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A view on barrier abnormalities in Schottky junctions

Murat Gülnahar[1]* and Yasemin Beyza GÜLNAHAR[2]

[1]*Department of Electric, Vocational School, Erzincan Binali Yıldırım University, 24200, Erzincan, Turkey*
[2]*Electrical-Electronics Engineering Department, Faculty of Technology, Gazi University, 06560, Ankara, Turkey*

*mgulnahar@erzincan.edu.tr *Email of the corresponding author*

Abstract **–** Potential distribution of the Schottky junctions allows the potential fluctuations model to be re-inspected depending on the temperature. In this work, the barrier anomalies are re-discussed in basis of the potential fluctuations model and is proposed a new approach of which predicts that there should be distinct barrier distribution for each one temperature in barrier. In addition, the potential structure of the junction predicts that the standard deviation values of the barrier should demonstrate a general temperature dependence. In these conditions, the thermoionic emission equation may be interpreted again. The theoretical results are performed successfully and it is obtained to the temperature dependence variations of the standard deviation and barrier height values at V=0 V. In consequence, it has been seen that the new approach may be applied succesfully to current-voltage data, and the results have enabled that the behaviors of the barrier anomalities in Schottky junctions are interpreted again.

Keywords – Schottky Diodes, Barrier Anomalies, Gaussian Distribution, Potential Fluctuations Model, Standard Deviation

I. INTRODUCTION

The current transport mechanism for a metal-semiconductor junction is called thermionic emission at the conditions in which all the carriers flows over the barriers and its general current equation is given by [1]

$$I = Io[exp((q(V - IRs))/nkT)] \qquad (1.a)$$

with

$$Io = AA * T2exp(-q\phi/kT) \qquad (1.b)$$

where T is the absolute temperature, k is the Boltzmann constant, q is the electronic charge, V is the applied voltage, n is the ideality factor, A* is the Richardson constant, ϕ is the apparent barrier height, A is the diode area and Rs is the series resistance. From a measured I-V curve using Eq. (1), ideality factor and apparent barrier height are determined easily with equations such as,

$$n = q/kT \;\; dV/(d(lnI)) \qquad (2.a)$$

$$\phi = -kT/q \; ln(Io/(AA * T2)) \qquad (2.b)$$

Ideality factor and apparent barrier height are important parameters which characterize the electronic properties of Schottky barrier. In addition, they can directly explain the performance of the junction.

The stability, reliability and performance of a diode are affected directly from the interface layer between the metal and semiconductor. The composition, quality and non-stoiometric structure of the interface, and the position of electrical charges in the interface are known as interface states. The interface states induce Schottky barrier inhomogeneities in the barrier and all barrier parameters such as ideality factor and barrier height are influenced from these anomalities.

n ideality factor includes the effects of the non-homogeneous dielectric interface layer. Why is it bigger than 1 is attributed to some factors such as tunelling currents in highly doped semiconductors [1], generation-recombination currents in the depletion region [1], interface states at a thin layer between the metal and semiconductor [2,3], image-force lowering of the Schottky barrier in electric field at the interface [4].

So far, various techniques and models have been developed to analyze the well-unknown nature of the interface [1,3-10]. However, the behaviour and structure of the interface is not understood well yet. One of the first important attempts relating to properties of the interface layer is the interface layer model which was firstly developed by Card and Rhoderick [2,5] and others [6]. The interface layer model suggests the idea of a thin insulating layer which has thickness and dielectric constant between metal and semiconductor. In addition, the localized electronic states exist in the oxidized insulator layer-semiconductor interface according to this approach [1,5]. Tung has considered that there are patches having different barrier heights which affect each other in a diode with pinch-off model [11]. The pinch-off effect takes into account the interaction among all the patches in a diode and it is to be the more interesting in the barrier conditions having large inhomogeneities. The parallel conduction model expresses the idea that the patches in the whole area of a diode do not affect each other and are not in an interaction among themselves [12]. According to this model, the total current is the sum of the currents flowing via the current filaments existing through the whole area. In the literature, it is seen that the models like the single-Gaussian [13], multi-Gaussian [10], constant [14] and log-normal [15] are frequently used to interpret Schottky barrier anomalies in the basis of the parallel conduction model. The Gaussian distribution functions are the preferred one due to their practicability and simplicity. Werner and Güttler's single-Gaussian distribution function is successful and meaningful to describe a barrier height distribution which has only a mean barrier height and standard deviation [13].

