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Modified approach to modeling barrier inhomogeneity in Schottky diodes

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Abstract

The conventional model describing barrier inhomogeneities in Schottky diodes with a single series resistance leads to many anomalies including crossing over effect in current–voltage–temperature (*I–V–T*) plots. A new model is therefore proposed here which entails a parallel combination of several diodes, each with its own series resistance. Further, the barrier heights follow a Gaussian distribution function $\rho(\varphi)$ with a mean barrier height ($\overline{\varphi}$) and standard deviation σ. The series resistance is believed to vary inversely with the $\rho(\varphi)$ value of the concerned barrier height and hence the area occupied. The occurrence of anomalies with the conventional model is examined in depth, and their effective elimination with the proposed model is discussed with the undertaken current simulations. In addition to predicting the increase in apparent barrier height with increase in temperature, decrease in ideality factor with increase in temperature, and elimination of modeling anomalies observed in the conventional model, the model is successful in predicting that apparent barrier height as a function of inverse thermal energy is a quadratic behavior even with a single distribution. This previously required unlikely scenarios involving multiple mean barrier heights and standard deviations with the conventional model. Finally, the description also explains the observed increase in the apparent barrier height with decrease in temperature of a Schottky diode when the values are deduced from the *C–V–T* data under reverse bias.

Keywords: Schottky contacts, inhomogeneity, barrier height

(Some figures may appear in colour only in the online journal)

Introduction

The Schottky junction is typically characterized by parameters such as barrier height and ideality factor. These parameters exhibit temperature dependence i.e. the barrier height measured increases with increase in temperature and the ideality factor decreases with increase in temperature and their nature has been explained based on various theories, and among them, the commonly accepted cause being the presence of barrier height inhomogeneities [1–8]. The impact of barrier height inhomogeneity has taken an important role recently with the advent of emerging alternatives in high power and high voltage electronics such as GaN or SiC and study of MIS structures with hybrid technologies employing interlayers such as conducting polymers, nanocomposites, graphene etc [9–16]. Since these materials systems and devices exhibit non-idealities whose sources may be varied in each system and varies from system to system, accurate modeling of each of the contributions allow for identification of the source of the anomalies and possibly their mitigation or elimination. Inhomogeneity implies that the barrier height φ is not constant, but, varies over the area of the Schottky junction and represented by a distribution function. Ballistic electron microscopy studies have provided evidence for the existence of a Gaussian distribution of the barrier heights [17]. The analytical model that was subsequently developed incorporating the Gaussian distribution assumed a parallel disposition of elemental diodes with a single series resistance for obtaining the expressions for the current, apparent barrier height (φ_{ap}) and apparent ideality factor (η_{ap}) [18]. However, several discrepancies appeared during simulation of the *I–V* characteristics of Schottky diodes at different temperatures using the analytical model, viz. (i) the saturation current turns out to be larger at a lower temperature than that at a higher temperature when the limits for the barrier height (φ) in the

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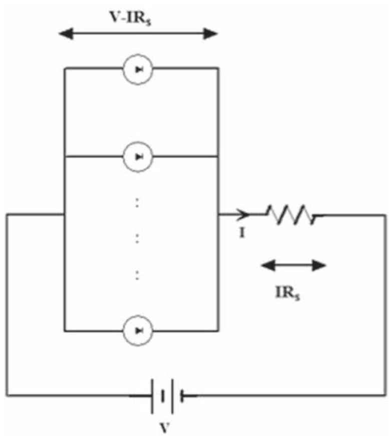

Figure 1. The equivalent circuit of a Schottky diode containing barrier inhomogeneities.

Gaussian distribution are set from $-\infty$ to ∞ and (ii) the phenomenon of crossing over is observed in which *I–V* curves of lower and higher temperatures intersect when the limits of (φ) are chosen from 0 to ∞ [19]. In this paper, a model is proposed where Schottky junction is believed to possess barrier inhomogeneities and described by a parallel combination of elemental diodes with Gaussian distribution of barrier heights, but each having its own φ and series resistance $R(\varphi)$ to explain its *I–V* characteristics satisfactorily with no anomalies reported earlier and predicting experimental observations that previously could not be satisfatorily ascribed to barrier inhomogeneity without invoking unlikely scenarios of voltage dependent distribution parameters or multiple standard deviations. Note that in this work, barrier height φ employs the unit V and $q\varphi$ employs energy unit eV.

Conventional model and associated anomalies

Conventional model [8, 9] assumes parallel combination of elemental diodes of different barrier heights, following a Gaussian probability distribution function $\rho(\varphi)$, such that

$$\rho(\varphi) = \frac{1}{\sqrt{2\pi}\,\sigma} \exp \frac{-(\varphi - \overline{\varphi})^2}{2\sigma^2}, \tag{1}$$

where φ is the barrier height, σ is the standard deviation and $\overline{\varphi}$ is the mean barrier height. The cross-sectional area of the elemental diode is just proportional to the probability of the corresponding barrier height (equation (1)). The parallel combination of diodes is connected to a single series resistance (R_s). Its equivalent circuit diagram is shown in figure 1. The thermionic emission diffusion current for a Schottky diode containing barrier inhomogeneities is then given by

$$I = \int_a^b I(\varphi, V)\rho(\varphi)\mathrm{d}\varphi, \tag{2}$$

where $I(\varphi, V)$ represents the thermionic emission current through an elemental diode of barrier height φ at a voltage V and expressed as

$$I(\varphi, V) = I_s(\varphi)\left\{\exp \frac{q(V - IR_s)}{kT} - 1\right\} \tag{3}$$

