



On the origin of increase in the barrier height and decrease in ideality factor with increase temperature in Ag/SiO₂/p-Si (MIS) Schottky Barrier Diodes (SBDs)

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In order to get more information on possible current conduction mechanisms (CCMs) through junction and the nature of barrier height (BH) at metal/semiconductor interface, the forward bias I-V characteristics of the Ag/SiO₂/p-Si (MIS) type Schottky barrier diodes (SBDs) have been investigated in temperature range of 200-360 K. We observed that there is an increase in zero-bias BH (Φ_{B0}) and a decrease in ideality factor (n) with increase in temperature. The value of effective Richardson constant (A^*) obtained from classic Richardson plot was also found much lower than the known theoretical value of n-Si. Therefore, Φ_{B0} vs $q/2kT$ was drawn to obtain an evidence of a Gaussian distribution (GD) of the BHs values over the diode area with the mean BH ($\bar{\Phi}_{B0}$) and standard deviation (σ_{s0}). The values of $\bar{\Phi}_{B0}$ and σ_{s0} were found from the slope and intercept of this plot as 0.786 eV and 0.082 V, respectively. Thus, the values of $\bar{\Phi}_{B0}$ and effective Richardson constant (A^*) were obtained from slope and intercept of the modified Richardson plot as 0.784 eV and 30,40 Acm⁻²K⁻², respectively. Thus the forward bias I-V characteristics of Ag/SiO₂/p-Si SBD can be successfully explained on the basis of thermionic emission (TE) mechanism with a GD of BHs. The series and shunt resistances (R_s and R_{sh}) of the SBD were also determined using Ohm's law for each temperature.

Keywords: Ag/SiO₂/p-Si (MIS) type SBDs; Temperature dependent conduction mechanisms; Gaussian distribution (GD) of barrier heights; Series and shunt resistance of diode;

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1. Introduction

Metal-semiconductor (MS) and metal-insulator-semiconductor (MIS) structures which are frequently called Schottky barrier diodes (SBDs) have some superior features such as very fast response time, low forward bias potential and fast switching. The current conduction mechanisms (CCMs) in these devices depend on various parameters such as the process of surface preparation, barrier height (BH) inhomogeneity at M/S interface, the doping concentration of donor or acceptor atoms, energy distribution of surface states (N_{ss}), series and shunt resistances (R_s and R_{sh}) of the diode

and applied bias voltage [1-7]. Usually, the analysis of the forward bias current-voltage (I-V) characteristics in SBDs only the based on thermionic emission (TE) theory reveals an abnormal increase in the zero-bias barrier height (Φ_{B0}) with increasing temperature, in which there is a positive coefficient BH ($\alpha = (\Delta\Phi_{B0}/\Delta T)$) that is in contrast with the negative temperature coefficient ($\alpha = \Delta E_g/\Delta T$) of forbidden energy band gap (E_g). Because band gap of a semiconductor gets smaller as the temperature is decreased, hence in such case the general expectation is that the BH also gets smaller too. Nevertheless, obtained temperature coefficient of BH does not have to be same as temperature coefficient of E_g . In addition, the value of n may be considerably larger than unity and the conventional Richardson plot deviated from the linearity especially at low temperatures, consequently the value of effective Richardson constant (A^*) may be very low compared to the theoretical value [7-10].

Analyzing the I-V characteristics of SBDs only at room temperature and above it cannot supply to us with

detailed information on the CCMs and the nature of BH formation at M/S interface. On the other hand when these measurements were carried out in the wide of temperature could allow us to gain insight in to different aspects of characteristics both CCMs and nature of BH. Because especially under room temperatures, in SBDs, additional to TE theory a number of CCMs thermionic field emission (TFE), field emission (FE), multistep tunneling (MT) via surface states or dislocations and Gaussian distribution (GD) of BHs compete unusually, one of them may dominate over the others in a certain temperature and applied bias voltage region [7-12]. Therefore, the possible CCMs especially under room temperatures become more complex rather room and above temperatures [13-19]. Therefore, a complete description of CCMs through junction and understanding of the nature of BH still remain a challenging problem especially at low temperatures. In recent years, the nature of the increase in the Φ_{B0} and a decrease in n with an increase in temperature has been successfully explained on the basis of a TE theory with a GD of the BHs [1-7,13-22].

