Effects of barrier height distribution on the behavior of a Schottky diode

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The current–voltage characteristics of a Schottky diode are simulated numerically using the thermionic emission-diffusion mechanism and considering a Gaussian distribution of barrier heights, with a linear bias dependence of both the mean and standard deviation. The resulting data are analyzed to get insight into the effects of distribution parameters on the barrier height, activation energy plots and the ideality factor over a temperature range 50–300 K. It is shown that with a Gaussian distribution of the barrier heights the system continues to behave like a single Schottky diode of apparently low zero-bias barrier height and a high ideality factor. Its barrier height decreases, activation energy plot becomes non-linear and ideality factor increases with a decrease in temperature. While the distribution parameters are responsible for the abnormal decrease of barrier height, their bias dependences account for the higher ideality factor at low temperatures. Also, the pivotal role played by series resistance in influencing the linearity of the $\ln(I)–V$ plots of Schottky diodes with a Gaussian distribution of barrier heights is discussed. © 1997 American Institute of Physics. [S0021-8979(97)01422-9]

I. INTRODUCTION

The classical model of a metal-semiconductor contact (or Schottky diode) assumes the junction to be abrupt with a fixed barrier height (BH). However, such a description fails to account for the observed temperature dependence of diode parameters determined from the corresponding current-voltage ($I–V$) characteristics on the basis of thermionic emission-diffusion (TED) theory.\textsuperscript{1–3} The discrepancies have, in fact, been attributed to the barrier inhomogeneities present in the Schottky diodes.\textsuperscript{4–16} To describe 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{11–14} Also, the barrier in the higher regions is considered to be quite large, typically a few tenths of a volt.\textsuperscript{11,12} However, low BH regions are known to get pinched off below a critical size (\textasciitilde the depletion region width, 0.2–1 $\mu$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{14} with an increase in 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 well 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 correspond 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 a 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{18} The Gaussian distribution function is widely accepted and is utilized to explain the difference in barrier heights observed from capacitance–voltage ($C–V$) and $I–V$ measurements in Al/$p$–InP (Ref. 8) and PtSi/Si,\textsuperscript{10} non-linearity in the Arrhenius plot and findings of photoresponse measurements in PtSi/ $p$–Si,\textsuperscript{7} direct images of Schottky barrier height fluctuations in Au–Si contacts,\textsuperscript{17} an abnormal decrease of BH and an increase of ideality factor ($\eta$) at low temperatures,\textsuperscript{15,16} etc.

An attempt was made here to simulate the $I–V$ characteristics of Schottky diodes on the basis of the TED current equation and by assuming a Gaussian distribution of barrier heights with linear bias dependence of its mean and standard deviation. The simulated $I–V$ data are analyzed in detail to examine the effects of distribution parameters and their bias dependences on the Schottky diode characteristics over a temperature range of 50–300 K. The aim is to identify the factors responsible for the abnormal decrease in BH and the increase in the ideality factor with a decrease in temperature.

II. METHOD OF ANALYSIS

The total current across a Schottky diode containing barrier inhomogeneities can be written as\textsuperscript{15,19}

\[ I(V) = \int i(V, \phi_b)\rho(\phi_b) d\phi_b, \]  

where $i(V, \phi_b)$ is the current at a bias $V$ for a barrier of height $\phi_b$ and $\rho(\phi_b)$ is the normalized distribution function giving the probability of occurrence of barrier height $\phi_b$. The implicit assumption is that there exists a number of parallel diodes of different barrier heights, each contributing to the current independently. For the case of a Gaussian distribution of barrier heights with mean $\bar{\phi}_b$ and standard deviation $\sigma$, $\rho(\phi_b)$ is given by:\textsuperscript{8–10,15,19}

\[ \rho(\phi_b) = \frac{1}{\sqrt{2\pi} \sigma} e^{-\frac{(\phi_b - \bar{\phi}_b)^2}{2\sigma^2}}, \]  

\[ I(V) = \int \frac{1}{\sqrt{2\pi} \sigma} e^{-\frac{(\phi_b - \bar{\phi}_b)^2}{2\sigma^2}} i(V, \phi_b) d\phi_b, \]  

and

\[ I(V) = \int \frac{1}{\sqrt{2\pi} \sigma} e^{-\frac{(\phi_b - \bar{\phi}_b)^2}{2\sigma^2}} \mathcal{F}(\phi_b; \mathcal{G}(\phi_b; \bar{\phi}_b, \sigma)) d\phi_b, \]  

where $\mathcal{F}(\phi_b; \mathcal{G}(\phi_b; \bar{\phi}_b, \sigma))$ is the normalized distribution function giving the probability of occurrence of barrier height $\phi_b$.
\[
\rho(\phi_b) = \frac{1}{\sigma \sqrt{2 \pi}} \exp \left( -\frac{(\phi_b - \bar{\phi}_b)^2}{2\sigma^2} \right),
\]

