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Inhomogeneous barrier height effect on the current–voltage characteristics of an Au/n-InP Schottky diode

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Abstract: We report the current–voltage (I–V) characteristics of the Schottky diode (Au/n-InP) as a function of temperature. The SILVACO-TCAD numerical simulator is used to calculate the I–V characteristic in the temperature range of 280–400 K. This is to study the effect of temperature on the I–V curves and assess the main parameters that characterize the Schottky diode such as the ideality factor, the height of the barrier and the series resistance. The I–V characteristics are analyzed on the basis of standard thermionic emission (TE) theory and the inhomogeneous barrier heights (BHs) assuming a Gaussian distribution. It is shown that the ideality factor decreases while the barrier height increases with increasing temperature, on the basis of TE theory. Furthermore, the homogeneous BH value of approximately 0.524 eV for the device has been obtained from the linear relationship between the temperature-dependent experimentally effective BHs and ideality factors. The modified Richardson plot, according to the inhomogeneity of the BHs, has a good linearity over the temperature range. The evaluated Richardson constant A^* was 10.32 A·cm^{-2}·K^{-2}, which is close to the theoretical value of 9.4 A·cm^{-2}·K^{-2} for n-InP. The temperature dependence of the I–V characteristics of the Au/n-InP Schottky diode have been successfully explained on the basis of the thermionic emission (TE) mechanism with a Gaussian distribution of the Schottky barrier heights (SBHs). Simulated I–V characteristics are in good agreement with the measurements [Korucu D, Mammadov T S. J Optoelectronics Advanced Materials, 2012, 14: 41]. The barrier height obtained using Gaussian Schottky barrier distribution is 0.52 eV, which is about half the band gap of InP.

Key words: simulation; SDB; Silvaco; InP; temperature; I–V–T
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1. Introduction

In recent years, indium phosphide (InP) has received a great deal of attention for the fabrication of optoelectronic and microwave devices as well as integrated circuits used in modern high-speed optical communication systems[1−5]. Schottky barrier contacts on n-InP have potential applications in solar cells, microwave field effect transistors (FETs), and high-speed charge-coupled devices. The choice of InP stems from the fact that it has an optimum band gap required for photovoltaic energy conversion and a large charge carrier mobility required for high-speed devices[6−10].

The current–voltage (I–V) characteristics of Schottky diodes obtained at room temperature do not give detailed information about the charge transport process and the nature of the barrier formed at the metal–semiconductor interface. The temperature dependent electrical characteristics, however, can provide information regarding the charge transport process through metal–semiconductor contacts and therefore give a better picture of the conduction mechanisms[11−14].

In this paper, we discuss the temperature dependence of the barrier height and the ideality factor on the basis of TE theory in which the barrier height has a Gaussian distribution around a mean value due to barrier height inhomogeneities at the metal–semiconductor interface. The I–V characteristics of Au Schottky contacts on an n-InP substrate are calculated over the temperature range of 280–400 K. The main purpose of this paper is to explain the inhomogeneity observed in the experimental I–V characteristics of Reference [15] (for example) using a numerical simulation.

2. Sample structure

The simulated device structure is presented in Figure 1. It includes a 0.7 μm epitaxial n-drift layer and a 300 μm epitaxial n$^+$ layer. The two layers are uniformly doped by 1×10^{16} cm^{-3} and 1×10^{18} cm^{-3} respectively. This structure is chosen to be the same as that of Reference [15] so that a comparison can be made.

3. Numerical simulation

In order to elucidate certain phenomena observed in semiconductor devices, extensive characterization has to be carried out. Furthermore, analytical modeling may be required. Experimental characterization can be very costly while analytical modeling may be just mathematical with no physical meaning. Numerical simulation can be very helpful in minimizing experimental and analytical modeling efforts. Many parameters can be varied to elucidate the observed phenomenon. In the present study the variable parameter is the temperature while the studied phenomenon is the effect of the inhomogeneous barrier height on the current-voltage characteristics. In this respect, the ATLAS module of the SILVACO software[16] is used

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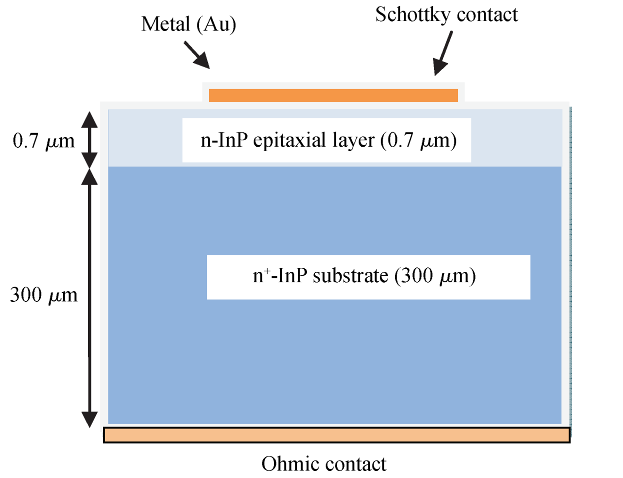

Figure 1. A two dimensional schematic cross section of the simulated Au/n-InP Schottky diode.