In this study, to get more information of the possible CCMs through junction and the nature of BH at M/S interface, the analysis of the forward bias I-V characteristics of the Ag/SiO₂/p-Si (MIS) type SBDs have been investigated both above and under room temperature. The analysis of experimental I-V characteristics revealed that there is an increase in the Φ_{B0} and a decrease in n with an increase in temperature and such behavior of Φ_{B0} and n can be successfully explained on the basis of the TE theory with GD of the BHs at M/S interface.

2. Experimental details

Ag/SiO₂/p-Si (MIS) type SBDs were fabricated on the B doped (p-type) single Si crystal wafer with (100) float zone, one side polished, 2 inch diameter, 1-4 Ωcm resistivity and 300 μm thickness. Wafers first went through an ultrasonic acetone, alcohol, deionize (DI) water with 18 MΩcm resistivity cleaning and a dilute HF dip to remove oxide formed on the surface. Then Si-wafer degreased in organic solvent of CH₂Cl₂, CH₃COCH₃ and CH₃OH etched in a sequence of H₂SO₄ and H₂O₂, 20% HF, a solution of 6HNO₃:1HF:35H₂O, 20% HF and then quenched DI water at 10 minutes in ultrasonic bath. After surface cleaning of p-Si wafer, 500 nm high purity (99.999%) Ag was thermally evaporated onto the whole backside p-Si wafer at 10⁻⁶ Torr in metal evaporation system. The ohmic back contact was prepared by sintering the evaporated Ag back contact at 600 °C for 60 minutes in flowing dry N₂ ambient at 2L/min. Thus both Ag was diffused in p-Si and at performed a thin SiO₂ insulator layer on the front of p-Si wafer. Finally, the rectifier contacts were formed onto front of p-Si wafer by evaporation of 1500 Å thick Al dots with 7.85x10⁻³ cm² in same high vacuum metal evaporation system.

For the current-voltage (I-V) measurements samples were placed on the copper holder with the help of silver paste and the electrical contacts were also made to the upper electrodes by the use of thin silver coated wires with silver

paste. The forward and reverse bias current-voltage (I-V) characteristics of the Ag/SiO₂/p-Si (MIS) type SBDs were performed in the temperature range of 200-360 K by the use Keithley 2400 source meter. All measurements were carried out with the help of a microcomputer through an IEEE-488 ac/dc converter card in a Janis vpf-475 cryostat. A simple illustration of measurement system was given in Fig.1.

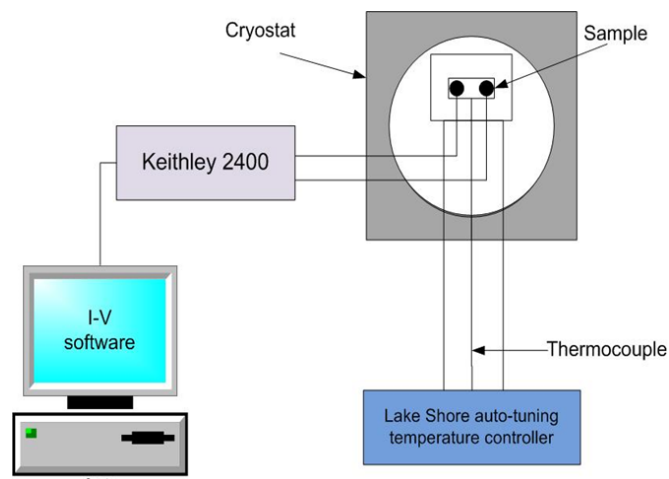


Fig. 1. A simple illustration of the experimental measurement system.

