Simulation to Study the Effect of Carrier Concentration on I-V Characteristics of Schottky Diode

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Abstract

The current-voltage characteristics for Au/n-Si Schottky diode are generated by simulation. The simulation performed using Newton-Raphson iteration method yields current-voltage characteristics over wide temperature range. The data is analyzed using TDE-mechanism to study the temperature dependence of barrier height and ideality factor. Results obtained from simulation studies show the barrier height and ideality factor are independent of temperature for pure TE-mechanism. Thus the simulation of I-V characteristics is performed by incorporating ideality factor, obtained on the basis of carrier concentration from 1022-1024 atoms/m3.

The result of analysis yield barrier height is still independent of temperature but the ideality factor becomes temperature dependent and this dependence of ideality factor on temperature increases with increase in carrier concentration. Further, the temperature dependence of barrier height and ideality factor is discussed and simulation of current-voltage characteristics is performed.

Keywords: Schottky barrier diode; Carrier concentration; Electrical parameters of schottky diode

Introduction

Current transport across Metal-semiconductor (MS) contact is of great interest for device and material scientists. A number of attempts have been made so far to understand this mechanism, but a complete description of the conduction mechanism across the MS interface is still a challenging problem. For an ideal Schottky diode, the current flow is only due to thermionic emission (TE) mechanism with ideality factor equal to unity (n=1). However, due to various factors such as device temperature, dopant concentration, device area, density of interface states, structural properties of interface etc., the current-voltage characteristics of Schottky contact exhibit deviations from TE-mechanism with temperature dependent ideality factor [1-4]. Generally, the ideality factor increases with decrease in temperature, the phenomena is commonly known as “To-effect” and was first proposed by Padovani and Sumner [5], where as the barrier height for these diodes is found to decrease with fall in operating temperature.

Taking into account the effect of above mentioned anomalies of the I-V characteristics, different methods have been suggested. Padovani and Stratton proposed, in case of degenerate materials (i.e., N_d \geq 10^{12} atoms/m^3) the above anomalies can be explained on the basis of quantum mechanical tunneling [1,2]. Hackam and Harrop suggested, the ideality factor should be incorporated in saturation current expression [6]. Further, Zs. J. Horvath proposed, any mechanism which enhances electric field at the MS interface is responsible to enhance multistep tunneling at the interface [7]. According to these models, the temperature dependence of ideality factor as well as barrier height (BH) of Schottky contacts can be explained on the basis of TFE-theory.

Another approach for explaining these anomalies is based on barrier inhomogeneity models. According to these models, barrier height of the contact will be affected by the non-uniformity of the interfacial layer and form a distribution over the contact. As a result, this fluctuation of the barrier height over Schottky contact may lead to non-ideal I-V characteristics [8,9].

Simulation is an emerging trend in the field of research and development and is widely used to study the I-V characteristics of Schottky diode also. S. Chand and J. Kumar [10] and S. Chand and S. Bala [11,12] have carried out a detailed study on Schottky diode by using simulation. However, all these studies are based on barrier inhomogeneity model (Gaussian). In present paper a different approach has been adopted to explain the temperature dependence of barrier height through simulation of I-V characteristics of Schottky diode.

Method of Simulation

On the basis of Bathe’s thermionic emission theory [13], the forward I - V characteristics of an ideal Schottky barrier diode can be expressed as

\[ I = I_s \exp \left( \frac{qV}{kT} \right) \]

where

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

\[ \phi_b \] is the diode area, \( A^* \) is the Richardson constant, \( S \) is the diode area, \( \phi_b \) is the barrier height, \( T \) is the temperature and \( k \) is the Boltzman constant. The simulation of I-V characteristics using eq. (1) is performed through computer programming (GW-Basic) using Newton-Raphson iteration method. Parameters used for simulation are: diode area \( S = 7.87 \times 10^{-7} \text{m}^2 \) (corresponding to diameter 1mm), effective Richardson constant \( A^* = 1.12 \times 10^{6} \text{A m}^{-2} \text{K}^{-2} \) (for n-type silicon), barrier height \( \phi_b \) = 0.8 eV (Au/n-Si device), and \( Rs = 100 \Omega \).