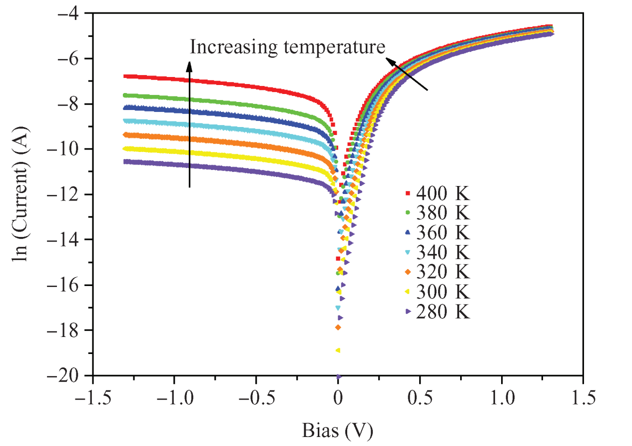

Figure 2. The simulated I–V characteristics of an Au/n-InP Schottky diode in the temperature range of 200–400 K.

to calculate current-voltage characteristics of the Au/n-InP at different temperatures. It is a physically-based two and three dimensional device simulator. It predicts the electrical behavior of a specified semiconductor structure and provides an insight into the internal physical mechanisms associated with device operation. The simulator is based on a mathematical model, which consists of a set of fundamental equations linking together the electrostatic potential and the carrier densities, within some simulation domain. The simplest model of charge transport that is useful is the drift–diffusion model[17], which is adequate for nearly all practical devices.

Poisson's equation, which relates the electrostatic potential to the space charge density, is given by:

$$\varepsilon\frac{d^2\psi}{dx^2} = -\rho(x), \tag{1}$$

where ψ is the electrostatic potential, ε is the local permittivity, and ρ is the local space charge density.

The continuity equations in steady state for electrons and holes are expressed, respectively by:

$$0 = \frac{1}{q}\frac{\mathrm{d}/n}{\mathrm{d}x} + G_\mathrm{n} - R_\mathrm{n}, \tag{2}$$

$$0 = \frac{1}{q}\frac{\mathrm{d}/p}{\mathrm{d}x} + G_\mathrm{p} - R_\mathrm{p}, \tag{3}$$

where n and p are the electron and hole concentration, J_n and J_p are the electron and hole current densities, G_n and G_p are the generation rates for electrons and holes, R_n and R_p are the recombination rates for electrons and holes, and q is the electron charge.

In the drift–diffusion model, the current densities are expressed in terms of the quasi-Fermi levels ϕ_n and ϕ_p as:

$$J_\mathrm{n} = -q\mu_\mathrm{n} n\frac{\mathrm{d}\phi_\mathrm{n}}{\mathrm{d}x}, \tag{4}$$

$$J_\mathrm{p} = -q\mu_\mathrm{p} p\frac{\mathrm{d}\phi_\mathrm{p}}{\mathrm{d}x}, \tag{5}$$

where μ_n and μ_p are the electron and hole mobilities, respectively. The quasi-Fermi levels are linked to the carrier concentrations and the potential through the two Boltzmann approximations:

$$n = n_\mathrm{i}\exp\left(\frac{\psi - \phi_\mathrm{n}}{k_\mathrm{B}T}\right), \tag{6}$$

$$p = n_\mathrm{i}\exp\left(-\frac{\psi - \phi_\mathrm{p}}{k_\mathrm{B}T}\right), \tag{7}$$

where n_i is the effective intrinsic concentration and T is the lattice temperature.

The electrical characteristics are calculated following the specified physical structure and bias conditions. This is achieved by approximating the operation of the device into a one-dimensional grid, consisting of a number of grid points called nodes. By applying the set of differential equations (Poisson's and continuity equations) onto this grid (or the equation's discretization), the transport of carriers through the structure can be simulated. The finite element grid is used to represent the simulation domain.

