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# The analysis of $I$–$V$ characteristics of Schottky diodes by thermionic emission with a Gaussian distribution of barrier height

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ABSTRACT

The current–voltage ($I$–$V$) characteristics of Al/p-Si Schottky barrier diode (SBD) with native insulator layer were measured in the temperature range of 178–440 K. The estimated zero-bias barrier height $\Phi_{Bo}$ and the ideality factor $n$ assuming thermionic emission (TE) theory have shown strong temperature dependence. Evaluation of the forward $I$–$V$ data have revealed an increase of zero-bias barrier height $\Phi_{Bo}$ but the decrease of ideality factor $n$ with the increase in temperature. The experimental and theoretical results of the tunneling current parameter $E_o$ against $kT/q$ were plotted to determine predominant current-transport mechanism. But the experimental results were found to be disagreement with the theoretical results of the pure TE, the thermionic-field emission (TFE) and the field emission (FE) theories. The conventional Richardson plot has exhibited non-linearity below 240 K with the linear portion corresponding to the activation energy of 0.085 eV and Richardson constant ($A^*$) value of $2.48 \times 10^{-9}$ A cm$^{-2}$ K$^{-2}$ which is much lower than the known value of 32 A cm$^{-2}$ K$^{-2}$ for holes in p-type Si. Such behaviours were attributed to Schottky barrier inhomogeneities by assuming a Gaussian distribution of barrier heights (BHs) due to barrier height inhomogeneities that prevail at interface. Thus, the modified $\ln(I_o/T^2) - q2\sigma o2/2k^2T^2$ vs q/kT has plotted. Then $A^*$ was calculated as 38.79 A cm$^{-2}$ K$^{-2}$ without using the temperature coefficient of the barrier height. This value of the Richardson constant 38.79 A cm$^{-2}$ K$^{-2}$ is very close to the theoretical value of 32 A K$^{-2}$ cm$^{-2}$ for p-type Si. Hence, it has been concluded that the temperature dependence of the forward $I$–$V$ characteristics of the Al/p-Si Schottky barrier diodes with native insulator layer can be successfully explained on the basis of TE mechanism with a Gaussian distribution of the barrier heights.



## 1. Introduction

The mechanisms of carrier transport and some structural parameters of SBDs have been studied both experimentally and theoretically in past decades, but little experimental information is available on Schottky barrier formation and electronic states at metal–semiconductor (MS) interface [1–24]. It has been generally assumed that the thin insulating layer between the metal and semiconductor is uniform and has distinct effect on the behaviour of MS-diodes. In recent years, there are a vast number of reports on experimental studies of characteristic parameters such as the barrier height and ideality factor in MS or, metal–insulator–semiconductor (MIS) Schottky diodes and solar cells [1–17]. Also theoretical studies based on the effect of a Gaussian distribution of barrier height (BH) on $I$–$V$ characteristics have also been reported in literature [25–42]. The performance and reliability of these devices especially depend on the formation of insulator layer between metal and semiconductor interface, inhomogeneities of Schottky barrier contacts and series resistance of diodes. The analysis of the $I$–$V$ characteristics of these devices on the basis of thermionic emission–diffusion (TED) theory of current transport usually reveals an abnormal decrease of zero-bias barrier height $\Phi_{Bo}$ and the increase of ideality factor $n$ with decrease of temperature [5–15]. This abnormal behaviour of $I$–$V$ characteristics of MS contacts at low temperatures has been attributed to the barrier inhomogeneities present in MS contacts. The decrease in the barrier height at low temperatures in fact leads to the non-linearity in the activation energy ($\ln(I_o/T^2)$ vs $1/T$ or $1/nT$) plot. Thus, it is found to be non-linear by the temperature dependence of the barrier height and the ideality factor.