In the potential fluctuations model, the applied bias is emphasized as an effective factor which influences barrier structure and parameters due to the existing potential distribution of the interface [8,9]. According to this model, the bias is a single parameter which affects the composition and potential structure of the interface. For example, this model does not consider the effect of temperature. However, in the literature, it is interpreted frequently that the barrier height and ideality factor are dependent on the temperature [8-12]. Therefore, the potential fluctuations model without considering the effects of the temperature is insufficient.

In this paper, our purpose is to analyze the effect of barrier inhomogeneities in a contact structure on some barrier parameters by depending on temperature. Therefore, we re-interpreted the potential fluctuations model and thermionic emission equation. The results were applied succesfully on temperature-dependence I-V data of an Al/p-Si sample [16].

II. MATERIALS AND METHOD

The thermionic emission theory predicts an abrupt junction structure having no interface between metal and semiconductor, but it is not true. Understanding the nature of the interface structure is a key point for junction studies. The interface is not atomically flat or spatially homogeneous, as seen in Fig. 1. However it is rough and complicated with its non-homogeneous thickness and composition [13]. In the interface, there are various mechanisms which affect its potential distribution and arise from the metal-interface and semiconductor-interface interactions. Dislocations and semiconductor donor atoms in the vicinity of the interface is one of these mechanisms. The

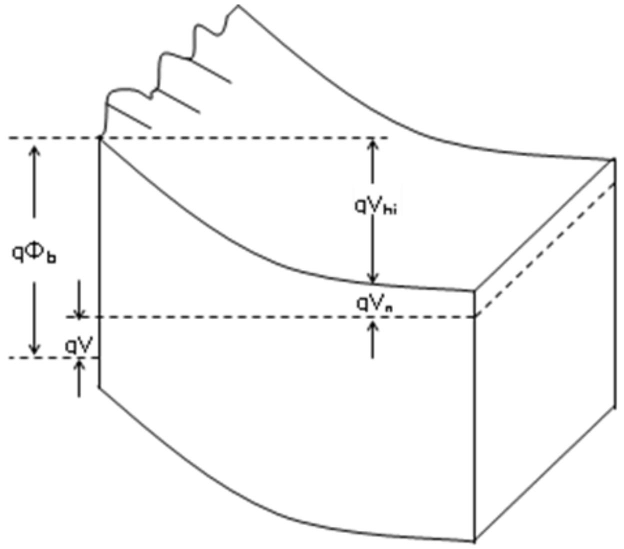

Figure 1. Two-dimensional band diagram according to potential fluctuations model of non-abrupt Schottky contact.

distances between the donors are irregular and are not arranged in regular lattices and are randomly distributed.

In the interface, there are various mechanisms which affect its potential distribution and arise from the metal-interface and semiconductor-interface interactions. Dislocations and semiconductor donor atoms in the vicinity of the interface is one of these mechanisms. The distances between the donors are irregular and are not arranged in regular lattices and are randomly distributed. Additionally, atomic steps, dislocations, grain boundaries in metal and/or polycrystalline structure and thickness modulation of the metal influence the interface structure. As a result, the potential distribution of the interface continuously presents the hills and valleys in the ridges of the potential barriers [13].

Fig. 2.(a) depicts the plot of n ideality factor versus V bias of an Al/p-Si/Al Schottky diode at 180 K. I-V curve at 180 K was arbitrarily chosen because it has a larger thermal emission region among the measured I-V curves depending on the temperature of Al/p-Si/Al. The values of n(V) may be obtained as a function of the temperature to compare their behaviours in different temperatures.