4. Results and discussion

First of all the simulated I–V characteristics of the Au/n-InP Schottky diode using Atlas-Silvaco, at different temperatures (IVT), are shown in Figure 2. They are in good agreement with the measured results in Reference [15] since the same structure is used.

In the forward bias, the $\ln I$ increases rapidly with increasing bias in the low bias region ($0.1 \leqslant V \leqslant 0.3$) but slows down considerably for higher voltages. The first part indicates that the I–V characteristics have the usual form while the second part indicates a series resistance effect, the interfacial insulator layer, and the interface states when the applied voltage is sufficiently large ($V \geqslant 0.3$). Also, the dark reverse current increases with increasing reverse bias and no saturation is observed. This may be due to defects which are simulated by setting the appropriate recombination rates in Equations (2) and (3).

The forward I–V characteristics for Schottky diodes are usually due to the thermionic emission theory[17], given by the expression:

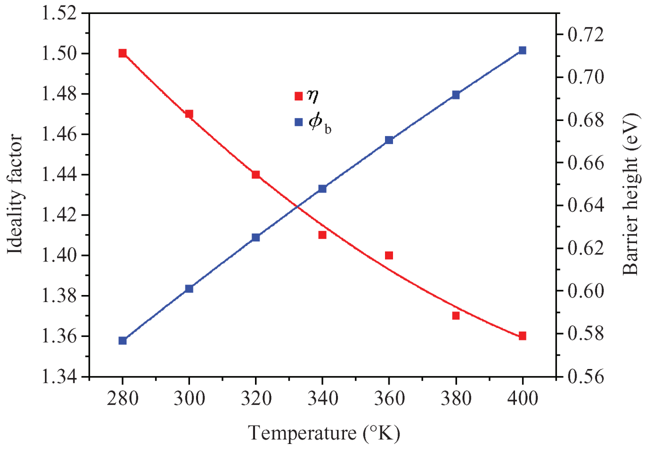

Figure 3. The extracted ideality factor n and the barrier height ϕ_B from the I–V characteristics of the Au/n-InP Schottky diode (Figure 2) in the temperature range 280–400 K.

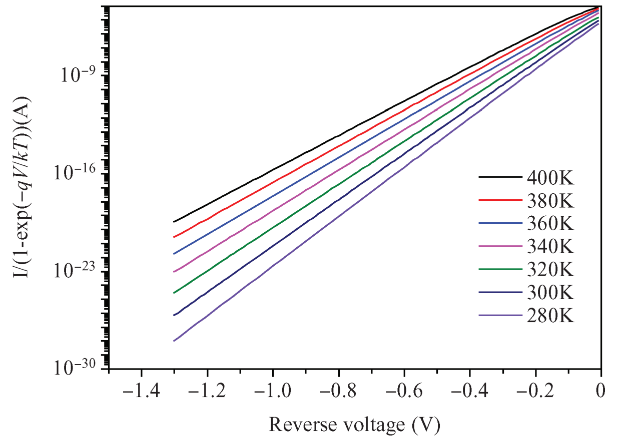

Figure 4. Semi-logarithmic *I/(1-exp(-qV/kT))* versus V plot from the reverse bias I–V data in Figure 2 for Au/n-InP SD in the temperature range of 280–400 °K.

$$I = I_0\left[\exp^{\frac{q(V-R_S I)}{nkT}} - 1\right], \tag{8}$$

where R_S is the series resistance of the diode, V is the applied voltage, q is the electronic charge, k is the Boltzmann constant, T is the absolute temperature, n is the ideality factor and I_0 is the saturation current given by:

$$I_0 = AA^* T^2 e^{(-q\phi_B/kT)}, \tag{9}$$

where A^* is the Richardson constant, A is the area of the diode, and ϕ_B is the barrier height. $A^* = 9.24$ A·cm^{-2}·K^{-2} for n-type InP[17].

For $V - R_S I \ll 3kT/q$, Equation (9) becomes:

$$I = I_0 \exp^{\frac{q(V-R_S I)}{nkT}}. \tag{10}$$

The knowledge of R_S, ϕ_B, n, and I_0 will clarify the conduction mechanism in the Schottky diode. For this purpose the Chung and Cung procedure is used to extract these parameters from the I–V characteristics[18].