In this study, the forward bias $I$–$V$ characteristics of Al/p-Si Schottky barrier diodes with native insulator layer were measured over the temperature range of 178–440 K. The experimental results shows that the barrier height and ideality factor determined from forward bias $I$–$V$ characteristics were found to be strong function of temperature. The ideality factor $n$ was found to decrease, while the BH increases with the increasing temperature. In addition, the experimental and theoretical results of the $E_o$ against $kT/q$ were plotted to determine predominant current-transport

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mechanism. But the experimental results were found to be disagreement with the theoretical results of the pure TE, TFE and FE theories. Such behaviours of Schottky barrier characteristics of the diodes were interpreted on basis of the existence of Gaussian distribution of the BHs around a mean value due to BH inhomogeneities prevailing at the metal–semiconductor interface.

## 2. Experimental procedure

The Al/p-Si diodes were prepared on a quarter of 2 in. diameter float zone ⟨1 0 0⟩ p-type (boron doped) single crystal silicon layer having thickness of 400 μm with 8 Ω cm resistivity. The samples were ultrasonically degreased by dipping into iso-propyl alcohol and washed with de-ionized water with resistivity of 18 MΩ cm. After chemically etched with a $CP_4$ ($HF:CH_3COOH:HNO_3$:1:1:2) solution for 5 min, the native oxide layer on the front surface of the substrate was removed in $HF:H_2O$ (1:10) solution and finally the wafer was rinsed in de-ionized water of 30 s. The aluminum (Al) back contact (with a thickness of 2000 Å) was thermally evaporated by means of a tungsten filament onto the whole back of silicon crystal under the pressure $2 \times 10^{-6}$ Torr. The low resistivity ohmic back contact to p-type Si wafers was made by using high purity Al, and followed by a temperature treatment at 450 °C for 15 min in dry nitrogen ($N_2$) atmosphere. The Schottky contacts were formed onto front face of Si by evaporation of high purity Al dotes with diameter of about 2 mm. The current–voltage (*I–V*) measurements were performed by the use of a Keithley 220 programmable constant current source, a Keithley 614 electrometer in the temperature range of 178–440 K using a temperature controlled Janes vpf-475 cryostat, which enables us to make measurements in the temperature range of 77–450 K. The sample temperature was always monitored by using a copper–constantan thermocouple close to the sample and measured with a dmm/scanner Keithley model 199 and a Lake Shore model 321 auto-tuning temperature controllers with sensitivity better than ±0.1 K.

## 3. Results and discussions

### 3.1. Temperature dependence of the forward bias I–V characteristics

Fig. 1 shows the semi-logarithmic *I–V* characteristics of the Al/p-Si Schottky barrier diodes with native insulator layer, measured at different temperatures over the range of 178–440 K. The current through a SBD at a forward bias ($V \geqslant 3kT/q$), according to TE theory, is given by [1]

$$I = I_o \exp\left(\frac{qV}{nkT}\right)\left[1 - \exp\left(-\frac{qV}{kT}\right)\right] \tag{1}$$

where $I_o$ is the reverse saturation current defined by

$$I_o = AA^{*}T^2 \exp\left(-\frac{q\Phi_{B0}}{kT}\right) \tag{2}$$

where $q$ is the electronic charge, $A^*$ is the effective Richardson constant and equals to 32 A $cm^{-2}$ $K^{-2}$ for p-type Si, $A$ is the effective diode area, $k$ is the Boltzmann constant, $T$ is the absolute temperature, $\Phi_{B0}$ is the zero-bias barrier height and $n$ is the ideality factor.

The reverse saturation current $I_o$ was obtained by extrapolating the linear intermediate voltage region of the curve to zero-applied voltage. The apparent zero-bias barrier height $\Phi_{B0}$ values was calculated at each temperature from Eq. (2) based on pure TE shown in Table 1. The experimental values of $\Phi_{B0}$ and $n$ were changed from 0.496 eV and 4.00 (at 178 K) to 1.131 eV and 1.41 (at 440 K). As seen is Table 1, while the ideality factor decreases with increasing temperature the zero-bias barrier height increases with increasing temperature. The temperature coefficient β of barrier height is calculated 2.4 meV (Fig. 2). This temperature dependence is an obvious disagreement with the reported negative temperature coefficient of $\Phi_{B0}$. Moreover the value of $\Phi_{B0}$ at 0 K is found to be 0.07 eV (Fig. 2) which is small when compared to usual value.