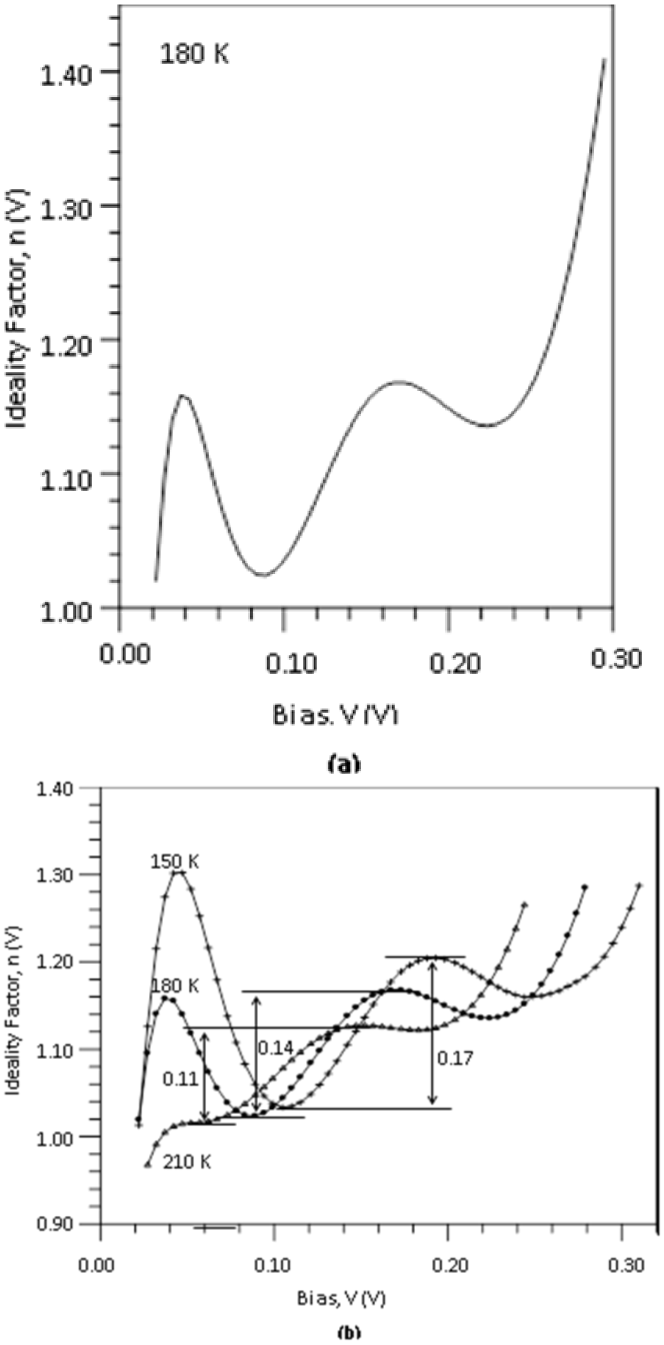

Figure 2 (a-b). **(a)** The variation of n (V) dependent to applied bias in 180 K. **(b)** The plot of n (V) versus applied bias for 150 K, 180 K and 210 K temperatures.

Fig. 2.(b) shows the plot of n(V) versus bias within the limitations of their thermal emission regions for 150 K, 180 K and 210 K of Al/p-Si/Al. In addition, the values of n(V) were calculated to be 1.20, 1.15 and 1.13 in 150 K, 180 K and 210 K for 0.2 V bias values chosen arbitrarily, respectively. Hence, it may be noted that it demonstrates dependence to the temperature even at a constant voltage. As seen in

Fig. 2.(b), the position of the peaks varies with temperature and follow each other in the direction of increasing bias. Height and width of the peaks increase generally with decreasing temperature, especially in the range of 0-0.1 V. Height of the peaks which follow each other for each temperature was obtained to be 0.17 between 0.1-0.19 V at 150 K, 0.14 between 0.09-0.17 V at 180 K, and 0.11 between 0.06-0.16 V at 210 K. Thus, it may be interpreted that the position and height of the peaks change depending on the temperature. As a result, temperature is effective on the fluctuation of n(V).

The ideality factor is a very effective parameter which reflects clearly the structure of the interface and barrier. The behaviour of n(V) in Fig. 2 (a-b) is due to Schottky barrier inhomogenities induced by the interface. The peaks in the plot of n(V) versus applied bias V are attributed to the existence of the interface states in the literature [17-22].

