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Barrier height determination in homogeneous nonideal Schottky contacts

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Abstract

A novel method is proposed to determine effective barrier heights in homogeneous nonideal Schottky contact from I–V measurements. This method takes into account the different mechanisms of current flow through the metal–semiconductor interface. The total current has been expressed as the sum of two independent terms which are: (1) the thermionic current where the ideality factor value is equal to one and (2) the contribution of different transport mechanisms. The second term responds to a general expression of the thermionic emission theory where the barrier height and the ideality factor are voltage dependent. The effective barrier height is found by means of subtraction of the transport mechanism terms from the total current. The method was applied to a group of I–V experimental curves which were reported by M Barus and D Donoval 1993 *Solid State Electron.* **36** 969.

1. Introduction

The study of the Schottky contact formation is vital for semiconductor devices. Thus, the understanding and control of the electrical properties of the interface can greatly improve the performance of the electronic circuits.

The band bending of the depletion layer of a Schottky contact is characterized by its barrier height. Generally, the barrier height is evaluated by current–voltage and capacitance–voltage measurements, as well as by internal photoemission and ballistic electron emission microscopy (BEEM). The current–voltage measurements are also used in order to determine the transport mechanisms on the metal–semiconductor interface [1, 2].

Current transport in Schottky contacts is due to majority carriers and it may be described by thermionic emission over the interface barrier [3]. The thermionic current may be written as:

$$I_{\text{ideal}} = I_0\left[\exp\left(\frac{qV}{kT}\right) - 1\right] \tag{1}$$

where

$$I_0 = AA^{**}T^2\exp\left(-\frac{q\phi_{B0}}{kT}\right) \tag{2}$$

is the thermionic current saturation, A is the diode area, A^{**} is the modified Richardson constant, T is the temperature, ϕ_{B0} is the Schottky barrier height and the other constants have their usual meaning.

However, in real Schottky contacts, an ideal behaviour deviation is frequently observed and the I–V curves cannot be fit by equation (1). The Schottky effect, series resistance, leakage resistance, the presence of other transport mechanisms [2] and inhomogeneous Schottky barrier heights [4–7] have been established by several authors as the most important causes of nonideal behaviour.

1.1. Schottky effect

The Schottky effect reduces the barrier height by an amount $\Delta\phi$ which depends on the applied voltage [2]. In consequence, the barrier height, ϕ_{B0}, in equation (1) can be replaced by the effective Schottky barrier height ϕ_{B} which is given by

$$\phi_{\text{B}} = \phi_{\text{B0}} - \Delta\phi - \beta V \tag{3}$$

where ϕ_{B0} is the zero voltage barrier height and β is positive, and

$$\frac{1}{n} = 1 - \beta \equiv 1 - \frac{\partial\phi_{\text{B}}}{\partial V}. \tag{4}$$

The coefficient n is a semi-empiric parameter which is called the ideality factor. Typically, n = 1–1.01 for homogeneous Schottky contacts. However, it is larger for real contacts.

For the particular case where there is no bias dependence of ϕ_B, $\Delta\phi$ is given as

$$\Delta\phi(V) = \left[\frac{q^3 N_d}{8\pi^2\epsilon_{SC}^2}\left(\phi_B - V - \xi - \frac{kT}{q}\right)\right]^{\frac{1}{4}} \tag{5}$$

where ξ is the energy difference between the Fermi level and the bottom of the conduction band or the top of the valence band.

1.2. Series resistance

Regarding the Schottky effects and the series resistance R_s, equation (1) is modified and can be rewritten as

$$I_1 = I_{01}\exp\left(\frac{qV_d}{nkT}\right)\left[1 - \exp\left(\frac{-qV_d}{kT}\right)\right] \tag{6}$$

where V_d is the diode voltage

$$V_d = V - I_1 R_s \tag{7}$$

and

$$I_{01} = AA^{**}T^2\exp\left[-\frac{q(\phi_{B0} - \Delta\phi)}{kT}\right]. \tag{8}$$

The effect of R_s is important when $V_d \ll I_1 R_s$. In this case, Norde [8], Lien *et al* [9] and Werner [10] have developed methods where plots of auxiliary functions are often used. These methods made it possible to evaluate the barrier height, the ideality factor and the series resistance.

1.3. Leak resistance

When the leakage current—which is characterized by leak resistance, R_L, and the voltage drop on the series resistance—is introduced into equation (6), the total current can be written as

$$I_L = I_1 + \frac{V_d}{R_L}. \tag{9}$$

In numerous cases, equation (9) reliably describes the behaviour of the Schottky diode.

1.4. Transport mechanism

The total current expressed by equation (9) can be replaced by other transport mechanisms such as tunnel, recombination-generation and injection minority carriers.

1.4.1. The quantum mechanical tunnelling through the barrier [11] is present at moderate values of voltage and the current has the form

$$I_2 = I_{02}\exp\left(\frac{qV_d}{E_0}\right)\left[1 - \exp\left(\frac{-qV_d}{kT}\right)\right] \tag{10}$$

where

$$E_0 = E_{00}\cot\left(\frac{qE_{00}}{kT}\right) \tag{11}$$

and

$$E_{00} = \frac{1}{2}\hbar\sqrt[2]{\frac{N_d}{m^*\varepsilon_{SC}}}. \tag{12}$$

I_{02} is a complicated function of temperature, barrier height and semiconductor parameters.

