

A Simulated Study on Charge Carrier Transport through the Barrier Inhomogeneity in MS Contact

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Abstract- The paper presents, a simulated study for charge carrier transport at metal semiconductor contact with respect to the Richardson constant. During simulation, the Richardson's constant has been determined from the intercepts of I-V curves. When the I-V curves of schottky diodes for different materials have been obtained by using their Richardson constant, then a change in their intersecting behavior at different temperatures as well as the value of barrier heights with linear bias dependence have been observed. This change in barrier height values with bias, affects the conduction mechanism through the metal-semiconductor. It has been concluded that the in order to develop MS contact, the material with high Richardson constant may be preferred to have high current density.

Index Terms- Barrier height; metal-semiconductor contact; schottky diodes.

1. INTRODUCTION

Metal- semiconductors play an important role in electronic and optoelectronic device based on semiconductors compounds in the form of schottky diode. The performance and reliability of a Schottky diode is drastically influenced by the interface quality between the deposited metal and the semiconductor surface. Schottky barrier diodes (SBDs) have been widely studied and many attempts have been made to understand the conduction mechanism across such Schottky diodes. The knowledge of the conduction mechanism across a Schottky barrier is essential in order to calculate the Schottky barrier parameters and explain the observed effects. Generally, the SBD parameters are determined over a wide range of temperatures in order to understand the nature of the barrier and the conduction mechanism. Thermionic emission (TE) theory is normally used to extract the SBD parameters [1-7], however, there have been several reports of certain anomalies [4, and 7-9] at low temperatures. The temperature dependence of the I-V characteristics of the metal-semiconductor helps us to understand different aspects of conduction mechanism. However, a complete description of the charge carrier transport through MS contact is still a challenging problem. The spatial variation of barrier heights in Schottky diodes is considered to explain the anomalous behavior with temperature dependence of diode parameters derived from experimental data. The variation of barrier heights (BHs) is described mainly by a Gaussian distribution function and is widely accepted to explain the experimental data [10-18]. Simulation performed to see the effect of such

inhomogeneities in barrier heights, which leads to the same temperature dependence of diode parameters as

observed from experimental current-voltage (I-V) characteristics [19, and 20].

The equation governing current flow through Schottky barrier diode for applied bias V is given by [21]

$$I(\phi_b, V) = A_d A^{**} T^2 \exp\left(\frac{-q\phi_b}{kT}\right) \left[\exp\left(\frac{qV}{kT}\right) - 1 \right] \quad \dots (1)$$

However, the barrier height is bias dependent and reported to increase linearly with forward bias [21, and 22]. Considering the linear bias dependence of barrier height, one can write

$$\phi_b(V) = \phi_{b0} + \gamma V \quad \dots (2)$$

Where, ϕ_{b0} is the barrier height at zero bias and γ is bias coefficient of barrier height. Substituting barrier height value from equation (2), equation (1) can be written as

$$I = I_0 \exp\left(\frac{-\gamma qV}{kT}\right) \left[\exp\left(\frac{qV}{kT}\right) - 1 \right] \quad \dots (3)$$

with

$$I_0 = A_d A^{**} T^2 \exp\left(\frac{-q\phi_{b0}}{kT}\right) \quad \dots (4)$$

the saturation current at zero bias. Now, introducing a parameter η such that $1/\eta = 1 - \gamma$, equation (3) can be written as

$$I = I_0 \exp\left(\frac{qV}{\eta kT}\right) \left[1 - \exp\left(\frac{-qV}{kT}\right) \right] \quad \dots (5)$$