Maeda [22] presents a defect model of Schottky barrier inhomogeneities on the basis of MIGS model. According to, Maeda's MIGS model, the relationship of the standard deviation with the applied voltage is expressed as,

$$\sigma 2 = \sigma o2\ (1 - V/\phi) \qquad (3)$$

In addition, the relationship between barrier height and ideality factor is expressed as [23],

$$\phi e = \phi b + (1 - 1/n)\mathrm{V} \qquad (4)$$

In Gaussian distribution model, σ is obtained by linear fittings of the distribution regions which present separate linear variations of the barrier height from the plot of versus 1/T according to the following equation,

$$\phi e = \phi b - \left(\frac{q\sigma 2}{2kT}\right) \qquad (5)$$

If Eqs. (4) and (5) are reorganized, the relationship between σ and n may be given by

$$\sigma 2 = -2kT/q\ (1 - 1/n)\mathrm{V} \qquad (6)$$

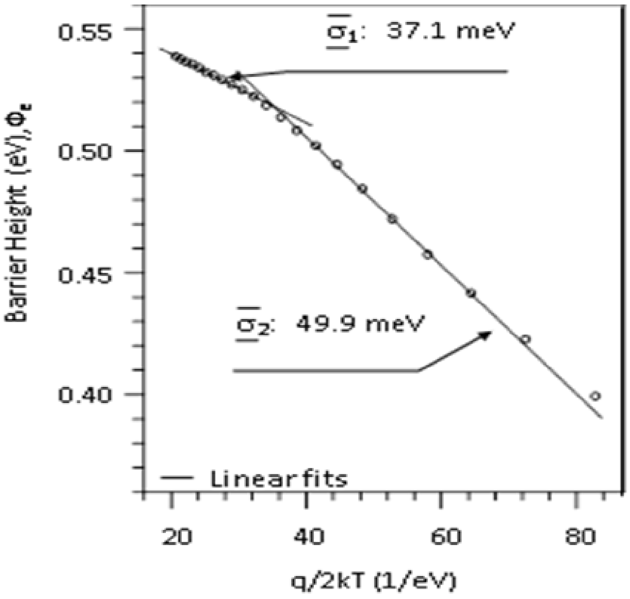

Figure 3. The variation of ϕ_e apparent barrier height versus q/2kT between 70-280 K temperature range of Al/p-Si/Al and discrete linearfits.

The values of barrier height ϕe and standard deviation σ have so far been calculated using Eq. (6) as the mean values for each distinct distribution region existing in the plot of versus 1/T. The values of barrier height and standart deviation have so far been calculated using Eq. (5) as the mean values for each distinct distribution region existing in the plot of versus 1/T.

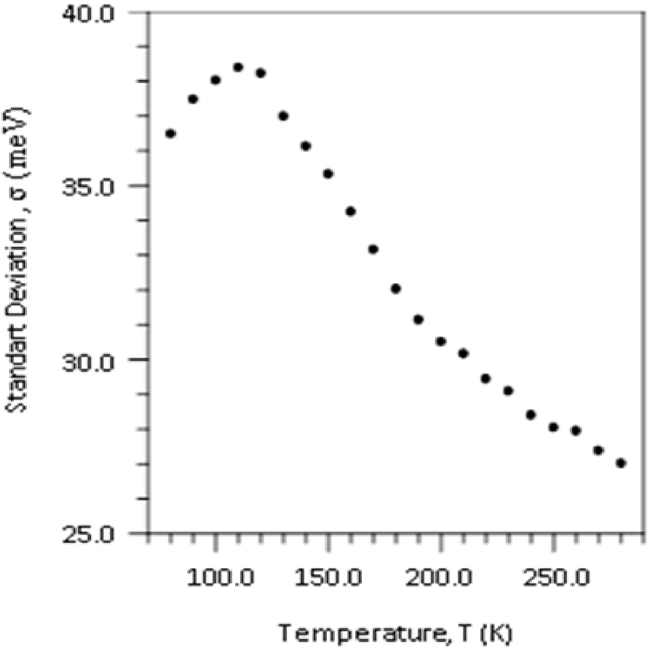

Figure 4. The plot of σ standart deviation versus temperature of Al/p-Si.