3. Result and discussion

Fig. 2 shows typical semi-logarithmic forward and reverse bias I-V characteristics of Ag/SiO₂/p-Si SBD in the temperature range of 200 K-360 K. As shown in Fig.2, lnI-V plot consists of a good linear behavior with different slopes in intermediate forward biases, but deviated from the linearity at high forward bias voltages especially due to the effect of R_s and interfacial SiO₂ layer. On the other hand, the effect of R_s at intermediate forward biases (linear region), can be neglected low. In the reverse bias (Fig.2), there is a non-saturation behavior and it can be explained in terms of image force lowering BH, generation-recombination and the existence of insulator layer [9-15]. When SBDs have R_s and n higher than unity, the forward bias I-V characteristics in terms of TE over the barrier can be expressed as [11, 12]:

$$I = AA^*T^2 \exp\left(-\frac{q}{kT} \Phi_{B0}\right) \left[\exp\left(\frac{q(V - IR_s)}{nkT}\right) - 1 \right] \quad (1)$$

The expressions in front of the brackets in Eq. 1 corresponds to reverse-bias saturation current (I_0) and it can be obtained from the intercept of the linear part lnI-V plot (Fig.2) at zero bias, Φ_{B0} is the zero-bias BH, V is the applied voltage drop across the diode, A^* is the effective Richardson constant (32 A/cm²K² for p-Si), the term of IR_s is the voltage drop across the R_s . Similarly, the value of n can be also extracted from the slope of the linear part of lnI-V plot for each temperature as following relation:

$$n = \frac{q}{kT} \left(\frac{dV}{d(\ln I)} \right) \quad (2)$$

Thus, the value of Φ_{Bo} can be calculated from Eq.3 by using the obtained experimental value of I_o and the diode area (A) of the SBD for each temperature:

$$\Phi_{Bo} = \frac{kT}{q} \ln \left(\frac{AA^*T^2}{I_o} \right) \quad (3)$$

Experimental I_o , n , and Φ_{Bo} for the fabricated Ag/SiO₂/p-Si SBD in the temperature range of 200 -380 K are tabulated in Table 1. All these parameters are found a strong function of temperature and they changed from 1.43x10⁻¹¹ A, 1.912, 0.590 eV (at 200 K) to 1.14 x10⁻⁵A, 1.537, and 0.676 eV (at 360 K). Such change in Φ_{Bo} with temperature and high value of n can be attributed to the existence of interfacial insulator layer, particular density distribution of surface states (N_{ss}) at Si/SiO₂ interface, in-homogeneities of BH at M/S interface, and the dominated conduction by interface recombination [15-23].

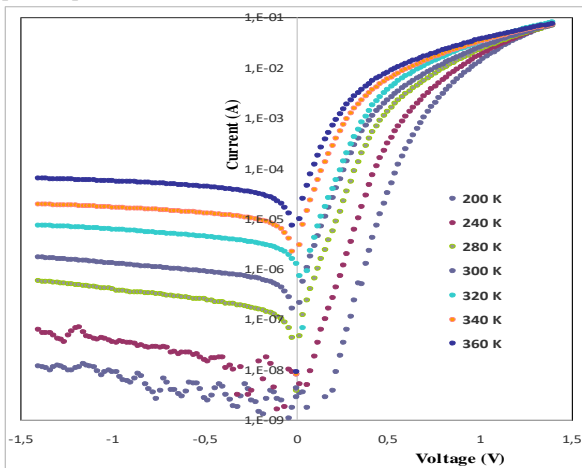


Fig. 2. Experimental forward and reverse bias I-V-T characteristics of the Ag/SiO₂/p-Si SBD.

Table. 1. The obtained some various electrical parameters from the forward bias I-V characteristics of the Ag/SiO₂/p-Si SBD for various temperatures.