The ideality factor is determined from the slop of the linear region of the forward bias ln(*I*)–*V* characteristics through the relation as

$$n = \frac{q}{kT}\left(\frac{dV}{d(\ln I)}\right) \tag{3}$$

**Table 1**
Temperature dependent values of various diode parameters determined from *I–V* characteristics of Al/p-Si Schottky barrier diodes in the temperature range of 178–440 K.

| *T* (K) | $I_o$ (A) | *n* | $\Phi_{B0}$ (eV) | *nT* |
|---|---|---|---|---|
| 178 | $9.5 \times 10^{-9}$ | 4.00 | 0.496 | 712 |
| 208 | $1.6 \times 10^{-8}$ | 3.35 | 0.576 | 697 |
| 240 | $3.2 \times 10^{-8}$ | 2.80 | 0.656 | 673 |
| 300 | $1.2 \times 10^{-7}$ | 2.33 | 0.797 | 700 |
| 440 | $7 \times 10^{-7}$ | 1.41 | 1.131 | 619 |

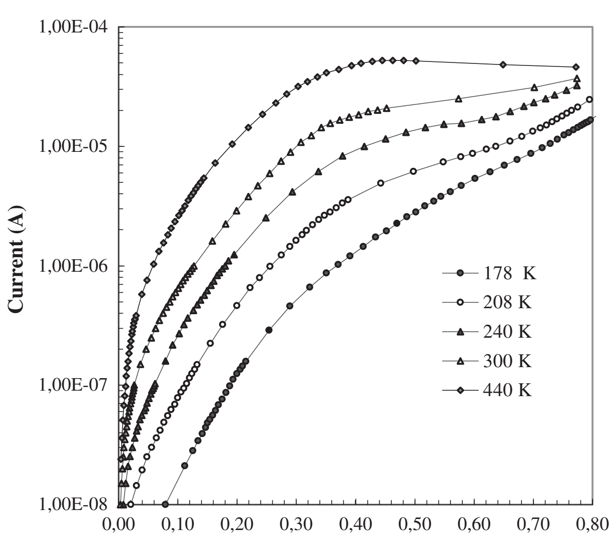


**Fig. 1.** The experimental forward bias *I–V* characteristics of the Al/p-Si Schottky barrier diode at various temperatures.