When $\eta = 1$ (or $\gamma = 0$), equation (3) reduces to pure thermionic emission-diffusion equation (1). The parameter η is called the ideality factor and usually

has a value greater than unity. This amounts to extra current arising due to other mechanisms or due to variation in barrier height. For example, thermionic-field emission, generation-recombination, tunneling, interface impurities, interfacial oxide layer, image forces all tend to increase current, and hence makes ideality factor η rises above unity. The neutral region of the semiconductor (between the depletion region and back Ohmic contact) offers resistance (R_s) and so a significant voltage drop occurs at large forward currents. This amounts to a reduction of the voltage across the barrier region from that actually applied to the terminals of the diode. This is accounted for by replacing the V by $V-IR_s$ in the equation (5). The current equation then becomes,

$$I = I_0 \exp\left(\frac{q(V-IR_s)}{\eta kT}\right) \left[1 - \exp\left(\frac{-q(V-IR_s)}{kT}\right)\right] \quad \dots (6)$$

In such a situation a plot of $\ln(I)$ versus V deviates from a straight line at high forward voltages. The Gaussian distribution of barrier heights, with a mean value of ϕ_b and standard deviation σ , has the form [14, 18, 21, and 22].

$$\rho(\phi_b) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\left(\frac{\phi_b - \bar{\phi}_b}{2\sigma^2}\right)^2\right] \quad \dots (7)$$

Where, the pre-exponential term is the normalized constant.

The total current across the Schottky contact at a forward bias is then given by

$$I(V) = \int I(\phi_b, V) P(\phi_b) d\phi_b \quad \dots (8)$$

Where, $i(\phi_b, V)$ is the current through an elementary diode of barrier ϕ_b and bias voltage V .

Substituting $i(\phi_b, V)$ and $\rho(\phi_b)$ from Eq. (1) & (7) and performing the integration of Eq. (8) from $-\infty$ to $+\infty$, we get [13, and 24]

$$I(V) = A_d A^{**} T^2 \exp\left[\frac{-q}{kT}\left(\bar{\phi}_b - \frac{\sigma^2 q}{kT}\right)\right] \exp\left(\frac{q(V-IR_s)}{kT}\right) \times \left[1 - \exp\left(\frac{-q(V-IR_s)}{kT}\right)\right] \quad \dots (9)$$

2. Methodology

Simulation of the I-V characteristics of inhomogeneous Schottky diodes with Gaussian distribution of barrier heights has been performed using analytical approach. Analytical approach is based on calculating the total current through an inhomogeneous diode by evaluating the current $I(V, \phi_b)$ through each elementary barrier by the Newton-Raphson iteration method using equation (1), after multiplying the current through each barrier

by its probability distribution function, $p(\phi_b)$ as given by equation (7). The total current is obtained after analytically solving the integral equation (1). The $\ln(I)$ - V curves of inhomogeneous Schottky contacts are generated using equation (9) and analyzed for conduction of the current through inhomogeneous barrier heights with materials of different Richardson's constant.

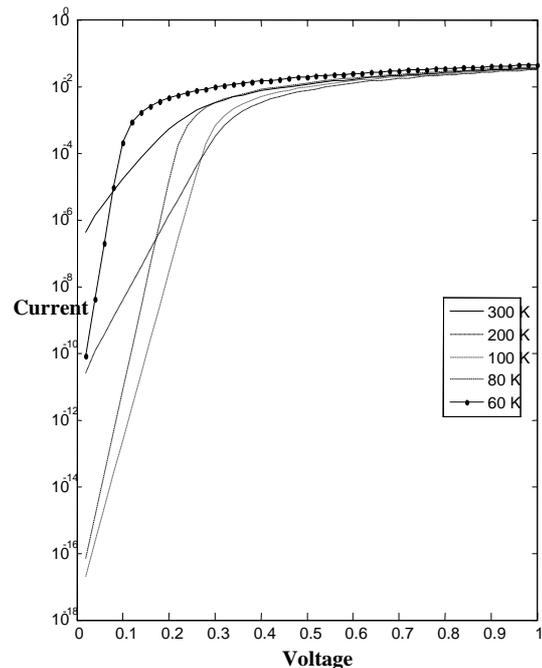


Fig. 1. $\ln(I)$ - V characteristics of Schottky diode for Si with effective Richardson's constant 1.12×10^6 for temperature range from 80K-300K