The saturation current I_0 is determined from the intercept of the ln$I$ versus V plot with the V-axis (at $V = 0$ V). Once I_0 is determined, the barrier height ϕ_B can be evaluated using Equation (9), thus $\phi_B = (kT/q)\ln(AA^*T^2/I_0)$. The ideality factor n is determined from the slope of the linear forward region of the ln$I$ versus V plot, hence $n = (q/kT)\mathrm{d}V/\mathrm{d}(\ln I)$. The variation of the extracted parameters n and ϕ_B in the temperature range 280–400 K from the I–V characteristics of Figure 2 are shown in Figure 3.

The ideality factor increases while the barrier height ϕ_B decreases with decreasing temperature.

The barrier height can also be evaluated from the reverse I–V characteristics. A plot of semi-logarithmic $I/(1\text{–}\exp(-qV/kT))$ versus V yields the saturation current I_0 as the intercept at $V = 0$ (Figure 4). Once I_0 is determined, the barrier height ϕ_B can be evaluated using Equation (9), thus $\phi_B = (kT/q)\ln(AA^*T^2/I_0)$.

The BH versus temperature plot from the reverse bias I–V characteristics is given in Figure 5 indicated by open triangles. The value of the SBH in the reverse bias characteristics ranges from 0.48 eV at 280 °K to 0.61 eV at 400 °K.

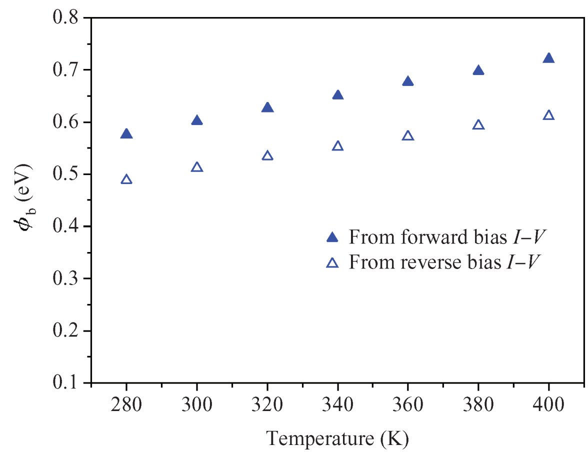

Figure 5. Barrier height versus temperature plot for the Au/n-InP SD in the temperature range of 280–400 K.

It has been seen from the forward and reverse bias SBH values in the temperature range of 280–400 K that there is a "systematic" BH difference of 0.09 eV between forward and reverse bias BHs. This is acceptable since it is very comparable to those of References [19, 20].

The Arrhenius plot of $\ln(I_0/T^2)$ versus $10^3/T$ gives the Richardson constant and the barrier height since Equation (9) can be rewritten as $\ln(I_0/T^2) = \ln(AA^*) - (q/kT)\phi_B$. The Arrhenius plot is shown in Figure 6.

The value of A^* obtained from the intercept of the linear portion of the ordinate is 1.78×10^{-5} A·cm^{-2}·K^2, which is much lower than the theoretically calculated value, which is ≈ 9.4 A·cm^{-2}·K^2 for n-type InP. A barrier height value of 0.259 eV is obtained from the slope of the straight line.

In the above extraction of the Schottky parameters, a homogeneous barrier was assumed which led to unacceptable values. This indicates that the homogenous barrier height model suffers from several inconsistencies such that:

(1) An increase in the barrier height BH ϕ_B and a decrease in the ideality factor n with an increase in the temperature.

(2) The Richardson constant obtained deviates largely from the theoretical value.

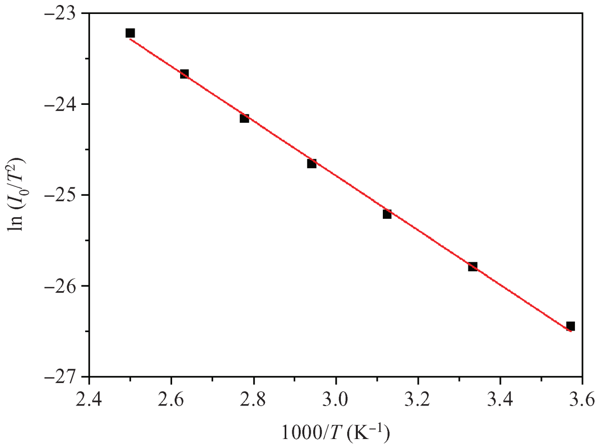

Figure 6. The Richardson plot of $\ln(I_0/T^2)$ versus $10^3/T$.