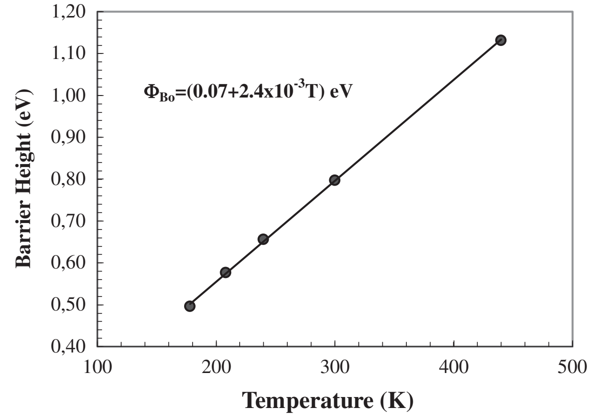


**Fig. 2.** Temperature dependence of zero-bias barrier height for Al/p-Si Schottky barrier diode.

Also, the voltage dependent ideality factor can be written from Eq. (1) as

$$n(V) = \frac{qV}{kT\ln(I/I_o)} \tag{4}$$

It is well known that $n = 1$ for an ideal diode. Ideality factors between 1.01 and 1.02 can be expected due to image force lowering of the Schottky barrier at the interface [35]. However, $n$ has usually a value greater than unity. High values of $n$ can be ascribe to the presence of the interfacial thin native oxide layer, series resistance, etc. [36]. However, the barrier inhomogeneities have been very important to explain for the higher values of the ideality factor. For example, interface defects may cause a lateral inhomogeneous distribution of barrier heights at the interface which results in larger ideality factors, and the charge transport across the interface only is no longer due to thermionic emission [37–40]. Fig. 3 shows a plot of the experimental BH versus the ideality factor for various temperatures. As can be seen in this figure the BHs become smaller as the ideality factors increase. The straight line in Fig. 3 is the least squares fit to the experimental data. That is, there is a linear relationship between experimental effective BHs and ideality factors of Schottky contacts.

This finding can be attributed to lateral barrier inhomogeneities in Schottky to be caused by grain boundaries, multiple phases, facets, defects, a mixture of different phases, etc. [38]. The extrapolation of the experimental BHs versus ideality factors plot to $n = 1$ has given a laterally homogeneous BH of approximately 1.17 eV. Thus, it can be said that the significant decrease of the zero-bias BH and increase of the ideality factor especially at low temperature are possibly caused by the BH inhomogeneities [37–44].

To evaluate the BH in another way, we use the Richardson plot of reverse saturation current $I_o$. By taking the natural logarithm of Eq. (2), one can obtain

$$\ln\left(\frac{I_o}{T^2}\right) = \ln(AA^*) - \frac{q\Phi_{B0}}{kT} \tag{5}$$

The conventional energy variation of $\ln(I_o/T^2)$ vs $1000/T$ plot is found to be non-linear in the temperature range measured. However, the $\ln(I_o/T^2)$ vs $1000/nT$ plot gives a straight line as shown in Fig. 4. The non-linearity of the $\ln(I_o/T^2)$ vs $1000/T$ plot is caused by the temperature dependence of the barrier height and ideality factor. However, the experimental data are shown to fit asymptotically with a straight line above 240 K, yielding an activation energy of 0.08 eV, and the Richardson constant ($A^*$) value of $2.48 \times 10^{-9}$ A cm$^{-2}$ K$^{-2}$ is determined from intercept at the ordinate of this experimental plot, which is much lower than the known value of 32 A cm$^{-2}$ K$^{-2}$ for p-Si. This deviation in the $A^*$ may be due to the spatial inhomogeneous barrier heights and potential fluctuation at the interface that consist of low and high barrier areas [8,16,17,27,35]. Furthermore, the value of the Richardson constant obtained from the I–V characteristics as a function of temperature may be affected by the lateral inhomogeneity of the barrier.