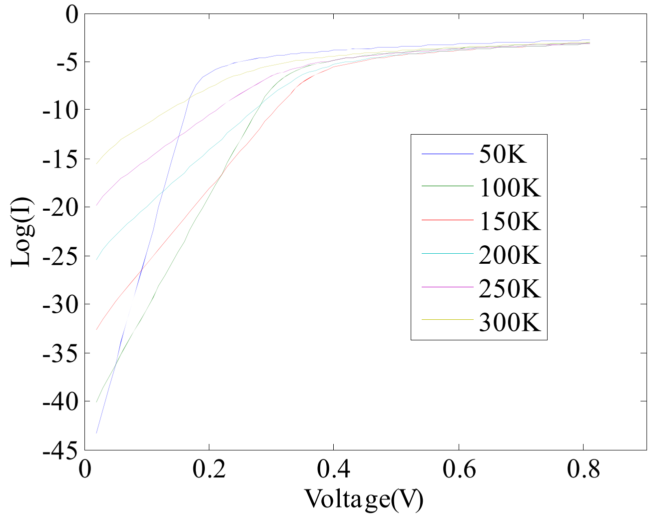

Figure 2. Simulated *I–V* characteristics with $R_s = 10\ \Omega$, $A_d = 7.87 \times 10^{-7}\ \mathrm{m}^2$, $\overline{\varphi} = 0.8$ V and $\sigma = 0.08$ V showing crossing over phenomenon.

with $I_s(\varphi) = A_d A^{**} T^2 \exp\left(-\frac{q\varphi}{kT}\right)$. Here A_d is the area of the contact, scaled by $\rho(\varphi)$, A^{**} is the effective Richardson constant, T is the temperature, q is the electronic charge, and k is the Boltzmann constant. The integral is simply the summation of the currents through all the elemental diodes. The integration limits a and b have been taken as either $-\infty$ and ∞ or 0 and $2\overline{\varphi}$, respectively [9]. The mean barrier height and the standard deviation have been assumed to be linear functions of voltage (that we will demonstrate later in this paper as unnecessary with our proposed modified approach) as $\overline{\varphi} = \overline{\varphi}_0 + \gamma V$ and $\sigma = \sigma_0 + \xi V$, where, $\overline{\varphi}_0$ is the mean barrier height at zero-bias, σ_0 is the standard deviation at zero-bias, and γ and ξ are their voltage coefficients, respectively. Introducing these substitutions and performing integration with limits $-\infty$ to ∞, the current expression takes the form [8]

$$I = A_d A^{**} T^2 \exp\left(-\frac{q\varphi_{\mathrm{ap}}}{kT}\right)\exp\left(\frac{q(V - IR_s)}{\eta_{\mathrm{ap}} kT}\right) \times\left[1 - \exp\left(\frac{-q(V - IR_s)}{kT}\right)\right], \tag{4}$$

where $\varphi_{\mathrm{ap}} = \overline{\varphi}_0 - \frac{\sigma_0{}^2 q}{2kT}$ and $\frac{1}{\eta_{\mathrm{ap}}} = 1 - \gamma + \frac{\sigma_0 q\xi}{kT}$ give the values of apparent barrier height and apparent ideality factor, respectively. It is obvious that the apparent barrier height decreases with decrease in temperature, becomes zero at $T = \frac{\sigma_0{}^2 q}{2k\overline{\varphi}_0}$ and even negative for $T < \frac{\sigma_0{}^2 q}{2k\overline{\varphi}_0}$. This results in an increase in saturation current (I_s) with decrease in temperature below $T = \frac{\sigma_0{}^2 q}{2k\overline{\varphi}_0}$, inconsistent with the thermionic emission diffusion theory itself and leads to an anomalous situation. The source of the above anomaly is traced to the negative limit of barrier height (i.e.$-\infty$) which is unrealistic but simplifies the integration process. To overcome this difficulty, limits for the barrier height are taken from 0 to $2\overline{\varphi}$ [9] and the ideality factor as unity. The solution of the integral (2) gives [9]

$$\tilde{I} = I \frac{\{\mathrm{erf}(f1) - \mathrm{erf}(f2)\}}{2}, \tag{5}$$

where I is given by equation (4) with $f1 = \left(\frac{\sigma^2 q}{kT} + \overline{\varphi}\right)\frac{1}{\sigma\sqrt{2}}$, $f2 = \left(\frac{\sigma^2 q}{kT} - \overline{\varphi}\right)\frac{1}{\sigma\sqrt{2}}$, $\varphi_{\mathrm{ap}} = \varphi$, and $\eta_{\mathrm{ap}} = \eta$

The simulated I–V curves at different temperatures for a typical diode using equation (5) are shown in figure 2. Clearly, the saturation current (i.e. y-intercept) now decreases monotonically with decrease in temperature. However, the crossing over phenomenon in which the I–V curves at 50 and 100 K intersect those at higher temperatures can also be observed. This contradicts the thermionic emission and diffusion theory as current at a specific voltage becomes the same at two temperatures (lower and higher). An effort is made here to understand this anomaly in the model.

Crossing over phenomenon

The crossing over phenomenon in a homogeneous Schottky diode can be examined through the minimum in the thermionic emission-diffusion current versus temperature plot at a given voltage.

For $(V\text{-}IR_s) \gg kT/q$, equation (4) yields

$$I = A_d A^{**} T^2 \exp\left(-\frac{q\varphi}{kT}\right)\left[\exp\left(\frac{q(V - IR_s)}{\eta kT}\right)\right]. \tag{6}$$

Taking logarithm on both sides, equation (6) becomes

$$\ln(I) = \ln(A_d A^{**}) + 2 \times \ln(T) - \frac{q\varphi}{kT} + \frac{q(V - IR_s)}{\eta kT}.$$

By differentiating with respect to temperature and equating to zero, the maxima–minima condition gives

$$T = \frac{-q(\varphi - \{(V - IR_s)/\eta\})}{2k}. \tag{7}$$

Thus, for a voltage drop $(V - IR_s) < \eta\varphi$, the temperature (T) is negative, i.e. no solution exists for maxima–minima condition for $T > 0$, and this makes physical sense as one would expect current to be a monolithically increasing function with temperature. However, for a voltage drop of $(V - IR_s) > \eta\varphi$, the temperature is positive. Obviously, there exists a temperature at which maxima–minima condition holds and corresponds to a minimum current represented by ($I_{\mathrm{min},}$, say). It essentially means that two temperatures exist invariably for any current above (I_{min}). This in fact indicates an intersection point of the current–voltage plots at two different temperatures. The anomaly of crossing over can therefore be observed if the voltage drop across the Schottky junction exceeds the barrier height (or the built-in potential). Thus, equation (6) is only valid for voltage drop across the junction lower than the barrier height itself. This implies that, for a voltage drop $(V - IR_s)$ greater than V_{bi} and less than $\eta\varphi$, the current is erroneous but not in the range to cause crossing over. But, for voltage greater than $\eta\varphi$ across the junction, error involved is enough to induce crossing over phenomenon.