T (K)	I _o (A)	n	Φ _{Bo} (eV)	R _s (at 1.2V) (Ω)	R _{sh} (at 1.2V) (Ω)
200	1.43x10 ⁻¹¹	1.912	0.590	33.00	1.13x10 ⁸
240	1.19 x10 ⁻⁹¹	1.770	0.624	30.14	1.80 x10 ⁷
280	4.67 x10 ⁻⁸	1.677	0.647	28.12	2.46 x10 ⁶
300	2.39 x10 ⁻⁷	1.630	0.654	26.89	7.99 x10 ⁵
320	8.48 x10 ⁻⁷	1.589	0.666	22.42	2.21 x10 ⁵
340	3.44 x10 ⁻⁶	1.557	0.670	23.77	6.60 x10 ⁴
360	1.14 x10 ⁻⁵	1.537	0.676	22.31	2.02 x10 ⁴

As can be seen in Table 1 and Fig.3, there is an increase in zero-bias BH (Φ_{Bo}) and a decrease in ideality factor (n) with increase in temperature. Such behavior of Φ_{Bo} with temperature is in agreement with the reported negative temperature coefficient of the BH and forbidden band gap (E_g) of the Si ($\alpha_{Si} \approx -4.73 \times 10^{-4} \text{ eV.K}^{-1}$) [26]. As explained in Refs. [14-19], when the current transport across the barrier is a temperature activated process; electrons at low temperature can easily surmount the lower BHs or patches. Thus the value of Φ_{Bo} starts to increase due to this excess current and so leads to an increase in ideality factor. On the other hand at high temperatures, more and more electrons have sufficient energy to overcome the higher BH and TE theory becomes more dominant rather than other CCMs [19-23].

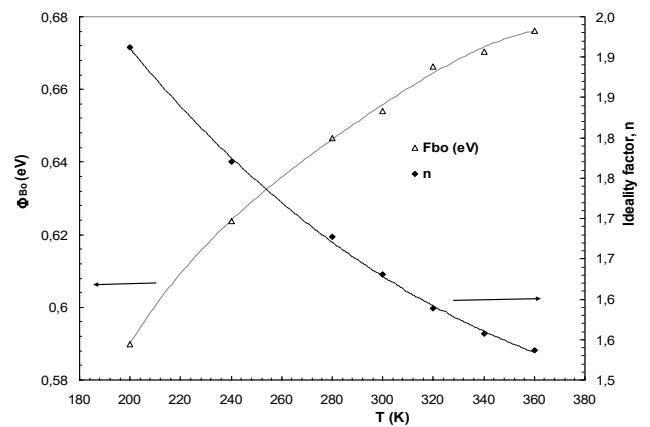


Fig.3. The variation in Φ_{Bo} and n with temperature for the Ag/SiO₂/p-Si SBD.

The second way to evaluate of BH or activation energy (E_a), one might also use the conventional Richardson plot as following relation.

$$\ln \left(\frac{I_o}{T^2} \right) = \ln(AA^*) - \frac{q\Phi_{Bo}}{kT} \quad (4)$$

As shown in Fig 4, the conventional Richardson plot shows a good linear straight line and the values of Φ_{Bo} (=E_a) and A^* were found as 0.482 eV and 0.045 A.cm⁻²K⁻² from the slope and intercept of it, respectively. This value of E_a is close to the mid-gap of E_g , but A^* is 711 times lower than the theoretical value of p-Si (32 A.cm⁻²K⁻²). These results and higher values of n confirmed that there is a deviation from ideal TE theory.