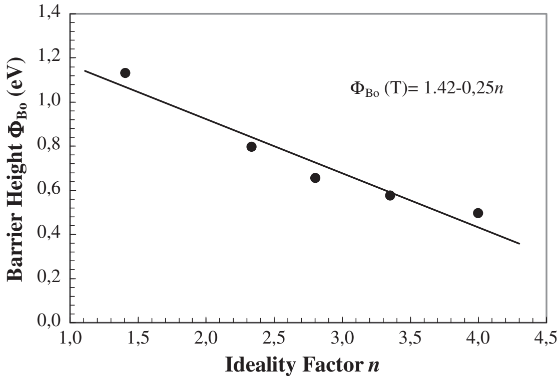


**Fig. 3.** Linear variation of apparent barrier height vs ideality factors at various temperatures.

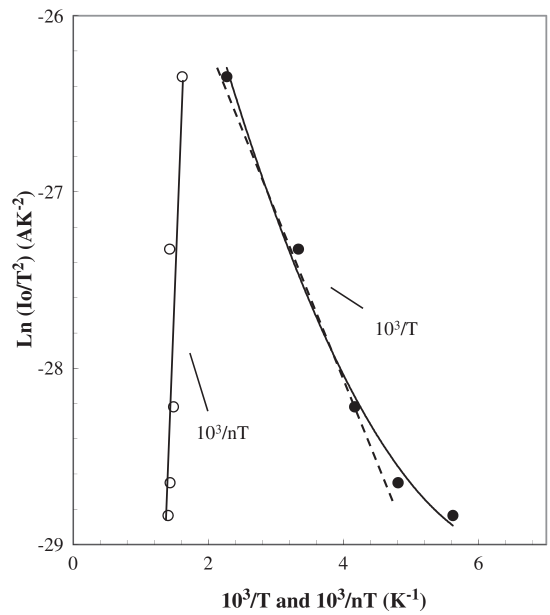


**Fig. 4.** Richardson plots of the $\ln(I_o/T^2)$ versus 1000/T and 1000/nT for Al/p-Si Schottky barrier diode.

The BH, obtained from Eq. (2) called apparent or zero-bias barrier height, which increase with the increasing temperature of Schottky contact depending on the electrical field across the contact and consequently on the applied bias voltage.

The ideality factor increasing with the decreasing temperature was found to change linearly in Fig. 5 with the inverse temperature as

$$n(T) = n_o + T_o/T \tag{6}$$

where the $n_o$ and $T_o$ are constant which were found to be −0.29 and 760.2 K, respectively. The increase in the ideality factor with the decreasing temperature is known as $T_o$ effect [39]. However, the

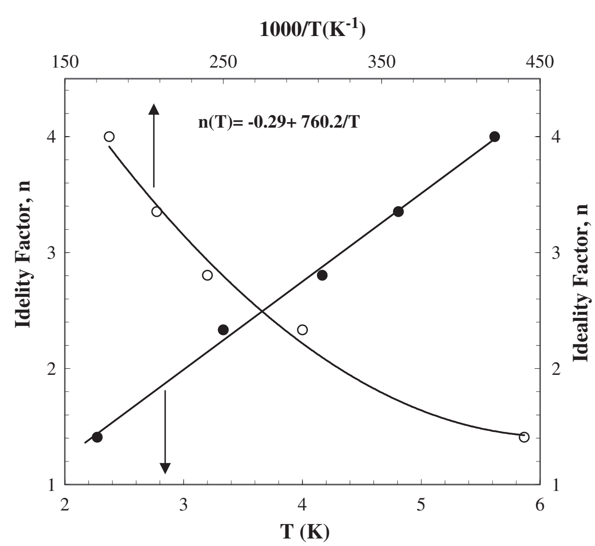


**Fig. 5.** The plot of $n$–$T$ and 1000/$T$ for the Al/p-Si Schottky barrier.

ideality factor is further analyzed by plotting $E_o$ (tunnelling current parameter) against $kT/q$ in Fig. 6 which shows the experimental and theoretical results of this plots to investigate the main dominant carrier transport mechanisms. The TFE theory requires a change in tunnelling current parameter $E_o$ with temperature according to relation of $E_o = nkT/q = E_{oo}\coth(qE_{oo}/kT)$ with $E_{oo} = h/4\pi(N_A/m^*\varepsilon_S)^{1/2}$ where $m^*$ is the effective mass of holes and $\varepsilon_S$ the permittivity of Si and the other symbol are of usual meaning [2,3,10]. The FE theory is an unlikely current-transport mechanism, since it would be predominate only at quite low temperatures for the semiconductor material having high doping concentrations, which is not the case for the Si substrate used in the present work. The TFE mechanism can be dominant in observed region, since $nT$ is not constant in this temperature range as shown in Table 1. However Padovani and Stratton [10] have pointed out that at only high temperatures and doping levels, TFE is responsible for current transport. Therefore, the possibility of the FE and TFE for our sample can easily be ruled out. The disagreement with the theoretical results of the pure TE, TFE and FE theories may be related to TE over a Gaussian barrier height distribution [8,33,45,46].