(2)

where \(1/\sigma \sqrt{2 \pi}\) is the normalization constant. The current \(i(V, \phi_b)\) through a Schottky barrier at a forward bias \(V\), based on the TED theory, is expressed \(^{20}\)

\[
i(V, \phi_b) = A_d A^{**} T^2 \exp \left( -\frac{q \phi_b}{kT} \right) \times \left[ \exp \left( \frac{q(V - IR_s)}{kT} \right) - 1 \right],
\]

(3)

where \(A_d\), \(A^{**}\), \(T\), \(q\), \(k\), and \(R_s\) are the diode area, effective Richardson constant, temperature, electronic charge, Boltzmann constant and diode series resistance, respectively. Thus, the current \(i(V, \phi_b)\) at a bias \(V\) for an elementary barrier of height \(\phi_b\) 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 \(\phi_b\) within the range 0–1.1 \(V\) in steps of 0.01 \(V\) and the total current is then estimated by performing the integration [Eq. (1)] using Simpson’s one-third rule. The process is repeated for each bias to obtain full \(I−V\) data at each temperature in the range 50–300 K. For this, the mean \(\bar{\phi}_b\) and standard deviations \(\sigma\) of the Gaussian distribution function are assumed to vary linearly with bias, i.e.,

\[
\bar{\phi}_b = \bar{\phi}_{b0} + \gamma V,
\]

and

\[
\sigma = \sigma_0 + \xi V,
\]

(4)

where \(\bar{\phi}_{b0}\) and \(\sigma_0\) are the mean and standard deviation at zero bias and \(\gamma\) and \(\xi\) are their voltage coefficients. The parameters chosen for performing the simulation are \(\bar{\phi}_{b0}=0.8\ \text{V}\), \(A_d=7.87 \times 10^{-7}\ \text{m}^2\) (for a diode of 1 mm diameter), \(A^{**}=1.12 \times 10^6\ \text{A m}^{-2}\ \text{K}^{-2}\) for \(n\)-type silicon,\(^{19}\) and \(R_s=10\ \Omega\). The values of voltage coefficients \(\gamma\) and \(\xi\) are taken as 0.06 and −0.05, respectively. These values were actually found recently from measured \(I−V\) data of the Pd_{2}Si/Si system.\(^{15,16}\) A computer program involving iteration has been used for least square fitting of the linear portion of the simulated \(\ln(I−V)\) characteristics in the TED current equation\(^{2,20}\)

\[
I(V) = I_s \exp \left( \frac{q(V - IR_s)}{\eta kT} \right) \left[ 1 - \exp \left( -\frac{q(V - IR_s)}{kT} \right) \right],
\]

(5)

with

\[
I_s = A_d A^{**} T^2 \exp \left( -\frac{q \phi_{b0}}{kT} \right),
\]

(6)

taking \(I_s\), \(\eta\) and \(R_s\) as adjustable parameters. Once \(I_s\) is known, \(\phi_{b0}\) can be easily found from Eq. (6) by introducing appropriate values of \(A_d\) and \(A^{**}\).