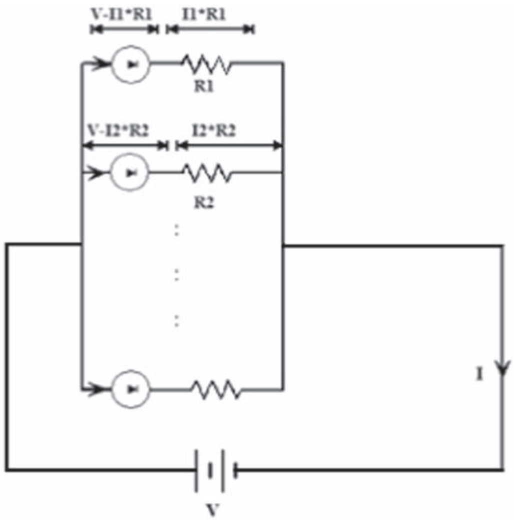

Figure 3. Equivalent circuit of Schottky diode containing barrier inhomogeneity described by a parallel combination of diodes with each having a specific series resistance.

Modified approach to modeling Schottky diode containing barrier inhomogeneities

Schottky diode containing barrier inhomogeneities is modeled as a parallel combination of elementary non-interacting diodes (figure 3), each with a specific barrier height and a series resistance. The barrier heights are represented by a Gaussian distribution function given by equation (1). Further, the area of each elemental diode is directly proportional to the value of its Gaussian distribution function $\rho(\varphi)$, i.e. higher $\rho(\varphi)$ value amounts to larger coverage of the Schottky junction by the elemental diode. On the other hand, its series resistance $R(\varphi)$ varies inversely with the area covered. Obviously, the series resistance $R(\varphi)$ of each elemental diode follows a distribution, such that

$$R(\varphi) = \frac{K}{\rho(\varphi)}, \tag{8}$$

where K is the proportionality constant. The series resistance associated with each elemental diode arises due to the neutral region in the semiconductor with a cross-sectional area $A_d\,\rho(\varphi)$ (A_d is the total cross-sectional area of diode) and has a value of $K/(\rho(\varphi)$. Since all elementary diodes lie in parallel, the net series resistance (R_s) of the neutral region can be obtained by integrating the reciprocal of the resistance distribution $R(\varphi)$:

$$\frac{1}{R_s} = \int_x^y \frac{\rho(\varphi)\mathrm{d}\varphi}{K}. \tag{9}$$

The limits x and y represent the region where the probability density function satisfies the condition

$$\int_x^y \rho(\varphi)\mathrm{d}\varphi = 1.$$

Thus, equation (9) gives $K = R_s$

From equation (8), one can write

$$R(\varphi) = \frac{R_s}{\rho(\varphi)} = R_s\sqrt{2\pi}\,\sigma\,\exp\frac{(\varphi - \overline{\varphi})^2}{2\sigma^2}. \quad (10)$$

An illustrative plot of log $R(\varphi)$ versus barrier height (φ) is shown in figure 4. The total current (I) through the Schottky diode at the applied voltage V is given by

$$I = \int_x^y I(\varphi, V)\rho(\varphi)\mathrm{d}\varphi, \quad (11)$$

where φ is the barrier height and $\rho(\varphi)$ is the probability density function describing the barrier inhomogeneity (being finite within the limits x and y and zero elsewhere). $I(\varphi, V)$ is the current through a Schottky diode of barrier height φ and cross-sectional area $A_d\,\rho(\varphi)$ at a voltage V. The term $I(\varphi, V)\rho(\varphi)$ is the current that flows through the elemental diode of barrier height φ and cross-sectional area $A_d\,\rho(\varphi)$ with an elemental series resistance of $R(\varphi)$. As mentioned earlier, the thermionic emission diffusion (TED) current equation can be used only if the voltage $[V - I(\varphi, V)\rho(\varphi) * R(\varphi)]$ is less than the built-in potential of the diode.

Hence, for $\{V - I(\varphi, V)\rho(\varphi)R(\varphi)\} < V_{\mathrm{bi}}$, the current through the elemental diode is given by

$$I(\varphi, V)\rho(\varphi)\mathrm{d}\varphi = i_s\left[\exp\left(\frac{q(V - I(\varphi, V)\rho(\varphi)R(\varphi))}{\eta kT}\right) - 1\right]\mathrm{d}\varphi, \quad (12)$$

where

$$i_s = A_d A^{**}T^2\rho(\varphi)\exp\left(-\frac{q\varphi}{kT}\right).$$

However, for $\{V - I(\varphi, V)\rho(\varphi)R(\varphi)\} > V_{\mathrm{bi}}$, an additional voltage appears across the series resistance, such that

$$I(\varphi, V)\rho(\varphi)\mathrm{d}\varphi = i_s\left[\exp\left(\frac{q(V_{\mathrm{bi}})}{\eta kT}\right) - 1\right]\mathrm{d}\varphi + \frac{V - V_{\mathrm{eq}}}{R(\varphi)}\,\mathrm{d}\varphi \quad (13)$$

where V_{eq} is the applied voltage for which $V - I(\varphi, V)\rho(\varphi)R(\varphi) = V_{\mathrm{bi}}$.