### 3.2. The analysis of the inhomogeneous barrier and modified Richardson plot

To explain commonly observed abnormal deviations from classical TE, some authors [7,34] have considered a system of discrete low-barrier regions embedded in a uniform background of higher-barrier material. These abnormal behaviours can be explained by assuming a Gaussian distribution of barrier height with a mean value $\overline{\Phi}_{B0}$ and standard deviation $\sigma_s$, which can be given as [16,21,27,31,32]

$$P(\Phi_B) = \frac{1}{\sigma_s\sqrt{2\pi}}\exp\left[-\frac{(\Phi_B - \bar{\Phi}_B)^2}{2\sigma_s^2}\right] \tag{7}$$

where $1/\sigma_s\sqrt{2\pi}$ is the normalization constant of the Gaussian barrier height distribution. The total $I(V)$ across a Schottky diode containing barrier inhomogeneities can be expressed as

$$I(V) = \int_{-\infty}^{+\infty} I(\Phi_B, V)P(\Phi_B)d\Phi \tag{8}$$

where $I(\Phi_B, V)$ is the current at a bias $V$ for a barrier of height based on the ideal TED theory and $P(\Phi_B)$ is the normalized distribution function giving the probability of accuracy for barrier height. Now, introducing $I(\Phi_B, \mathrm{V})$ and $P(\Phi_B)$ into Eq. (10) from (1) and (9), and performing the integration from $-\infty$ to $+\infty$, one can obtain the current $I(V)$ through a Schottky barrier at a forward bias $V$, similar to Eq. (1) and (2) but with the modified barrier

$$I(V) = AA^*T^2 \times \exp\left[-\frac{q}{kT}\left(\bar{\Phi}_{B0} - \frac{q\sigma_s^2}{2kT}\right)\right]\exp\left(\frac{qV}{n_{ap}kT}\right)\left[1 - \exp\left(-\frac{qV}{kT}\right)\right] \tag{9}$$

with

$$I_o = AA^*T^2\exp\left(-\frac{q\Phi_{ap}}{kT}\right) \tag{10}$$

where $\Phi_{ap}$ and $n_{ap}$ are the apparent barrier height and apparent ideality factor, respectively, and are given by [6,31]

$$\Phi_{ap} = \bar{\Phi}_{B0}(T=0) - \frac{q\sigma_s^2}{2kT} \tag{11}$$

$$\left(\frac{1}{n_{ap}-1}\right) = \rho_2 - \frac{q\rho_3}{2kT} \tag{12}$$

It is assumed that the mean BH $\overline{\Phi}_{B0}$ and $\sigma_s$ are linearly bias dependent on Gaussian parameters, such as $\overline{\Phi}_{B0} = \overline{\Phi}_{B0} + \rho_2 V$ and standard deviation $\sigma_s = \sigma_{so} + \rho_3 V$, where $\rho_2$ and $\rho_3$ are voltage coefficients which may depend on temperature, quantifying the voltage deformation of the BH distribution [29,31,33]. The temperature dependence of $\sigma_s$ is usually small and can be neglected [13]. It is obvious that the decrease of zero-bias barrier height is caused by the existence of the Gaussian distribution and the extent of influence is determined by the standard deviation itself. Also, the effect is particularly significant at low temperatures. Fitting of the experimental data in Eqs. (2), (12) and in Eq. (3) gives $\Phi_{ap}$ and $n_{ap}$ at zero-bias respectively which should obey Eqs. (13) and (14). Thus, the plot of $\Phi_{ap}$ vs $q/2kT$ (Fig. 7) should be a straight line that gives $\overline{\Phi}_B$ $(T = 0) = 1.19$ eV and $\sigma_s = 0.17$ V from the intercept and slope, respectively. Clearly, the diode with the best rectifying performance presents the best barrier homogeneity with the lower value of standard deviation. It was seen that the value of $\sigma_s = 0.17$ V is not very small compared to the mean value of $\overline{\Phi}_B = 1.19$ eV, indicating the presence of the interface inhomogeneities. Furthermore the temperature dependence of $\Phi_{ap}$ (Fig. 7) is nearly temperature independent. As was reported in certain Refs. [25,27,29,34,36], barrier inhomogeneities can occur as a result of inhomogeneities in the composition of the interfacial oxide layer thickness. The standard deviation is a measure of the barrier inhomogeneity. The lower value of $\sigma_s$ corresponds to a more homogeneous barrier height. Nevertheless, this inhomogeneity and potential fluctuation dramatically affect low temperature $I$–$V$ characteristics.