III. RESULTS AND DISCUSSION

The simulated \(\ln(I−V)\) curves are shown in Fig. 1 for various values of the standard deviation (\(\sigma_0\)) at 300 and 200 K. These plots initially reveal that with increasing standard deviation \(\sigma_0\) the linear region becomes less pronounced. This behavior actually results due to the series resistance \(R_s\) (=10 \(\Omega\)) associated with each elementary barrier. With an increase of \(\sigma_0\), more barriers of low barrier height (that are effective) appear which, in turn, contribute increased current at any given bias. The probability of the occurrence of these barriers decreases, however, as one moves away from the mean value. As a consequence, the product \(i(V, \phi_b)\rho(\phi_b)\) of the integral in Eq. (1) assumes appreciable values over a BH range below the mean of the distribution and makes the \(IR_s\) term effective at relatively low bias. Moreover, for each elementary barrier, the saturation in its \(I−V\)
curve begins at a different bias. Thus, the addition of each $i(V, \phi_b)\rho(\phi_b)$ term over a range of barrier heights makes the resultant $\ln(I-V)$ plot non-linear in nature. This effect of series resistance is more for higher $s_0$ as the non-linearity/saturation initiation then shifts towards low bias. Interestingly, for zero series resistance, $\ln(I-V)$ plots remain linear for all values of $\sigma_0$ and do not exhibit saturation effects (Fig. 1). These results amply demonstrate that the non-linearity in the current–voltage characteristics arises due to series resistance in a subtle way when a number of non-interacting parallel diodes with a Gaussian distribution of barrier heights act simultaneously. Consequently, the nature of non-linearity in the $\ln(I-V)$ plot becomes complex and therefore this very region should not be considered for extraction of barrier parameters (viz., $\phi_b$ and $\eta$).

The values of the barrier height and the ideality factor are depicted in Figs. 2 and 3 as a function of temperature for various standard deviations. Clearly, the barrier height decreases while the ideality factor increases slowly at low and rapidly at high values of the standard deviation. Further, these parameters are less sensitive to the standard deviation at higher temperatures but become progressively $\sigma_0$ dependent as the temperature is lowered. Figs. 2, 3, 5 and 6 suggest that decreasing temperature and increasing standard deviation have similar effects on the barrier parameters, i.e., both lead to a decrease in the barrier height and an increase in the ideality factor.

The results of simulation carried out with constant values of the mean and standard deviation (i.e., $\gamma=0$, $\xi=0$) show the nature of barrier height and Richardson plots to be exactly as shown in Figs. 2 and 4, respectively. However, the ideality factor is found to be close to unity for all the
diodes. In contrast, Dobrocka and Osvald obtained high change in slope bias dependence of the mean factor with a decrease in the temperature is caused by the'

\[ \ln(I) - V \] plots. This means that an increase in the ideality factor with a decrease in the temperature is caused by the bias dependence of the mean \( \bar{\phi}_0 \) and the standard deviation \( \sigma \) of the Gaussian distribution of barrier heights in Schottky diodes. In contrast, Dobrocka and Osvald obtained high values of the ideality factor under a similar situation and attributed them to the standard deviation. It needs to be emphasized that non-linearity has not arisen due to \( \sigma \) alone; if it had, that trend should have been present in case of zero series resistance as well. Instead, the \( \ln(I) - V \) plots are found to be linear—showing a shift for different values of \( \sigma_0 \) and a change in slope (amounting to an increase of the ideality factor) as shown in Fig. 3. The linear portion of any \( \ln(I) - V \) plot corresponds to the regime where the TED is dominant and the effect of bending due to series resistance is absent/negligible. Dobrocka and Osvald confined their analysis to the current interval that lies in the non-linear region (where the slope varies continuously with bias) and ignored altogether the low bias linear portion in evaluating the barrier parameters. This is perhaps the reason for their obtaining high values of the ideality factor without even considering the bias dependence of barrier parameters. In fact, the ideality factor in such cases should invariably be unity.

Alternatively, Eq. (1) can be solved analytically by making substitutions (2) and (3) and integrating within the limit of \(-\infty \) to \( +\infty \). This exercise using Eq. (4) for linear bias dependence of the mean (\( \bar{\phi}_0 \)) and standard deviation (\( \sigma \)) leads to an expression similar to Eq. (5), on neglecting the term involving \( \xi^2 V^2 \), with apparent barrier height (\( \phi_{ap} \)) and ideality factor (\( \eta_{ap} \)) given by

\[ \phi_{ap} = \bar{\phi}_0 - \frac{\sigma_0^2 q}{2kT}, \]

and

\[ \frac{1}{\eta_{ap}} = 1 - \gamma + \frac{\sigma_0 q \xi}{kT}. \]