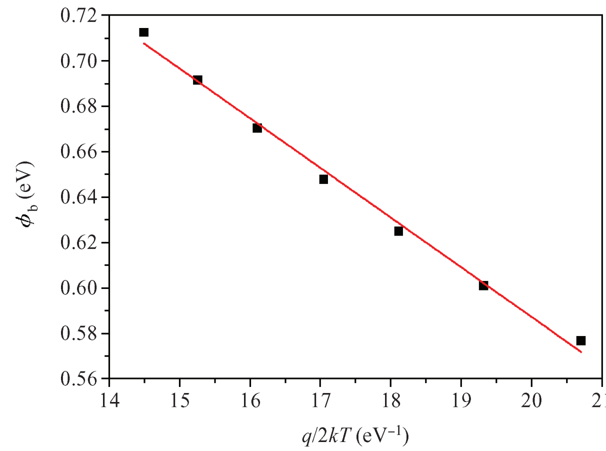

Figure 7. The apparent barrier height versus $q/2kT$ curves of the Au/n-InP Schottky barrier diode according to a Gaussian distribution of BHs.

In order to describe the abnormal behaviors mentioned above, an analytical potential fluctuation model using different types of distribution function at the interface on the spatially inhomogeneous SBDs has been proposed by different workers[22, 23]. A spatial distribution of the barrier height at the metal–semiconductor interface of Schottky contacts by a Gaussian distribution ρ (ϕ_B) with a standard deviation (σ_0) around a mean SBH (ϕ_{B0}) value has been suggested by Werner and Guttler[22], thus:

$$\rho(\phi_B) = \frac{1}{\sigma_0\sqrt{2\pi}} e^{-\frac{(\phi_B - \bar{\phi}_{B0})^2}{2\sigma_0^2}}. \tag{11}$$

The pre-exponential term is the normalization constant. Then, the total current across the Schottky barrier diode at a forward bias is given by:

$$I = \int i(V, \phi_B)\rho(\phi_B)\mathrm{d}\phi_B, \tag{12}$$

where $i(V, \phi_B)$ is the current at a bias V for a barrier of ϕ_B based on the thermionic emission model. It is assumed that the mean BH ϕ_B and σ are linearly bias dependent on Gaussian parameters, such as $\phi_B = \phi_{B0} + \rho_2 V$ and standard deviation $\sigma = 0 + \rho_3 V$, where ρ_2 and ρ_3 are voltage coefficients which may depend on T. The temperature dependence of σ is usually small and may be neglected[21, 22]. Substituting Equations (5) and (9) into Equation (10), and performing the integration it becomes[21, 22]

$$I = I_0 I = I_0 \left(e^{\frac{q(V - B_S I)}{n_{ap} kT}} - 1\right). \tag{13}$$

I_0 is then given by:

$$I_0 = AA^* T^2 e^{-\frac{q\phi_{Bap}}{kT}}, \tag{14}$$

where ϕ_{Bap} and n_{ap} are the apparent BH and apparent ideality factor, respectively, and are given by

$$\phi_{Bap} = \phi_{B0} - \frac{q\sigma_0^2}{2kT}, \tag{15}$$

$$\frac{1}{n_{ap}} - 1 = -\rho_2 + \frac{q\rho_3}{2kT}\frac{q\sigma_0^2}{2kT}. \tag{16}$$

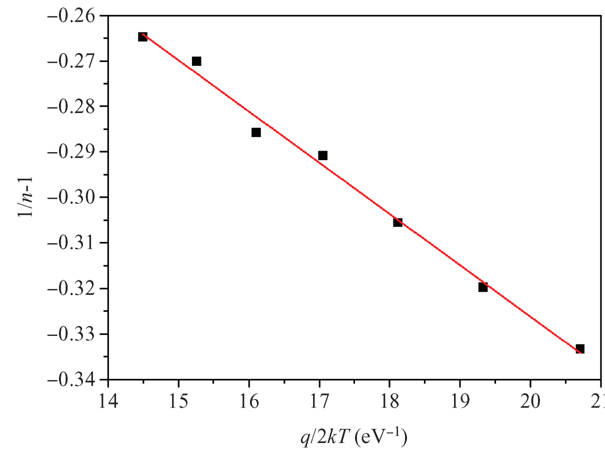

Figure 8. The $1/n-1$ versus $q/2kT$ curve of the Au/n-InP Schottky barrier diode according to a Gaussian distribution of BHs.

The graphical representation of the barrier and the ideality factor as a function of $q/2kT$ helps to characterize the behavior of the inhomogeneous potential barrier. Figure 7 represents the variation of the potential barrier as a function of $q/2kT$. This plot is a straight line that is in good agreement with the theoretical equation of the inhomogeneous model proposed by Werner and Guttler[22].