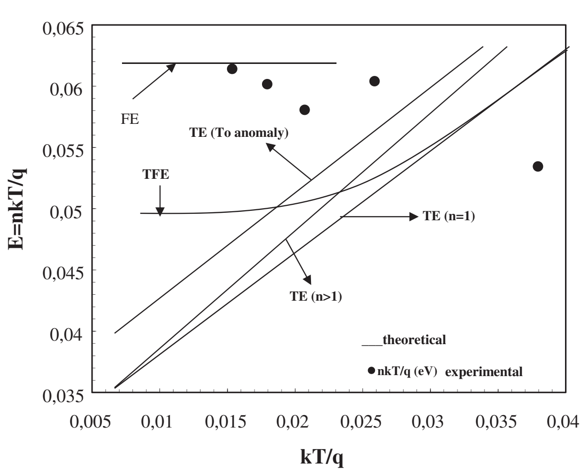


**Fig. 6.** The experimentally and theoretically found tunnelling current parameter $E_o$ ($nkT/q$) vs $kT/q$ for Al/p-Si Schottky diode.

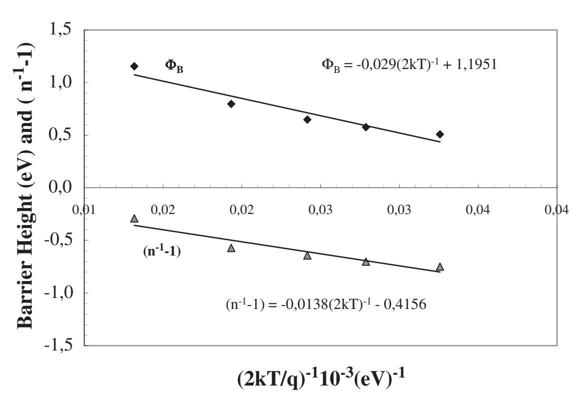


**Fig. 7.** Zero-bias apparent barrier height and ideality factor vs $1/T$ curves of the Al/p-Si Schottky diode according to Gaussian distribution of barrier height.

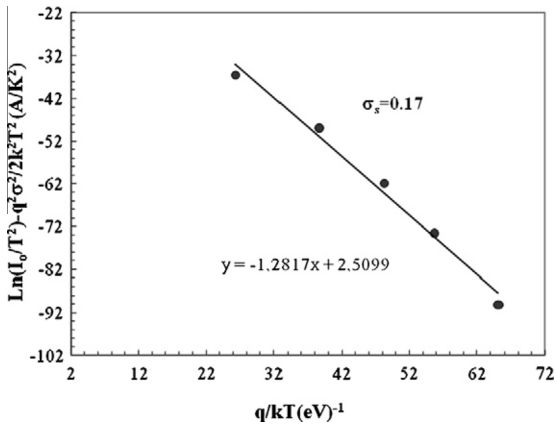


**Fig. 8.** Modified Richardson Ln($I_0/T^2$)-$q^2\sigma^2/2kT^2$ vs $1/T$ plot for the Al/p-Si Schottky diode according to Gaussian distribution of barrier height.