Results and Discussion

At any temperature, for \( V >> 3kT/q \), eq (1) predicts, the \( \ln(I) \) vs V plot should be a straight line with unit slope and its intercept at zero-

\[ I = I_s \exp \left( \frac{qV}{kT} \right) \]

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bias give \( I_s \). Whereas \( \ln(I_s/ST^2) \) vs \( 1/T \) plot (eq. 2) should be another straight line with intercept at \( 1/T = 0 \) and slope gives the value of \( A^* \) and \( \varphi_{bo} \) respectively. The \( \ln(I) - V \) plots thus obtained at various temperatures are shown in Figure 1. These curves are linear over several orders of current, \( I-V \) data so obtained is analyzed using thermionic emission diffusion (TED) theory to obtain the BH and ideality factor.

Figure 2 shows the BH and ideality factor obtained from simulated data at various temperatures. The barrier height and ideality factor are found to be independent of temperature as expected for the case of pure thermionic emission. But in actual practice the barrier height and ideality factor is generally temperature dependent. Also, on the basis of pure TE – mechanism the simulation is possible upto 125K only. This is because the value of saturation current \( I_s \) below 125K is extremely low.

However, for diode from heavily doped semiconductor or with imperfection junction, the equation (1) is no longer valid. Podovani and Sumner [5] reported their non-ideal forward \( I-V \) characteristics to the expression.

**Figure 3:** Simulated \( I-V \) characteristics of Schottky diode with BH = 0.8 eV, \( R_s = 10 \ \Omega \) and \( N_D = 5 \times 10^{24} \ \text{m}^{-3} \) at various temperatures using eq. (3).

**Figure 4:** Plot showing the variation of ideality factor and barrier height with temperature obtained from \( I-V \) data of Figure 1.

\[
\eta = A^* \exp \left( \frac{-\varphi_{bo}}{kT} \right) \exp \left( \frac{qV}{kT + \varphi_{bo}} \right)
\]

where \( T_c \) is called excess temperature. Atalla and Soshea [14] fit their non-ideal \( I-V \) characteristics to the expression

\[
I = A^* \exp \left( \frac{-\varphi_{bo}}{kT} \right) \exp \left( \frac{qV}{kT + \varphi_{bo}} \right)
\]

where \( \eta \) is the ideality factor. Padovani and Stratton and later Rhoderick and Williams proposed, if current transport is controlled by the thermionic field emission theory, the relation between current and voltage can be expressed as [1]

\[
I = I_s \exp \left( \frac{V}{F_c} \right)
\]

where \( F_c = E_c \coth \left( \frac{qE_c}{kT} \right) = \eta kT \) and \( E_c = 18.5 \times 10^{-15} \left( \frac{N_p}{m_c} \right)^{\frac{3}{2}} \)

The analysis of (4) shows, the ideality factor is temperature dependent through carrier concentration \( (N_p) \). Thus, \( I-V \) data at different temperatures for various values of \( N_p \) is simulated by incorporating ideality factor in eq. (1).

The \( I-V \) data so obtained, at \( N_p = 5 \times 10^{24} \ \text{atoms/m}^3 \) only, is presented in Figure 3. Plot shows the \( I-V \) curves are still linear over several orders of current but these are not converging at higher bias voltage in spite of constant value of series resistance \( (R_s) \). Moreover they are shifting downward and this shift is more prominent at lower temperature. The simulation of \( I-V \) data is still possible upto 125K as there is no change in the saturation current. The ideality factor and barrier height obtained from the slope and intercept of \( \ln (I) \) vs \( V \) plot at various temperatures and for different carrier concentrations are presented in Figure 4. Analysis of plot shows, the ideality factor is temperature dependent as observed in most of the cases but the barrier height is still constant (i.e., independent of temperature).