In order to have a simplified form of total current expression, let $I(\varphi, V)\rho(\varphi) = I_\rho(\varphi, V)A/V$ where $I_\rho(\varphi, V)$ can be considered as the current per barrier height element, which when integrated over the entire range of barrier heights yields the total current.

Thus, equations (12) and (13) take the form

$$I_\rho(\varphi, V) = i_s\left[\exp\left(\frac{q(V - I_\rho(\varphi, V)R(\varphi))}{\eta kT}\right) - 1\right], \quad (14)$$

$$I_\rho(\varphi, V) = i_s\left[\exp\left(\frac{q(V_{\mathrm{bi}})}{\eta kT}\right) - 1\right] + \frac{V - V_{\mathrm{eq}}}{R(\varphi)}. \quad (15)$$

The total current given by equation (11) can be rewritten as

$$I = \int_x^y I_\rho(\varphi, V)\mathrm{d}\varphi, \quad (16)$$

where x and y are limits that represent the range of barrier heights. In the proposed approach, the standard deviation is assumed to be constant with respect to voltage in contrast to the previous model where the standard deviation was taken as a linear function of voltage to explain the temperature variation of apparent ideality factor. However, as shown later via simulation, the changes in ideality factor are due to barrier inhomogeneities themselves. The success of the approach lies in accurate estimation of the TED current through each elemental diode in the entire temperature and voltage ranges.

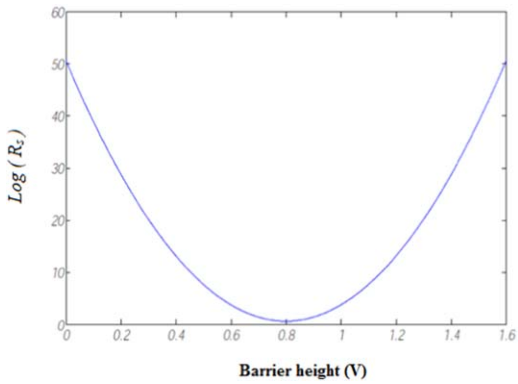

Figure 4. The distribution of series resistance with barrier height with $R_s = 10\,\Omega$, mean barrier height $= 0.8$ V and standard deviation $= 0.08$ V.

Range of barrier heights

The limits (maximum and minimum) of the barrier height have been under consideration ever since a Gaussian distribution function was proposed to represent inhomogeneity in a Schottky diode. Initially, the limits were assumed to be from $-\infty$ to ∞ as it leads to simplification in the integration process [8]. These were subsequently found unrealistic and changed as 0 to $2\overline{\varphi}$ [9] with exclusion of negative barrier heights. Such an omission does improve the model and reduces the possible errors. However, the minimum limit of the barrier height as zero remains, even though it is finite and equal to ζ, the energy difference between Fermi level and bottom of the conduction band. If the work function of metal (φ_{m}) is larger than that of the semiconductor (say n-type), a Schottky junction is formed with the barrier height equal to $q(\varphi_{\mathrm{m}} - \chi)$. So, with decrease in φ_{m}, the barrier height decreases. If the work functions of the metal and semiconductor are identical, the barrier height becomes just equal to ζ with no depletion region or built-in potential and resulting contact is ohmic in nature. When φ_{m} is further lowered, the contact continues to have the same barrier height ζ with no depletion region and ohmic character. Hence, the lower limit for the barrier height can be reasonably taken as ζ. The upper limit of the barrier height (φ) has been retained at $2\,\overline{\varphi}$ for the purpose of numerical analysis or integration as the contributions from barrier heights beyond $2\overline{\varphi}$ are negligible because of (i) the exponential decrease in the corresponding elemental diode current and (ii) low probabilities of such barriers.

Simulation of I–V characteristics

The simulation of currents has been carried out using equations (14)–(16) with the Gaussian distribution limits of barrier heights as ζ and $2\overline{\varphi}$. The integral was numerically solved