The temperature dependence of ideality factor can be understood on the basis of Eq. (14). Fitting showing ideality factor $n$ in Fig. 7 is a straight line that gives voltage coefficient $\rho_2$ and $\rho_3$ from the intercept and slope of the plot where $\rho_2 = -0.0138$ V and $\rho_3 = -0.415$ from the experimental data. The linear behaviour of the plot shows that the ideality factor expresses the voltage deformation of the Gaussian distribution of the SBD. Based on [16], Yıldırım and Türüt [47] stated that the coefficients $\rho_2$ and $\rho_3$ quantify the voltage deformation of the BH distribution, that is, the voltage dependencies of the mean BH and the barrier distribution width are given by coefficients $\rho_2$ and $\rho_3$, respectively. According to Eq. (6) in [47], the coefficients $\rho_2$ and $\rho_3$ are not dependent of temperature. In fact, one of the central features of this model is that it identifies the ideality factor as a representation of the voltage deformation at an inhomogeneous interface [47].

If the value of $\rho_2$ is negative, the BH should decrease with increasing forward bias, which is in the opposite sense to image force lowering [47]. The value of $\rho_3$ is indeed negative and thus the BH increases with increasing forward bias [47]. Furthermore, the increase of the BH with increasing forward bias is only possible because the decrease of the mean BH with increasing bias is compensated by a reduction of the value of $\sigma_s$ in Eq. (7) in Ref. [47]. This phenomena reveal the limitation of the special case of voltage-independent ideality factors, thus the effective BH $\Phi_B(V)$ varies linearly with bias, essentially the high ideality factor arises due to the bias dependence of the BHs. This bias dependence of BHs in the distribution through mean BH and standard deviations leads to the temperature-dependent ideality factor in inhomogeneous Schottky diodes [47].

To explain the discrepancy in the activation energy which deviates from linearity, Eq. (10) can be rewritten by Eqs. (12) with (13) as follows

$$\ln\left(\frac{I_o}{T^2}\right) - \left(\frac{q^2\sigma_s^2}{2k^2T^2}\right) = \ln(AA^*) - \frac{q\bar{\Phi}_{B0}}{kT} \tag{13}$$

The modified $\ln(I_o/T^2) - q^2\sigma_s^2/2k^2T^2$ vs $q/kT$ plot according to Eq. (15) should give a straight line with the slope directly yielding the mean $\bar{\Phi}_{B0}$ and the intercept (=ln$AA^*$) at the ordinate determining $A^*$ for a given diode area $A$ (Fig. 8). In Fig. 8, the modified $\ln(I_o/T^2) - q^2\sigma_s^2/2k^2T^2$ vs $q/kT$ plot gives $\bar{\Phi}_{B0}$ ($T = 0$) and $A^*$ as 1.28 eV and 38.79 A cm$^{-2}$ K$^{-2}$, respectively.

## 4. Conclusions

In conclusion, it was shown that the $I$–$V$ characteristics of the Al/p-Si SBD in the temperature range of 178–440 K can be interpreted on the basis of the TE with Gaussian distribution of the barrier height of $\bar{\Phi}_{B0}$ ($T = 0$) = 1.19 eV and standard deviation of $\sigma_s = 0.17$ V. As is known, the distribution of the barrier height is caused by inhomogeneities that are present at the interface. Furthermore, the experimental results of $\Phi_{ap}$ and $n_{ap}$ fit very well for the theoretical equation related to the Gaussian distribution of $\Phi_{ap}$ and $n_{ap}$. Again the $\ln(I_o/T^2)$ versus $1/T$ plot and $1/nT$ plots yield an unreasonable effective Richardson constant although the flat band temperature coefficient was used in the calculation. But, the Richardson value of 38.79 A cm$^{-2}$ K$^{-2}$ obtained by means of the modified Richardson plot considering Gaussian distribution of the barrier heights is closer to theoretical value of 32 A cm$^{-2}$ K$^{-2}$ for holes in p-type Si.

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