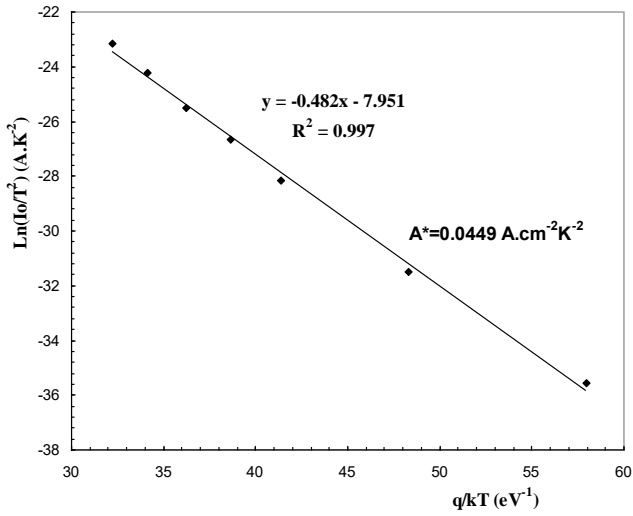


Fig.4. Richardson plot of the $\ln(I_o/T^2)$ vs q/kT for the Ag/SiO₂/p-Si SBD.

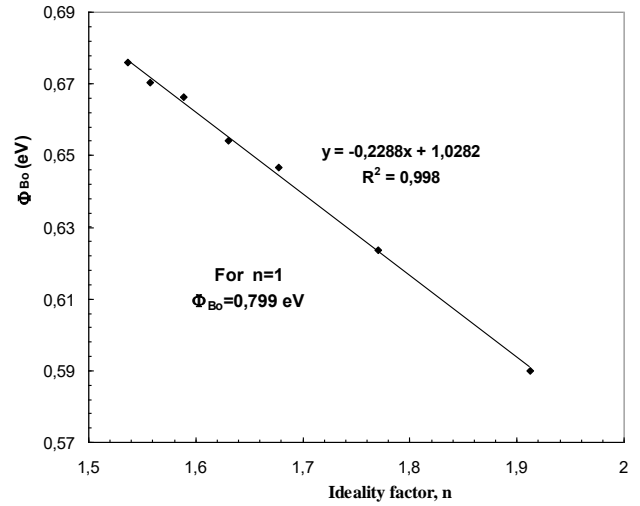


Fig.5. Temperature dependent Φ_{B0} vs n plot for the Ag/SiO₂/p-Si SBD.

According to Tung and co-workers [20], the increase in Φ_{B0} with increasing temperature can be explained the existence of lower BHs or “patches” imbedded in a higher background uniform BH. Mönch [18] was also found a linear relationship between the Φ_{B0} and n to evidence the GD of BH at M/S interface. Therefore, Φ_{B0} vs n plot was drawn for Ag/SiO₂/p-Si SBD and it (Fig. 5) shows a linear behavior and the extrapolation this plot to $n=1$ has given at about mean value of BH (Φ_{B0}) as 0.799 eV. These results can be explained by the lateral distribution of BH and it has a Gaussian distribution (GD) of the BH values over the diode area with the mean BH (Φ_{B0}) and standard deviation (σ_{so}) [24]. According to this theory, the changes in the Φ_{B0} and n with temperature can be expressed by the following relations [14-18]:

$$\Phi_{ap} = \bar{\Phi}_{B0} - \frac{q\sigma_s^2}{2kT} \quad (5)$$

$$\frac{1}{n_{ap}(T)} - 1 = -\rho_1(T) = -\rho_2 - \frac{q\rho_3}{2kT} \quad (6)$$

In Eq.5, the σ_s is almost independent of temperature or usually can be neglected low. The quantities of Φ_{ap} and n_{ap} are called as apparent BH and n which are corresponding to the Φ_{B0} and n , respectively. The quantities of ρ_1 , ρ_2 and ρ_3 are the voltage deformation coefficients quantify the voltage deformation of the BH distribution. By using Eqs. 5 and 6, both Φ_{B0} vs $q/2kT$ and $(n^{-1}-1)$ vs $q/2kT$ plots were drawn and given in Fig. 6.