3. Results and Discussion:

The total current through the Schottky diode can be calculated by solving equation (9) using iteration method. It has been usual practice to find the total current through an inhomogeneous Schottky contact in this way. Since equation (7) represents the total current through an inhomogeneous Schottky diode, which has a Gaussian distribution of BHs, it is possible to calculate the current by numerically solving it using a computer program for iteration at any mean and standard deviation. In the present study, $\ln(I)$ - V curves of inhomogeneous Schottky diodes with Gaussian distribution of BHs are generated using numerical simulation of Eq. (9), with diode area, $A_d = 7.87 \times 10^{-7} \text{ m}^2$, corresponding to 1 mm diameter metal dot, effective Richardson constant $A^{**} = 1.12 \times 10^6 \text{ Am}^{-2} \text{ K}^{-2}$ (for n-type Silicon), $\bar{\phi} = 0.8 \text{ V}$, $\sigma = 0.08 \text{ V}$ and $R_s = 20 \Omega$. Fig. 1 represents the I-V curves of

inhomogeneous Schottky diode in temperature range of 60-300K, with analytical method. From, the graph it is clear that curves at lower temperature intersecting the curves at higher temperature [25]. Similar intersecting behavior is observed for the I-V curves generated for different materials with different effective Richardson's constant as shown in figs.(2, 3, and 4).

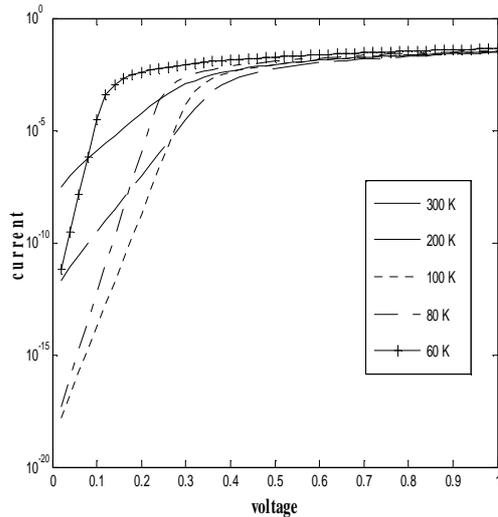


Fig. 2 In (I)-V characteristics of Schottky diode at temperature range from 80K-300K for Ge with effective Richardson's constant $8.16 \text{ A cm}^{-2} \text{ K}^{-2}$

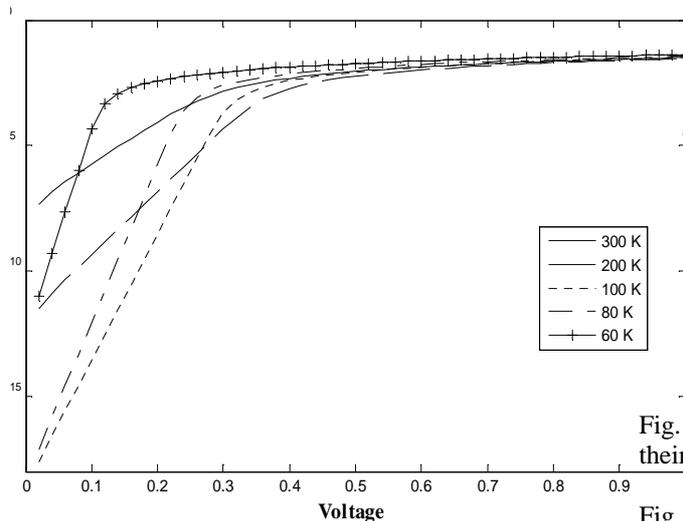


Fig. 3 In (I)-V characteristics of Schottky diode at temperature range from 80K-300K for Ag with effective Richardson's constant $12.89 \text{ A cm}^{-2} \text{ K}^{-2}$

From the I-V characteristics (figs. (1, 2, 3, and 4)) of schottky diodes for different materials by using their Richardson constant are generated, it is clear that a change in their intersecting behavior occurs at different temperatures. With the change in the

intersection point of the I-V curves the value of the barrier heights also vary with linear bias dependence. This change in value of barrier heights with voltage, affects the conduction mechanism through the metal-semiconductor contact.