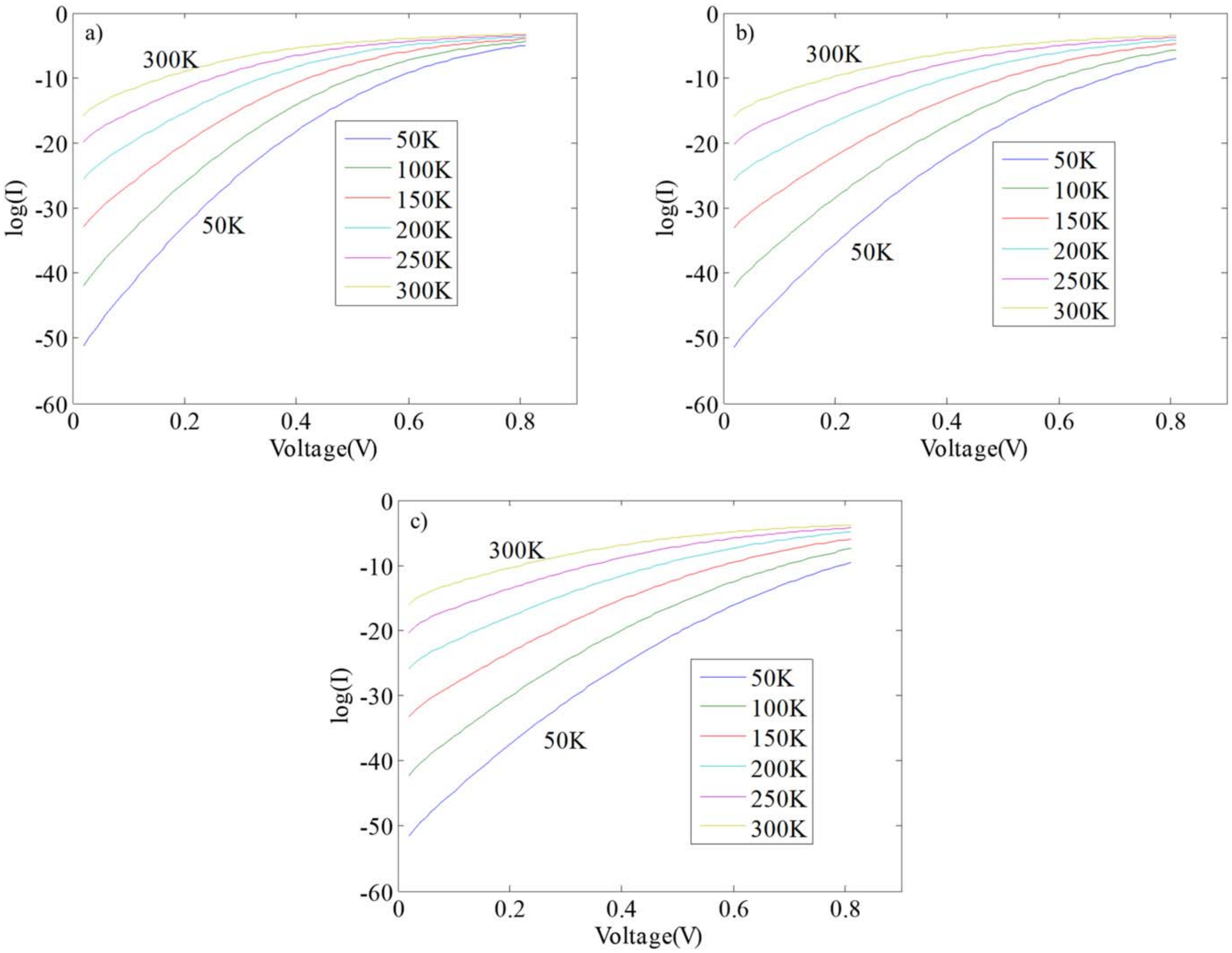

Figure 5. *I–V* characteristics on a semi-log scale simulated using the proposed model between limits $\zeta = 0.05$ V and $2\overline{\varphi}$ with $R_s = 10\ \Omega$, $A_d = 7.87 \times 10^{-7}\ \mathrm{m}^2$, $\overline{\varphi} = 0.8$ V and $\sigma = 0.08$ V for (a) $\eta = 1$ (b) $\eta = 1.2$ and (c) $\eta = 1.4$ showing well behaved curves at all temperatures with no signs of crossing over.

with Simpson's one third rule and the current estimated with equations (14) and (15) using Newton–Raphson method. The simulated *I–V* characteristics in the temperature range of 50–300 K are shown in figure 5 for ideality factors 1, 1.2 and 1.4. The increase in separation between the current-voltage plots at different temperatures with increase in ideality factor can be clearly noticed. The diode parameters, viz. apparent barrier height and apparent ideality factor, have been deduced from the linear region of the log(*I*) vs. *V* characteristics. While the slope determines the apparent ideality factor, the *y*-intercept gives the apparent barrier height. The parameters used here are the same as employed in conventional model to obtain the *I–V* curves, shown in figure (2). Clearly, the *I–V* curves produced with the new approach are well behaved and show no sign of anomalies including crossing over phenomenon observed before and mentioned above. Figure 6(a) shows rise in ideality factor with decrease in temperature even though standard deviation of the barrier height distribution is taken as constant and independent of voltage. The deduced values of apparent ideality factor listed in table 1 indicate increase with decrease in temperature at all η (= 1, 1.2, and 1.4). Earlier, with the conventional model, the change in ideality factor was explained by assuming standard deviation as dependent on bias and barrier height inhomogeneity by itself was unable to explain this dependence. Our work indicates that the assumption of the barrier height distribution dependent on applied bias is unnecessary to explain any observed dependence of ideality factor on temperature and barrier height inhomogeneity is responsible and sufficient to explain it. Further the function of the inverse slope on thermal energy as shown in figure 6(b) shows a transition from a non-ideal function with a large and continuously changing ideality factor towards a more ideal linear function with constant slope in agreement with Tung [20]. The model predicts an increase in barrier height with increase in temperature as depicted in figure 7(a). Furthermore, the calculated dependence of apparent barrier height with apparent ideality factor is shown in figure 7(b). These predictions of the proposed model are in good agreement with observed Schottky contact behavior [7, 10, 12–16, 20–22] in many systems. The success of the model is seen in figure 7(c), where by plotting apparent barrier height as a function of inverse thermal energy, a quadratic behavior is extracted which has been seen experimentally [12, 14]. This