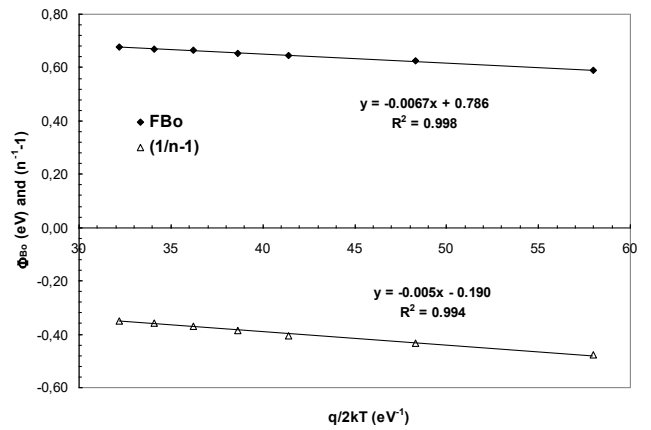


Fig. 6. Φ_{B0} and $(n^{-1}-1)$ vs $q/2kT$ plots for the Ag/SiO₂/p-Si SBD.

The values of $\bar{\Phi}_{B0}$ and σ_s were found as 0.786 eV and 0.067 V the intercept and slope of the Φ_{B0} vs $q/2kT$ plot, respectively, and this value of σ_s is not small compared to $\bar{\Phi}_{B0}$. This is an evidence of the interface in-homogeneities. The values of ρ_2 and ρ_3 were also found as -0.190 V and -0.005 V the intercept and slope of the $(n^{-1}-1)$ vs $q/2kT$ plot. Figs. 4-6 show that a single GD of the BHs at Ag/p-Si interface. In order to explain such behavior of A^* and low value of E_a , the modified Richardson plot can be rewritten as following [3,21-25].

$$\ln\left(\frac{I_o}{T^2}\right) - \left(\frac{q^2\sigma_o^2}{2k^2T^2}\right) = \ln(AA^*) - \frac{q\bar{\Phi}_{bo}}{kT} \quad (7)$$

Thus the modified Richardson plot was drawn by using Eq.7 and it represented in Fig.7. The values of $\bar{\Phi}_{B0}$ and A^* were found as 0.784 eV and 30.40 A.cm⁻²K⁻² the intercept and slope of the this plot, respectively. It is clear that this value of A^* is very close to the theoretic value of 32 A.cm⁻²K⁻² for p-Si crystal [11,12]. The obtained experimental value of $\bar{\Phi}_{B0}$ from

the modified Richardson plot is also very close to the obtained 0.799 and 0.786 eV values which are obtained from Fig. 5 and 6, respectively. As a result, the temperature dependence of current transport in Ag/SiO₂/p-Si (MIS) type SBD can be successfully explained by using TE theory with GD of the BHs due to the inhomogeneous BHs at Ag/p-Si interface.

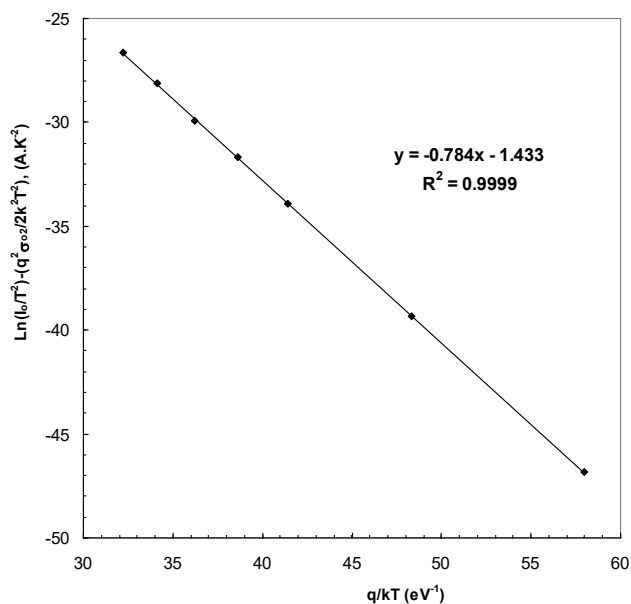


Fig. 7. Modified. Richardson plot of the $\ln(I_0/T^2)$ vs q/kT for the Ag/SiO₂/p-Si SBD.