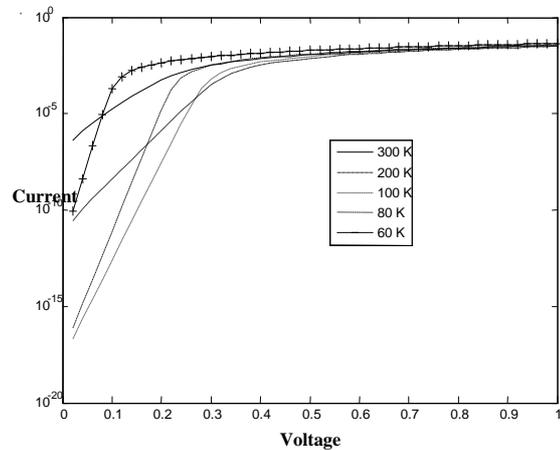


Fig. 4 In (I)-V characteristics of Schottky diode at temperature range from 80K-300K for Au with effective Richardson's constant $118.75 \text{ A cm}^{-2} \text{ K}^{-2}$

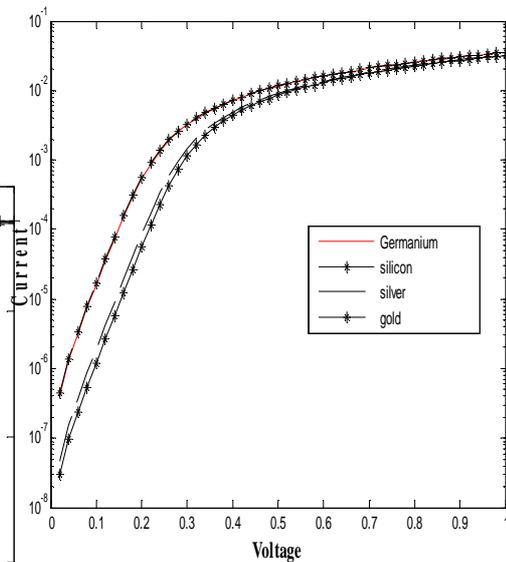


Fig. 5 In (I)-V curves for different materials with their effective Richardson's constant at 300K

Fig. 5 shows the I-V curves of semiconductor materials with different Richardson constant. From the fig. it is clear that the effect of series resistance for different material is different. We assume that resistance starts to show its effect at the mean value of barrier height. Therefore, it appears that the current at low bias due to low barrier heights while that at higher bias it is contributed by high barrier heights around the mean value. This observation that the current at low bias due to low BHs and at high bias due to high

barrier in the distribution is in accordance with the thermionic diffusion equation [26]. The saturation current of curves is different with respect to the bias dependence of voltage. It is well known that the forward current of a real Schottky diode is composed of two components. One is the current over entire contact area with a uniform barrier height and the other is the current through small patches with low barrier height. The latter has much larger series resistance than the former due to local pinch-off effect around the patch [17, 26, and 27], thus it dominates usually only at the small current region and causes the excess current, i.e. at the case of small bias and low temperature.

4. Conclusion

The current-voltage characteristics of inhomogeneous Schottky diodes were generated using analytically solved thermionic-emission diffusion equation incorporating Gaussian distribution of barrier heights and by direct numerical integration at any mean value of barrier height and standard deviation. It is shown that different effective Richardson's constant attributed to elementary barriers show different saturation current for the contact. The different saturation currents represent the number of barrier heights at low and high bias. The region covering the number of patches of barrier heights add a strong contribution to the total current density of the diode. Thus the charge carrier transport through the metal-semiconductor contact also depends on the Richardson's constant of the materials.

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