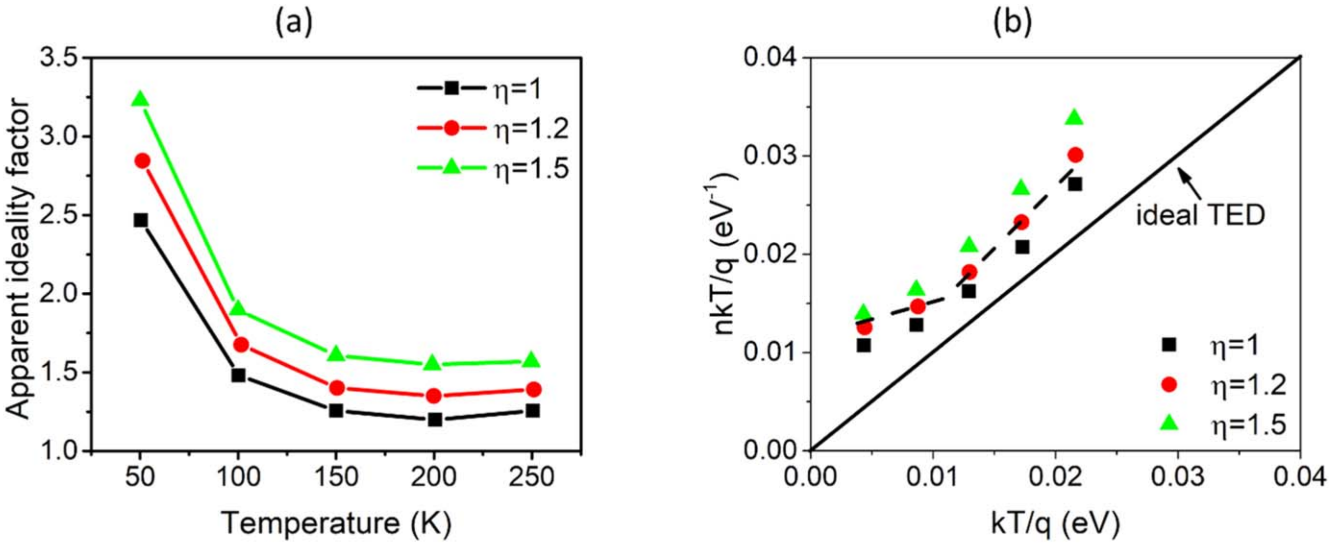

Figure 6. (a) Plot of apparent ideality factor versus temperature derived from the simulated *I–V* curves and (b) the plot of inverse slope (nkT/q) as a function of thermal energy (kT/q) for $\eta = 1$, $\eta = 1.2$ and $\eta = 1.5$. The black line represents ideal thermionic emission diffusion current.

Table 1. The apparent ideality factor as deduced from *I–V* curves at different temperatures for different values of η.

	Apparent ideality factor		
Temperature (K)	$\eta = 1$	$\eta = 1.2$	$\eta = 1.4$
50	2.46	2.84	3.23
100	1.46	1.68	1.9
150	1.22	1.41	1.6
200	1.19	1.36	1.54
250	1.23	1.39	1.56

behavior previously had to be interpreted as multiple mean barrier heights and different slopes corresponding to different standard deviations as shown in figure 7(c), an unlikely scenario, since the conventional model predicts the behavior to be linear. It is obvious from our improved model, a single distribution with one mean barrier and one standard deviation is actually responsible for the experimentally observed quadratic behavior which was not predicted by the conventional model and the requirement of multiple distributions was only an artifact of the conventional model due to its limitations. It is clear from the figures 6 and 7 that the temperature variation of barrier height and ideality factor manifested by barrier inhomogeneities can be well explained with the proposed approach suggested here.

It has to be noted that we have developed a model to accurately describe the effects of barrier inhomogeneity on thermionic emission diffusion current overcoming the limitations of the conventional model. However, explaining measured *I–V* characteristics in Schottky diodes on various emerging materials including GaN, SiC and Ga_2O_3 requires multiple models that includes various types of tunneling (thermionic field emission, field emission, defect assisted etc) at different barrier heights in addition to the barrier inhomogeneity model proposed in this work. For example, a large ideality factor at lower temperatures that decreases with increasing temperatures as a consequence of thermionic field emission, field emission or transitions from them to thermionic diffusion currents has been discussed in detail by Tung [20]. Similarly, the behavior of the inverse slope in figure 6(b) is similar to thermionic field emission and it is necessary to determine and differentiate the sources by other consequences such as barrier height dependence on temperature. Similarly, a shunt resistance parallel to the diodes may be required to model diode leakage that affects ideality factor at low forward bias [23]. It is obvious that modeling of actual devices requires simultaneous application of multiple models via TCAD software and our model is a valuable addition whose application is important with emerging materials (such as III-Nitrides, SiC, oxides etc) whose surface is not as well controlled as Si. Finally, there have been observations of crossover or intersecting behavior of current plotted for different temperatures in MIS structures [21, 24]. However, such crossovers occur at applied voltages much larger than the barrier height i.e. flat band conditions. The most likely cause is a series resistance that is expectedly dependent on temperature i.e., probably an increased resistance with increased temperatures due to decreased carrier mobility thereby resulting in lower currents at higher temperatures and hence a crossover in the I-V at applied forward bias voltages much larger than the barrier height. In contrast, the crossover phenomenon described in this work is at voltages lower than the barrier height and is a consequence of deficiencies in the conventional model.

C–V–T characteristics of Schottky diodes

Capacitance (C) of a Schottky diode in reverse bias is predominantly due to depletion region and is given by

$$C = \frac{\varepsilon_s A_d}{W}, \tag{17}$$

where ε_s is the dielectric constant of the semiconductor, A_d is the cross-sectional area, and W is the width of the depletion