Both R_s and R_{sh} are more important parameters which influence the CCMs especially at low temperature. Therefore, their values were obtained from the I-V data by using Ohm's law ($R_i = dV_i/dI_i$) and the obtained voltage dependent profile of R_i was given in Fig. 8 for each temperature. As seen in Fig. 8, the value of R_i becomes almost constant for each temperature at adequate high forward biases ($V \geq +1.2V$) which corresponds to the real value of R_s for the Ag/SiO₂/p-Si SBD. Similarly, at adequate low reverse biases ($V \leq -1.2V$) it again goes to a constant value which corresponds to the real value of R_{sh} . Both the R_s and R_{sh} values decrease with increasing temperature as expected. It is clear that the change in R_s and R_{sh} with temperature (Table 1) becomes more effective at low temperatures.

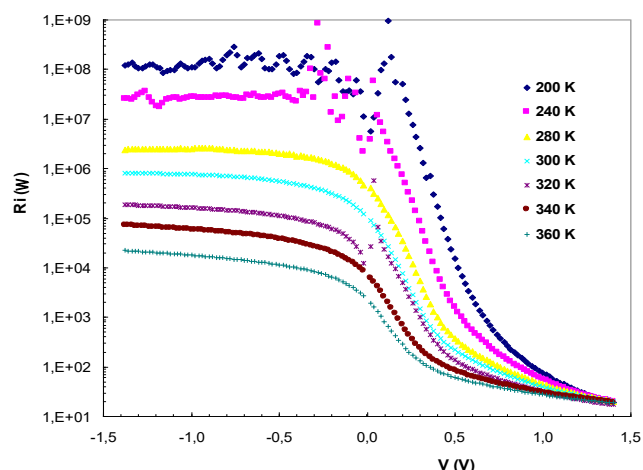


Fig. 8. The variation in R_i with applied voltage for various temperature in Ag/SiO₂/p-Si SBD.

4. Conclusions

In this study, the possible CCMs through junction and the nature of BH at Ag/p-Si interface have been investigated in the temperature range of 200 K-360 K. Experimental results show that the main electrical parameters such as I_0 , n , Φ_{B0} , R_s and R_{sh} values of the sample determined based on TE theory were found a strong function of temperature and they changed from $1.43 \times 10^{-11} A$, 1.912, 0.590 eV, 33Ω and $113 M \Omega$ (at 200 K) to $1.14 \times 10^{-15} A$, 1.537, 0.676 eV, 22.31Ω and $20.2 k \Omega$ (at 360 K), respectively. It is clear that there is an increase in Φ_{B0} and a decrease in n with increase in temperature. The value of A^* obtained from classic Richardson plot was also found as $0.045 A \cdot cm^{-2} K^{-2}$ which is 711 times lower than the known theoretical value of p-Si ($32 A \cdot cm^{-2} K^{-2}$). Therefore, Φ_{B0} vs $q/2kT$ was drawn to obtain an evidence of a GD of the BHs values over the diode area with the Φ_{B0} and σ_{so} . The values of Φ_{B0} and σ_{so} were found from the slope and intercept of this plot as 0.786 eV and 0.082 V, respectively. Thus, both the value of Φ_{B0} and A^* were obtained from slope and intercept of the modified Richardson plot as 0.784 eV and $30.40 A \cdot cm^{-2} K^{-2}$, respectively. As conclusion, the forward bias I-V characteristics of Ag/SiO₂/p-Si SBD can be successfully explained on the basis of thermionic emission (TE) mechanism with a GD of BHs. In order to see the effects of R_s and R_{sh} on the electrical characteristics of the SBD their values were also determined using Ohm's law for each temperature. The change in R_s and R_{sh} with temperature becomes more effective at low temperatures.

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