Equations (7) and (8) express the barrier height and the ideality factor in terms of distribution parameters (\( \bar{\phi}_0 \) and \( \sigma_0 \)) and their bias coefficients (\( \gamma \) and \( \xi \)) and temperature. Equation (8) is, in fact, valid under the assumption \((1 - \gamma + \sigma_0 q \xi/kT)V \gg \xi^2 V^2/2\). Also, Eqs. (7) and (8) actually correspond to parameters \( \phi_{ap} \) and \( \eta_{ap} \) derived from the data of the linear region in the \( \ln(I) - V \) plots, where the influence of series resistance (\( R_s \)) on each significant current component \( i(V, \phi_b) \), defined by Eq. (3), is absent/negligible. As pointed out earlier, the effect of series resistance is to cause a deviation from linearity in the \( \ln(I) - V \) plots. The point of initiation shifts towards lower bias with (i) an increase in \( \sigma_0 \) at a fixed non-zero \( R_s \) (Fig. 1) and (ii) an increase of \( R_s \) for a particular value of \( \sigma_0 \) (Fig. 7). If \( R_s \) is zero, linearity persists at all the temperatures in the entire \( \ln(I) - V \) plot for every \( \sigma_0 \) (Figs. 1 and 8). However, for the case of \( \sigma_0 = 0 \), i.e., no distribution of barrier heights or a fixed \( \phi_b \) at the interface, deviation from linearity invariably results, leading to saturation in the \( \ln(I) - V \) plots (Fig. 8). The effect of inhomogeneities (i.e., the simultaneous act of independent elementary barriers having a distribution of heights) on the non-linearity of \( \ln(I) - V \) plots at a given value of series resistance (\( R_s = 10 \Omega \)) is shown in Fig. 9. Actually, non-linearity begins at progressively lower bias as the value of \( \sigma_0 \) increases and amounts to a reduction in current that results due to a homogeneous barrier of an effective height \( \phi_{ap} \) and ideality factor \( \eta_{ap} \) given by Eqs. (7) and (8), respectively.

It may be mentioned that Eqs. (7) and (8) were also derived by Werner and Guttler when they considered the linear bias dependence of both the mean barrier height (\( \bar{\phi}_b \)) and the square of the standard deviation (\( \sigma^2 \)). As a consequence, the expression for the ideality factor (\( \eta_{ap} \)) contains a bias coefficient (\( \rho_0 \)) of \( \sigma^2 \) as opposed to the product of \( \sigma_0 \)

\[ \eta_{ap} = 1 - \gamma + \frac{\sigma_0 q \xi}{kT}. \]
and $\xi$ in the third term of Eq. (8), such that $\rho_3 = 2\sigma_0\xi$. This means that the ideality factor is a function of the bias coefficient of $\phi_b$ and the variance $\sigma^2$ besides temperature. On the other hand, according to Eq. (8), the ideality factor is determined not by the bias coefficients of $\phi_b$ and $\sigma$ alone but by the value of the standard deviation ($\sigma_0$) at zero bias as well. Therefore, $\eta_{ap}$ should actually vary with the value of $\sigma_0$ (as indicated in Fig. 3), instead of remaining constant as reported by Werner and Guttler. Needless to say, the emphasis here is on the simulation of $I$–$V$ characteristics of a Schottky diode by assuming a spatial Gaussian distribution of the barrier heights and considering the linear bias dependence of mean $\phi_b$ and standard deviation $\sigma$ for the first time. The values of $\phi_{ap}$ and $\eta_{ap}$ (marked by symbols) calculated using Eqs. (7) and (8), respectively, with $\phi_{b0} = 0.8$ V, $\gamma = 0.06$, $\xi = -0.05$ for various $\sigma_0$ and $T$ show excellent agreement with the results (shown by continuous curves) derived from the simulated $I$–$V$ plots (see, e.g., Figs. 2, 3, 5 and 6).

**IV. CONCLUSIONS**

The $I$–$V$ characteristics of Schottky diodes containing barrier inhomogeneities were simulated based on the thermionic emission-diffusion mechanism and the Gaussian distribution of barrier heights with linear bias dependence of both the mean and the standard deviation. While the existence of the Gaussian distribution leads to (1) a decrease in the zero-
bias barrier height with a decrease in temperature and (ii) non-linearity in the activation energy plots at low temperatures, the bias dependence of the distribution parameters (i.e., mean and standard deviation) accounts for the abnormal increase of the ideality factor with a decrease in temperature. Also, non-linearity in the thermionic emission-diffusion current-voltage characteristics of Schottky diodes results due to the finite series resistance in a subtle way through the standard deviation and is a consequence of the coexistence and simultaneous action of a large number of elementary barriers of different heights.

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