The plot of ϕ_B versus $q/2kT$ is a straight line with the intercept on the ordinate determines the zero mean barrier height ϕ_{B0} ($T = 0$ K) and the slope gives the zero bias standard deviation σ_0. The values obtained are 1.02 eV and 0.14 V for ϕ_{B0} and σ_0 respectively.

The plot of $1/n - 1$ as a function of $q/2kT$ is shown in Figure 8. The plot is a straight line, which is in accordance with that proposed by Werner and Guttler[22].

The analysis of this plot gives the values of the following voltage coefficients: $\rho_2 = 0.1$ V and $\rho_3 = -0011$ V. These values have the same order as those[15, 24, 25] of a similar structure.

The conventional Richardson plot deviates from linearity at low temperatures due to the barrier inhomogeneity; it can be modified by combining Equations (14) and (15) as follows:

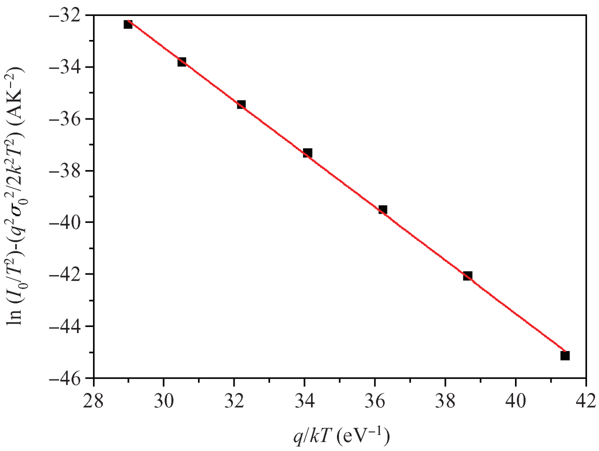

Figure 9. The modified Richardson $\ln(I_0/T^2)-(q^2\sigma_0^2/2k^2T^2)$ versus q/kT plot for the Au/n-InP Schottky barrier diode according to a Gaussian distribution of BHs.

$$\ln\frac{I_0}{T^2}-\frac{q^2\sigma_0^2}{2k^2T^2}=\ln AA^*-\frac{q\phi_{B0}}{kT}. \tag{17}$$

The plot of modified $\ln(I_0/T^2)-(q^2\sigma_0^2/2k^2T^2)$ versus q/kT plot according to Equation (17) should give a straight line with the slope and intercept at the ordinate directly yielding the mean barrier height ϕ_{B0} and A^* respectively. The modified Richardson plot is shown in Figure 9.

Using the least square curve fitting of the data, the values of ϕ_{B0} and A^* obtained are 1.02 eV and 10.32 A cm^{-2} K^{-2} respectively. As can be seen, the value of $\phi_{B0}=1.02$ eV is in close agreement with the value of $\phi_{B0}=1.02$ eV obtained from the plot of ϕ_B versus $q/2kT$ (Figure 7). Also the modified Richardson constant $A^*=10.32$ A cm^{-2} K^{-2} is in close agreement with the theoretical value (9.4 A cm^{-2} K^{-2}).

5. Conclusion

In this work we have used a numerical simulation to simulate the I–V of an Au/n-InP Schottky diode (SD), to investigate the influence of temperature on the evolution of these curves and assess the main parameters that characterize the Schottky diode such as the ideality factor and the height of the barrier. Analysis of the I–V characteristics of the Schottky structure based on the TE mechanism presents some deficiencies such that the decrease in the barrier height (Φ_B) and increase of ideality factor (n) with increasing temperature. The origin and nature of this behavior have been successfully explained on the basis of the thermionic emission with a Gaussian distribution of the barrier heights. It is seen that the value of σ_0 (0.14 V) is not small compared to the mean value of ϕ_{B0} which is 1.02 eV, indicating large inhomogeneities at the interface and thus potential fluctuations. The effective Richardson constant was found to be 10.32 A·cm^{-2}·K^{-2} from the modified Richardson plot, which is much closer to the theoretical value of 9.4 A·cm^{-2}·K^{-2}. These values are in good agreement with the values given in the literature, which also provides a good understanding of the physical behavior of the metal–semiconductor structure. In summary the importance of our simulation work is a successful comparison with measurements of Reference [15]. We have also discussed the inhomogeneity interface barrier. In our analysis the ideality factor, the barrier height and the Richardson coefficient were successfully compared with the literature.

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