Origin of non-ideal current-voltage characteristics of metal-semiconductor contact: A numerical study

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The current-voltage (I-V) characteristics of Schottky diodes having spatial inhomogeneities are simulated using thermionic emission-diffusion mechanism and assuming a Gaussian distribution of barrier heights. The contact interface is assumed to have a number of non-interacting parallel diodes each with different barrier height within the distribution limits. Simulations of I-V characteristics of Schottky diodes were carried out both with mean and standard deviation of the distribution as constant or bias dependent. The resulting data are analysed to get insight into the effects of distribution parameters on the barrier height, activation energy plots and ideality factor over a temperature range 60-300 K. Simulation results show that a Schottky contact exhibiting Gaussian distribution of barrier heights with constant mean and standard deviation continues to behave as a homogeneous diode of apparently low barrier height with close to unity ideality factor. However, simulations carried out considering the linear bias dependence of mean and standard deviation yields a log(I)-V curve which correspond to the same low barrier height but with high ideality factor. These effects increase with increasing the value of the standard deviation. The series resistance plays a pivotal role in influencing the linearity of the log(I)-V curves of Schottky diodes exhibiting Gaussian distribution of barrier heights. Thus, it is shown that simulation of I-V data of Schottky diodes by incorporating barrier inhomogeneities give rise to non-ideal characteristics with low barrier height, high ideality factor and non-linear activation energy plot.

An abnormal decrease of the zero-bias barrier height and increase of ideality factor are usually observed with decrease in temperature (T) in Schottky diodes when current-voltage data are analysed in terms of thermionic emission-diffusion (TED) theory\textsuperscript{1,3}. Further, the decrease in barrier height (BH) at low temperatures is shown to cause non-linearity in the activation energy [ln(I_s/T^\alpha) vs 1/T] plot, I_s and T being the saturation current at zero-bias and diode temperature, respectively\textsuperscript{1,3}. The discrepancies have, in fact, been attributed to the barrier inhomogeneities present in the Schottky diodes\textsuperscript{4,16}. For describing the barrier inhomogeneities, two different approaches are adopted. In the first, one assumes the coexistence of low and high BH regions with the former occupying a very small fractional area\textsuperscript{4,14}. Also, the difference in the barrier heights is considered to be quite large, typically a few tenths of volt\textsuperscript{11,12}. However, low BH regions are known to get pinched-off below a critical size (=the depletion region width, 0.2-1 \textmu m). Since the variation in BH occurs even at a scale much smaller than the depletion region width\textsuperscript{17}, the interaction between patches should invariably lead to pinch-off of the conduction path of the low BH regions. Also, according to Sullivan et al.\textsuperscript{11}, with increase of size (say, beyond 0.06-0.1 \mu m), pinch-off ceases and low BH regions become active as well. This means that the interaction between patches is negligible much below the depletion region width regime and so low BH areas act even with low coverage quite independently of the high BH regions. Further, if patches cover comparable areas of the diode and corresponding to nearly the same barrier heights, pinch-off cannot occur at all and they operate simultaneously like non-interacting ideal diodes. In these cases, the activation energy plot is required to fit well with two straight lines, the slope of each giving the corresponding value of the barrier height. The I-V characteristics of Schottky diodes, however, lead to continuous variation in the activation energy plot\textsuperscript{1,3}. In the second approach, the spatial barrier inhomogeneities are described with some distribution function, e.g., Gaussian\textsuperscript{8,10,15,16} or log-normal\textsuperscript{8,18}. Gaussian distribution function has been widely accepted and invoked to explain the difference in barrier heights observed from capacitance-voltage (C-V) and I-V measurements in Al/p-InP\textsuperscript{8} and PtSi/Si\textsuperscript{10}, non-linearity in the Arrhenius plot and findings of
photoresponse measurements in PtSi/p-Si, abnormal decrease of BH and increase of ideality factor ($n$) at low temperatures,$^{15,16}$ etc. Palm et al$^{17}$ have even shown direct images of Schottky barrier height fluctuations in Au-Si contacts using ballistic electron emission microscopy (BEEM) and represented them with a Gaussian distribution function. Recently, Vanalme et al$^{19}$ have also shown BEEM spectra representing Gaussian distribution of BHs in Au/III-V semiconductors (GaAs, InP, AlGaAs and InGaAs).