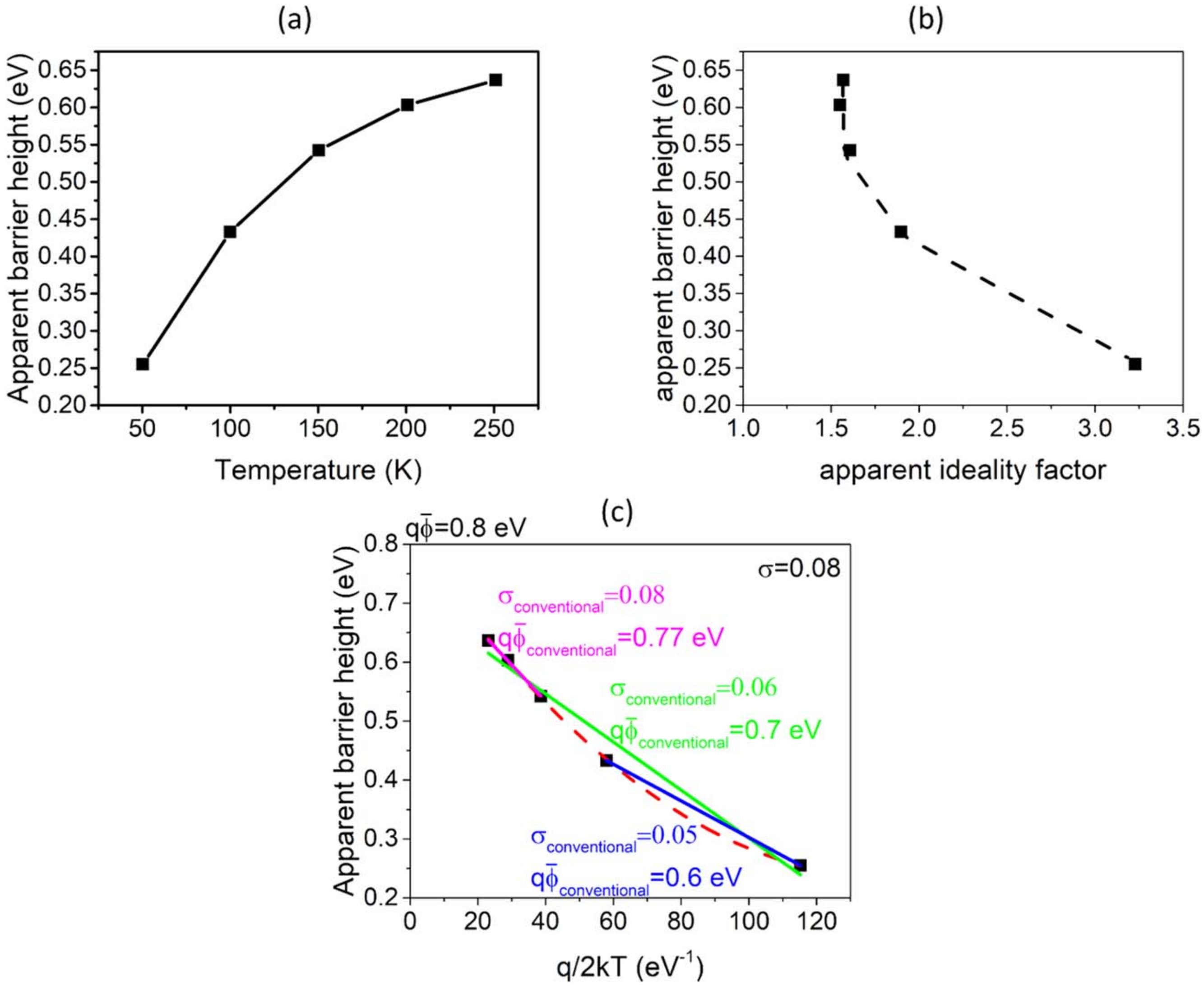

Figure 7. (a) Plot of apparent barrier height versus temperature derived from the simulated I–V curves ($\eta = 1.5$) using the proposed model and (b) relationship between apparent barrier height and apparent ideality factor $\eta = 1.5$ and (c) the function of apparent barrier height as a function of inverse thermal energy showing a quadratic (dashed line) behavior consistent with experiments.

region. The width 'W' is defined as

$$W = \sqrt{\frac{2\varepsilon_s}{q}\frac{1}{N_D}(\varphi - \zeta - kT/q + V)}, \tag{18}$$

where N_D is the dopant concentration, V is the reverse bias, φ is the barrier height, ζ is the difference in energy between the bottom of the conduction band and the Fermi level. The 'ζ' is expressed as

$$\zeta = (kT/q)\ln(N_C/N_D), \tag{19}$$

where N_C is the effective density of states.

Combining equations (17) and (18) and rearranging, one gets

$$\frac{1}{C^2} = \frac{2}{q\varepsilon {A_d}^2 N_D}\left(\varphi - \zeta - \frac{kT}{q} + V\right). \tag{20}$$

Equation (20) suggests that the $1/C^2$ versus V plot should be a straight line with slope providing the doping concentration (N_D) and the intercept on the ordinate giving the barrier height. For a metal-semiconductor junction displaying barrier inhomogeneities, figure 4 is modified such that each elemental diode is represented with its equivalent capacitance under reverse bias condition

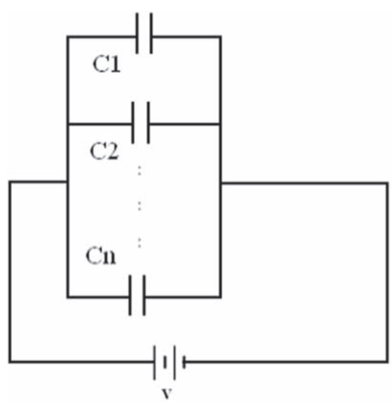

Figure 8. Equivalent circuit of Schottky junction having parallel combination of elemental diodes, each of capacitance C_i.