One method to explain the temperature dependence of barrier height and ideality factor is barrier inhomogeneities [8,9], which establishes a relation between barrier height and ideality factor also.
But this method talks about TED - theory only. Hackam and Harrop [6] proposed diode equation, for non ideal I-V forward characteristics, as

\[ I = A' ST^2 \exp \left( -\frac{\varphi_0}{\eta kT} \right) \exp \left( \frac{qV}{\eta kT} \right) \]  (5)

Accordingly, the ideality factor should be included in the expression for saturation current. As the effects that cause deviation from \( \eta = 1 \) at higher bias voltage are present at zero-bias voltage also. Later, Bhuiyan [15] and more recently Rajinder [16,17], fitted their data by incorporating ideality factor into saturation current.

So, the inclusion of ideality factor in saturation current makes barrier height temperature dependent i.e.,

\[ \varphi_b = \frac{\varphi_{bo}}{\eta(T)} \]  (6)

Thus, the simulation of the I-V data of Schottky diode with different carrier concentration has been performed using eq (5) and (6). The I-V data thus obtained is further analyzed on the basis of TED - theory to study the effect of temperature as well as carrier concentration barrier height and ideality factor.

Figure 5a shows I-V curves from 50-300K at \( N_D = 5 \times 10^{24} \) atoms/m\(^3\) only and Figure 5b shows I-V curves at 300, 200 and 125K for various values of \( N_D \). A look at plot Figure 5a shows, the I-V characteristics are linear over several orders of current. These curves become more and more linear and linearity of curves shifts towards higher bias voltage with decrease in temperature. This is because of excess current at low temperature due to low barrier height. Also Figure 5b shows there is increase in current with increase in carrier concentration and variation becomes more prominent with decrease in temperature.

The I-V data so obtained, for various values of \( N_D \), is analyzed on the basis of thermionic emission theory. The barrier height and ideality factor as a function of temperature are shown in Figure 6. Plot shows the barrier height decreases and ideality factor increases with decrease in temperature in the same manner as most of the practical Schottky diodes exhibit and these changes become more prominent with increase in the donor concentration (\( N_D \)) and decrease in temperature.

The value of \( I_o \) at each temperature, obtained from Figure 5a, is used to plot ln(\( I_o/T^2 \)) vs 1/T as shown in Figure 7, the usual Richardson plot (curve-a). For an ideal diode this should be a straight line with intercept and slope yielding the value of \( A' \) and BH respectively. But

\[ R_s = 10 \text{ ohms} \]

\[ N_D = 5 \times 10^{24} \] 24 atoms/m\(^3\) at various temperatures using eq. (4) only and Figure 5b shows I-V curves at 300, 200 and 125K for various values of \( N_D \). A look at plot Figure 5a shows, the I-V characteristics are linear over several orders of current. These curves become more and more linear and linearity of curves shifts towards higher bias voltage with decrease in temperature. This is because of excess current at low temperature due to low barrier height. Also Figure 5b shows there is increase in current with increase in carrier concentration and variation becomes more prominent with decrease in temperature.

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the extracted data exhibit linearity up to 200K only with $A^* = 2.15 \times 10^3$ Am$^2$K$^{-2}$ and $BH = 0.60$ eV. Clearly the values of $A^*$ and $BH$ so obtained are very less as compared to the values used for simulation. This discrepancy is because of extra current at low temperature. Further, the data is analyzed by using modified Richardson plot i.e., $\ln(I_s/T^2)$ vs $1/T$. Such a plot is shown in Figure 7 (curve-b), exhibit linearity over entire temperature range yielding the value of $A^* = 1.13 \times 10^3$ Am$^2$K$^{-2}$ and $BH = 0.8$ eV and these values are in good agreement with those used for simulation.

**Conclusion**

The $I-V$ characteristics of Schottky diodes are simulated over wide temperature range. The $I-V$ data for Au/n-Si Schottky diode is generated with and without ideality factor as well as by incorporating ideality factor in saturation current equation. The data so obtained fitted into the pure TED-equation to see the temperature dependence of ideality factor and barrier height. For $I-V$ characteristics with $\eta=1$, the barrier height and ideality factor are independent of temperature. Whereas incorporation of ideality factor in saturation current makes barrier height temperature dependent. It is also observed that the temperature dependence of barrier height becomes stronger with increase in carrier concentration. Finally it is concluded that the temperature dependence of barrier height is due to the factors which are responsible for the deviation of $I-V$ characteristics of Schottky diodes at higher bias voltage.

**References**