Dobrocka and Osvald$^{20}$ have reported the influence of Gaussian distribution parameters and temperature on the barrier height and ideality factor of Schottky diodes using numerical simulation, in which they have assumed the mean and standard deviation to be independent of bias. The barrier height is, however, known to increase with increase in the forward bias. Obviously, if the barrier inhomogeneities are indeed represented by a Gaussian distribution function, the entire distribution profile is expected to change with bias. Hence, the bias dependences of both the mean and the standard deviation are to be considered for simulation of I-V characteristics of Schottky diodes. Moreover, Dobrocka and Osvald$^{20}$ have confined their analysis to current interval $2.6 \times 10^{-5}$ - $2.6 \times 10^{-3}$ A at 300 K for deriving the values of the barrier height and the ideality factor. The corresponding portion of the log(I)-V curve, in fact, exhibits non-linearity and therefore the slope varies continuously with bias. This led to low and high values of barrier height and ideality factor, respectively, which they attributed to the standard deviation itself. Actually, only the linear portion of the log(I)-V curve is suitable for deriving these parameters on the basis of TED current Eqs (2,3). Thus, taking non-linear portion at high bias instead of linear region of the log(I)-V curve at low bias is not at all justified. An attempt has therefore been made here to simulate the I-V characteristics of Schottky diodes containing barrier inhomogeneities on the basis of TED current equation and assuming Gaussian distribution of barrier heights with and without considering the linear bias dependence of its mean and standard deviation. The simulated I-V curves are analysed in the usual way$^5$ to understand the effect of distribution parameters and their bias dependences on the Schottky diode characteristics over a temperature range of 60-300 K.

**Method of Numerical Simulation**

The total current across a Schottky diode containing barrier inhomogeneities can be written as$^{15,20}$

$$I(V) = \int i(V, \phi_h) \rho(\phi_h) \, d\phi_h \quad \ldots (1)$$

where, $i(V, \phi_h)$ is the current at a bias $V$ for a barrier of height $\phi_h$ and $\rho(\phi_h)$ is the normalized distribution function giving the probability of occurrence of barrier height $\phi_h$. The implicit assumption is that there exists a number of parallel diodes of different barrier heights, each contributing to current independently. For the case of Gaussian distribution of barrier heights with mean ($\bar{\phi}_h$) and standard deviation $\sigma$, $\rho(\phi_h)$ is given by$^{15,20}$

$$\rho(\phi_h) = \frac{1}{\sqrt{(2\pi)}} \exp\left[\frac{-(\phi_h - \bar{\phi}_h)^2}{2\sigma^2}\right] \quad \ldots (2)$$

where, $1/\sqrt{(2\pi)}$ is the normalization constant. The current $i(V, \phi_h)$ through a Schottky barrier at a forward bias $V$, based on the TED theory, is expressed as$^{21}$

$$i(V, \phi_h) = A_d A^* T^2 \exp(-q\phi_h/kT) \times \left[\exp(q(V-\phi_h)/kT)-1 \right] \quad \ldots (3)$$

where, $A_d$, $A^*$, $T$, $q$, $k$ and $R_S$ are the barrier area, effective Richardson constant, temperature, electronic charge, Boltzmann constant, and diode series resistance, respectively. Thus, the current $i(V, \phi_h)$ at a bias $V$ for an elementary barrier of height $\phi_h$ is determined numerically by solving Eq. (3) at any temperature $T$ for a given value of $R_S$ using a computer program. It is then multiplied by the probability for that barrier height, as obtained from Eq.(2), to determine the actual current contribution. This way, the current has been computed for each barrier height $\phi_h$ within the range 0-1.1 V in a step of 0.01 V and the total current is then estimated by performing integration (1) using Simpson one-third rule. The process is repeated for each bias to obtain a complete I-V data at each temperature in the range 60-300K. For this, the mean $\phi_h$ and standard deviation of the Gaussian distribution function are assumed to be either independent of or vary linearly with bias, i.e., $\bar{\phi}_h = \bar{\phi}_h + \gamma V$ and $\sigma = \sigma_0 + \chi V$ where $\phi_h$ and $\sigma$ are mean and standard deviation at zero bias and $\gamma$ and $\chi$ stand for their voltage coefficients. The parameters chosen for performing the simulation are: $\phi_h$ = 0.8 V, $A_d$ = $7.87 \times 10^{-7}$ m$^2$ (for a diode of 1 mm diameter), $A^*$ = $1.12 \times 10^6$ Am$^{-2}$ K$^{-1}$, and $R_S$ = 0 and 10 $\Omega$. The values of voltage coefficients $\gamma$ and $\chi$ are taken as 0.06 and -0.05,
respectively, keeping in view the experimental findings.15,16