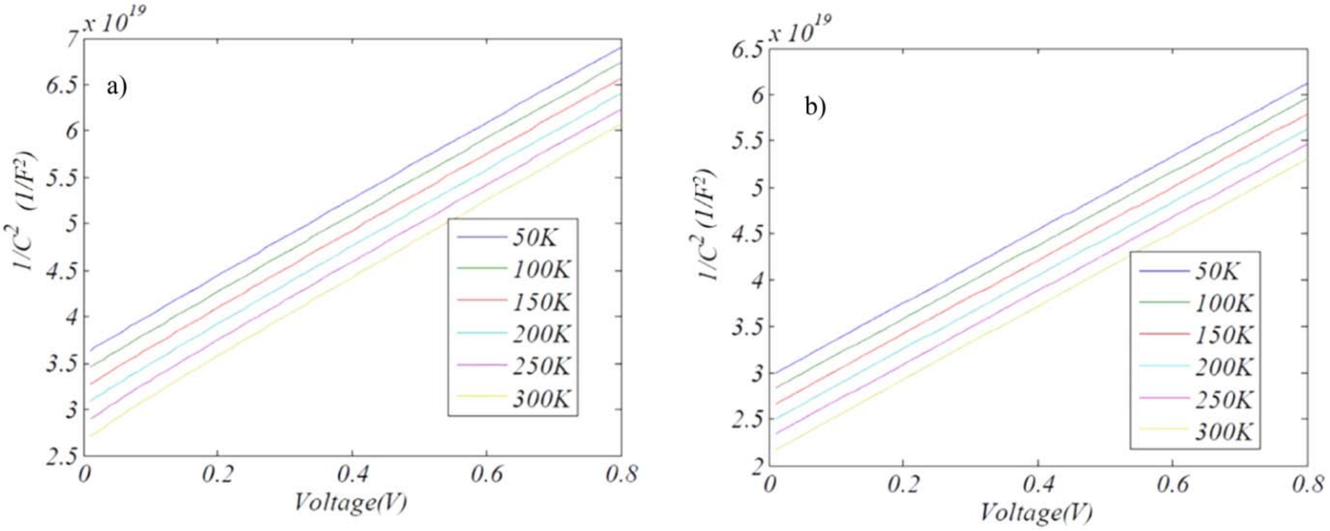

Figure 9. *C–V–T* characteristics of Schottky diodes simulated assuming a mean barrier height and standard deviation values as (a) 1 V and 0.25 V (b) 0.8 V and 0.08 V, respectively and a doping level of $5 \times 10^{15}\ \mathrm{cm}^{-3}$.

Table 2. Effective barrier height (φ_{eff}) deduced at different temperatures from simulated *C–V* curves.

Temperature (K)	$q\varphi_{\mathrm{eff}}$ (eV) ($\sigma = 0.25$V)	$q\varphi_{\mathrm{eff}}$ (eV) ($\sigma = 0.08$V)
50	0.960	0.794
100	0.956	0.794
150	0.952	0.793
200	0.948	0.793
250	0.944	0.792

(figure 8). The capacitance C_i of each diode depends on its effective area and expressed as

$$C_i(\varphi) = \frac{\varepsilon A_d \rho(\varphi)}{W(\varphi)}, \tag{21}$$

where $A_d\ \rho(\varphi)$ is the area and $W(\varphi)$ is the depletion width of the elemental diode (barrier height φ). The total diode capacitance (C) due to parallel combination of elemental capacitances is given by

$$C = C_1 + C_2 + C_3 + \cdots C_n = \sum_{1}^{n} C_i. \tag{22}$$

Since the Gaussian distribution function of barrier heights is continuous, the summation can be replaced by integration and the equation (22) in the limits ζ and $2\overline{\varphi}$ becomes

$$C = \int_{\zeta}^{2\bar{\varphi}} \frac{\varepsilon A_d \rho(\varphi) \mathrm{d}\varphi}{W(\varphi)}. \tag{23}$$

The equation (23) is numerically solved by summation method (with appropriately small interval to get the desired accuracy) to obtain *C–V* plots at various temperatures, taking $N_D = 5 \times 10^{15}\ \mathrm{cm}^{-3}$, mean barrier height ($\overline{\varphi}$) = 0.8 V and 1 V, and standard deviation $\sigma = 0.08$ and 0.25 V, mainly to ascertain the effect of barrier inhomogeneities. The $1/C^2$ versus V plots at various temperatures are shown in figure 9. The effective barrier height at each temperature is deduced

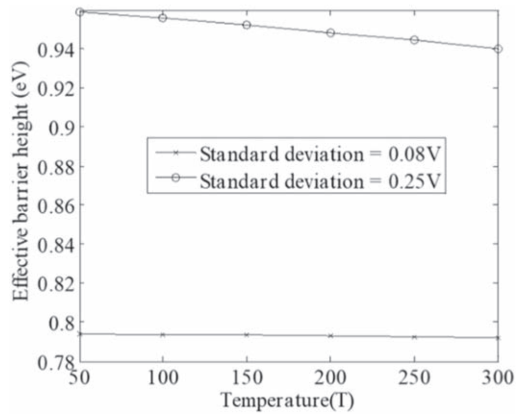

Figure 10. Effective barrier height versus temperature plot for Schottky diodes represented by Gaussian distribution function for barrier inhomogeneities.

from the intercept at the ordinate using equation (20). Table 2 summarizes the values of effective barrier height at various temperatures. Figure 10 shows the temperature variation of effective barrier height with parameters of distribution function as (i) $\overline{\varphi} = 0.8$, $\sigma = 0.08$ and (ii) $\overline{\varphi} = 1$ V, $\sigma = 0.25$ V. It may be noted that the effective barrier height extracted from *C–V* plots increases marginally with decrease in temperature due to prevalence of barrier height inhomogeneities at the Schottky junction. Experimental data reported indeed display similar behavior for Schottky diodes [25] and provide justification for the model proposed here.

Conclusions

The Schottky junction displaying barrier inhomogeneities and described by a parallel combination of elemental diodes with a single series resistance is not suitable and leads to unrealistic simulated *I–V* characteristics at low temperatures. The associated anomalies being (i) the saturation current larger at a lower temperature vis-à-vis higher temperature, (ii) the thermionic emission-diffusion current same at two temperatures for a forward bias, and (iii) the crossing over of *I–V* plots of different temperatures. If each elemental diode is assigned a series resistance of its own with the value inversely proportional to the area occupied, the anomalies in behavior can be eliminated. Simulated *I–V* characteristics suggest that the proposed model is robust and described the Schottky junction well with the limits of barrier heights as ζ and $2\overline{\varphi}$. The proposed model is well behaved and is successful in eliminating the anomalies of the conventional model. Further, it is successful in predicting that apparent barrier height as a function of inverse thermal energy is a quadratic behavior even with a single distribution. This previously required unlikely scenarios involving multiple mean barrier heights and standard deviations with the conventional model. Further, the description also explains the observed increase in the apparent barrier height with decrease in temperature of a Schottky diode when the values are deduced from the *C–V–T* data under reverse bias.

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