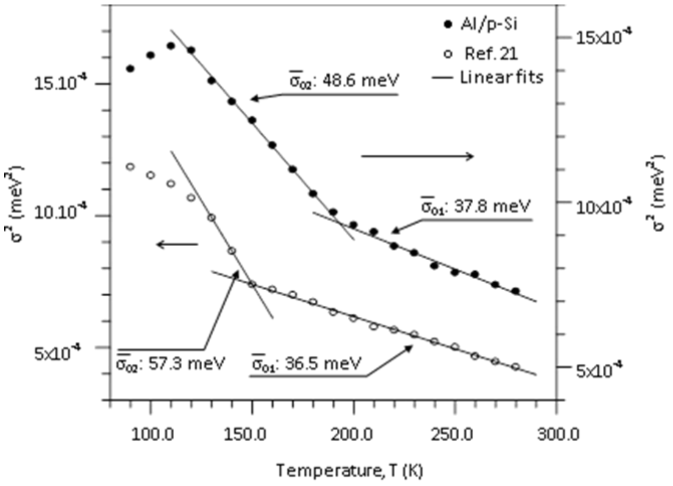

Figure 5. The plot of σ^2 versus temperature of Au/p-GaTe in Ref. [17] and Al/p-Si/Al and discrete linear fits.

Fig. 3 presents the plot of ϕ versus 1/T for the Al/p-Si sample in which it is clear that two distinct linear regions exist. These linear regions express that there are two Gaussian distribution regions for Al/p-Si. From Fig. 3, the mean values of σ and ϕ according to classic, single-Gaussian approaches are calculated to be 37.1 meV and 49.9 meV, and 0.567 eV and 0.604 eV by linear fits to the distribution regions using Eq. (5).

The values of the standard deviation σ and the barrier height ϕ at 280 K and 110 K were calculated to be 27.0 meV and 38.3 meV and, 0.553 eV and 0.557 eV, respectively using Eqs. (5) and (6). In addition, the variation of σ versus temperature is presented in Fig. 4. As seen in Fig. 5, σ increases steadily until nearly 110 K with decreasing temperature and deviates unsteadily for temperatures lower than nearly 110 K.

In contact structures which are ideal or close to ideal, it is expected that the values of standard deviation σ and ideality factor n should be 0 and 1, respectively. However, as seen in Fig. 4, the values of σ are very big than 0 especially at low temperatures due to the barrier anomalies. σ increases more rapidly at low temperatures. This variation of σ with the temperature demonstrates clearly that the barrier inhomogeneities and interface state density change with the temperature.

Fig. 5 shows the plot of σ^2 versus T for Au/p-GaTe/In [17] and Al/p-Si samples. In Fig. 5, two linear regions exist for the standard deviation values, as seen in the variations of ϕ versus for both Al/p-Si and Au/p-GaTe/In [17]. Thus, it may be expressed that there are distinct distribution regions for the standard deviation σ, as shown for the barrier height distribution in Fig. 4. These regions for σ are due to the effect of inhomogeneities which are close to each other in the same distribution region.

III. CONCLUSION

The potential distribution of the interface has a structure which causes the spatial barrier inhomogeneities and can change the current mechanism of the junction. The n ideality factor relates closely to the potential distribution of the interface in the junction. We have reviewed dependence of n the ideality factor on applied bias and have determined that n ideality factor fluctuates with bias. In addition, these fluctuations of n(V) are related to the Schottky barrier inhomogeneities and have grown and expanded when the temperature is reduced. As a result, an idea were developed showing that temperature and bias together are active parameters in potential distribution of the interface.

The temperature is an effective parameter in the Schottky barrier. When the temperature of the junction is reduced, the n ideality factor increases, the barrier height decreases generally due to the effect of increasing barrier anomalies. In reality, the barrier can have distribution regions because of existing potential structure of the junction and these distribution regions are not independent from the temperature.

Finally, we have discussed here the potential fluctuations model in detail and proposed a new approach on the basis of this model. We have reported that there are distinct barrier distributions for each temperature, and the patch currents are functions of the temperature. σ values of our samples are calculated for each measurement temperature.

Consequently, it should be noted that our model is appropriate to characterize I-V measurements. Our results suggest that the potential barrier distribution of a real contact structure cannot be depicted with a single-Gaussian distribution model which assumes that the barrier parameters are independent from the temperature.

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