A computer program involving iteration has been used for least square fitting of the linear portion of the simulated log(I)-V curve in TED current equation

\[ I(V) = I_s \exp\left[\frac{q(V-I_R S)\eta kT}{11kT}\right] \times \left[1-\exp\left\{-\frac{q(V-I_R S)\eta kT}{kT}\right]\right] \]

... (4)

with

\[ I_s = A_d A^{\ast} T^2 \exp\left(-\frac{q\phi_b}{kT}\right) \]

... (5)

taking \( I_s \), \( \eta \) and \( R_s \) as adjustable parameters. Once \( I_s \) is known, \( \phi_b \) can be easily found using Eq. (5). Unlike Dobrocka and Osvald20, who confined fitting to a current interval (i.e., \( 2.6 \times 10^{-5} - 2.6 \times 10^{-3} \) A at 300 K), no current restriction is applied here and fitting extended right upto the point where non-linearity begins to appear in the log(I)-V curve. The ideality factor \( \eta \) can also be obtained from the slope of the linear region of log(I)-V curve. Needless to say, a homogeneous Schottky diode is characterized by a single barrier height which may be taken as being independent or varying linearly with bias as before. The total current in such a case is given by Eq. (4) itself.

Results and Discussion

Fig. 1 shows the simulated log(I)-V curves of inhomogeneous Schottky diodes with various values of standard deviation at 300 K and 200 K. These plots initially reveal that with increasing \( \sigma_0 \), the linear region becomes less pronounced. This behaviour actually results due to finite series resistance \( R_s \) associated with each elementary barrier. Actually, with increase of \( \sigma_0 \), more barriers of low BH appear which, in turn, contribute increased current at any given bias. The probability of the occurrence of these barrier decreases, however, as one moves away from the mean value. As a consequence, the product \( \int(V,\phi_b)\rho(\phi_b) \) or argument of the integral in Eq. (1) assumes appreciable values over a BH range below the mean of the distribution. This makes the \( iR_s \) term effective at relatively low bias. Moreover, for each elementary barrier, the saturation in its log(I)-V curve begins at different bias. Thus, the addition of each \( i(V,\phi_b)\rho(\phi_b) \) term over a range of barrier heights makes the resultant log(I)-V curve non-linear in nature. This effect of series resistance is more for higher values of \( \sigma_0 \) as the non-linearity/ saturation initiation then shifts towards low bias. Interestingly, for zero \( R_s \) these curves remain linear for all values of \( \sigma_0 \) and do not exhibit saturation effects (Fig.1). Thus non-linearity in log(I)-V curves is arising due to the series resistance as well and can not be attributed to the standard deviation alone.

In order to know the nature of integrated curve over a bias range at any temperature, the data were analysed further to find barrier parameters. As these curves are identical to those for a real Schottky diode the values of barrier parameters, i.e., barrier height and ideality factor are obtained by usual fitting method. Fig. 2 shows the apparent BH as obtained from the simulated curves at various temperatures for

![Fig. 1 — Simulated log(I)-V curves of Schottky diodes for various \( \sigma_0 \), taking mean barrier height \( \phi_{b0} = 0.8 \) V and \( R_s = 10 \) \( \Omega \)]
different values of the standard deviation. Clearly, increase in standard deviation leads to a lowering of the apparent barrier height. Interestingly, the ideality factor (not shown here) is almost close to unity for all these curves. This means that ideality factor is independent of the standard deviation. In other words, a Schottky contact exhibiting Gaussian distribution of barrier heights with constant mean and standard deviation continues to behave as a homogeneous diode of apparently low barrier height with close to unity ideality factor.

