/GaAs diodes have the most imperfect contact interface amongst the sample diodes tested in this work.

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