Fig. 3 shows log(I)-V curves simulated considering the linear bias dependence of the mean and the standard deviation of the Gaussian distribution of BHs (The parameters are $\Phi_0 = 0.8$ V, $\gamma = 0.06$, $\chi = -0.05$ and $R_s = 10 \Omega$). The similar voltage dependence has been extended here to mean and standard deviation of Gaussian distribution of BHs for generating the I-V data (shown in Fig. 3) for an inhomogeneous Schottky contact.

In both the cases above, with and without linear bias dependence of distribution parameters, the apparent barrier height exhibits similar variation as shown in Fig. 2, the corresponding activation energy plots in the two cases are also identical. The effect of inhomogeneities on the Richardson ($\ln(I_s) / T^2$ vs $1/T$) plot is shown in Fig. 6 for various values of $\sigma_0$. It is
Thus, non-linearity in the log(I)-V curve is a consequence of large spread in the barrier height and occurs even at low voltages for reasons cited above. This leads artificially to somewhat higher ideality factor than unity. Dobrocka and Osvald\textsuperscript{20} have however used the curved portion of the log(I)-V curves, leaving the linear region observed at low voltages. As a consequence, they obtained high values of ideality factor and attributed them to the standard deviation. It needs to be emphasized that non-linearity in log(I)-V curves has not arisen due to \( \sigma_0 \) alone, as otherwise, it should have also been observed in the curves corresponding to zero series resistance. On the contrary, log(I)-V curves shown in Fig. 1 are found to be linear and parallel to each other - showing merely a shift for different values of \( \sigma_0 \) and thus no change in the ideality factor at all. The linear portion of the curve, in fact, corresponds to the region where TED is dominant and the effect of the bending due to series resistance is absent/negligible. There is no justification for ignoring the low bias linear region of the curve in the process of data fitting and evaluation of barrier parameters. This is perhaps the reason why Dobrocka and Osvald\textsuperscript{20} found high ideality factors in their work.

It is pointed out above that the series resistance influences the linearity of log(I)-V curves and, in turn, gives high values of the ideality factor. Actually, with no series resistance, linearity prevails for the entire bias range and one obtains parallel straight lines for...
different values of the standard deviation at any given temperature. The ideality factor therefore is constant. Also, for a finite series resistance with a single barrier height (i.e., zero standard deviation), bending occurs in log(I)-V curve at a particular current level at all the temperatures and leads to saturation\(^{22}\). The point where deviation initiates, however, shifts towards lower current with increase in the value of the series resistance. With finite series resistance and a Gaussian distribution of barrier heights (i.e., non-zero standard deviation), bending in the log(I)-V curve becomes prominent at high values of the standard deviation (Fig. 1). This feature can be understood as follows:

The Gaussian distribution of barrier heights is essentially equivalent to the existence of a large number of parallel diodes, each having a different barrier height. If each acts independently, the current contribution depends on the barrier height and the probability of its occurrence. For barrier heights below the mean of the distribution, no doubt increases but the probability of occurrence decreases progressively. The product \(i(\phi_b,V)p(\phi_b)\) then gives the current contribution of all elementary diodes each having of barrier height \(\phi_b\). The current therefore becomes appreciable over a BH range (which increases with the value of \(\sigma_b\)) below the mean of the distribution. Also, it makes deviation of log(I)-V curve at different bias levels. Consequently, when currents of all the elementary barriers are added up, the resulting log(I)-V curve exhibits non-linearity over a bias range.

Thus, it is amply clear that consideration of Gaussian distribution of barrier heights (with and without bias dependent \(\phi_b\) and \(\sigma\)) for simulation of I-V data of a Schottky diode by incorporating barrier inhomogeneities give rise to non-ideal characteristics with low barrier height, high ideality factor and non-linear activation energy plots.

**Conclusions**

The I-V characteristics of a Schottky diode containing barrier inhomogeneities can be simulated on the basis of TED theory and assuming a Gaussian distribution of barrier heights and invoking the model of non-interacting parallel diodes. The mere existence of the Gaussian distribution of barrier heights leads to decrease in the zero-bias barrier height and causes non-linearity in the activation energy plots.

The bias dependences of the mean and the standard deviation are responsible for the high ideality factor. However, this bias dependence make no change in the barrier height and the activation energy plots. The series resistance causes non-linearity in the current voltage characteristics of a Schottky diode in a subtle way when there exist barrier inhomogeneities such that a large number of non-interacting parallel diodes with Gaussian distribution of barrier heights act simultaneously.

**References**