For low temperatures, where $kT/E_{00} \ll 1$, field-emission tunnelling is expected. At high temperatures $kT/E_{00} \gg 1$ and thermionic field emission occurs when $kT/E_{00} \approx 1$.

1.4.2. The recombination in the space-charge region [12] appears at low voltages. Generally it is accompanied by thermionic current. The expression used to evaluate the current can be written as

$$I_3 = I_{03}\exp\left(\frac{qV_d}{2kT}\right)\left[1 - \exp\left(\frac{-qV_d}{kT}\right)\right] \tag{13}$$

where

$$I_{03} = \frac{qn_i wA}{2\tau_R}. \tag{14}$$

n_i is the intrinsic carrier concentration, w is the width of the space-charge zone and τ_R is the recombination lifetime.

1.4.3. The injection of minority carriers into the semiconductor [13] is another possible transport mechanism and it affects the current at high forward voltage.

1.5. Inhomogeneous Schottky barrier

The effective Schottky barrier height disappears when the inhomogeneous Schottky barrier is present, and it is replaced by a barrier height distribution.

The barrier height distribution has been found in two ways. One of these has been developed by Tung *et al* [14–18]. They have established that a locally varying Schottky barrier height may be expressed as a linear combination of a potential for a uniform Schottky barrier height and a potential due to a dipole layer with a moment per area, placed at the metal–semiconductor interface [15]. The other way has assumed that several parallel diodes of different barrier heights exist, each one contributing to the current independently. For this case, the barrier height distribution is represented by a Gaussian function where the mean and the standard deviation are assumed to vary linearly with bias [19, 20].

Consequently, the barrier height determination from I–V measurements is considered an arduous problem. Previous papers have proposed methods where the barrier height is calculated from I–V measurements in homogeneous contacts [2, 8–10, 21, 22]. A widely-accepted method is to fit the I–V experimental curves with equations (6) and (8) where the three fitting parameters are R_s, n and ϕ_B [2]. Another method reported by Barus and Donoval [21] is based on the effect that the presence of different transport mechanisms produces on I–V characteristics. The theoretical expression of each mechanism is introduced into a computer in order to fit the experimental forward I–V where R_s, n, τ_R and ϕ_B are the fitting parameters.

The main advantages and limitations of the above-mentioned methods are analysed in many reports [2, 10, 23, 24]. Although the fitting procedure attains more accurate results than other methods in the presence of experimental noise [23], the numerical coincidence between the measured and the fitting data is not sufficient to prove the validity of the diode model

[10]. The common approach of these methods is that all Schottky parameters are assumed to be voltage independent.

Other methods have considered the analysis of Schottky contacts with a voltage-dependent ideality factor $n(V)$. One of the most widely applied procedures uses the partial differentiation of equation (6) [2]. However, a total differentiation is required [22]. In this condition, the voltage dependence of n is

$$f(n) = \frac{kT}{q}\frac{\mathrm{d}}{\mathrm{d}V}(\ln I) \equiv \frac{1}{n} - \frac{V}{n^2}\frac{\mathrm{d}n}{\mathrm{d}V}. \qquad (15)$$

Consequently, the exact value of the ideality factor should be obtained by integration of the differential equation (15) but this procedure is complicated due to the unknown boundary condition [25]. Another method where the function $n(V)$ is calculated at each point of the I–V measurement has been reported by Ishida and Ikoma [26]. Generally, this method requires the determination of the saturation current.

In this paper, a new method to determine the effective barrier height takes into account that the barrier height and ideality factor are voltage dependent. This method is based on the effect of the transport mechanisms on the I–V curve of homogeneous Schottky contacts with low leakage current. The proposed method quantifies the influence of the ideal thermionic emission current and these effects are subtracted posteriorly.

2. Method

The method considers that any I–V curve of an homogeneous nonideal Schottky contact with low leakage current can be represented as

$$I_{\text{total}} = I_{\text{ideal}} + \sum_{i=1}^{n} I_i + \frac{V_\mathrm{d}}{R_\mathrm{L}} \qquad (16)$$

where I_{ideal} is the known thermionic current of a Schottky contact with $n = 1$ and barrier height, ϕ_{B0}. $\sum_{i=1}^{n} I_i$ contains all the transport mechanisms that cause the deviation of the ideal behaviour.

Regarding the voltage dependence of the ideality factor and the barrier height, the current I_i can be written as

$$I_i = I_{0_i}\exp\left(\frac{qV_\mathrm{d}}{n(V,T)_{0_i}kT}\right)\left[1-\exp\left(\frac{-qV_\mathrm{d}}{kT}\right)\right] \qquad (17)$$

where

$$I_{0_i} = AA^{**}T^2\exp\left(-\frac{q\phi_0(V,T)_i}{kT}\right). \qquad (18)$$

The general expressions of 'apparent barrier height' and 'apparent ideality factor' are as follows:

$$\phi(V,T)_i = \phi_0(V,T)_i + \beta_0(V,T)_i V \qquad (19)$$

and

$$\beta_0(V,T)_i = 1 - \frac{1}{n_0(V,T)_i}. \qquad (20)$$

To apply the method it was necessary to define a $Z(V,T)_i$ function from equations (17) and (18) as

$$Z(V,T)_i = \frac{kT}{q}\ln\frac{I_i}{AA^*T^2\left[1-\exp\left(-(qV_\mathrm{d}/kT)\right)\right]} \qquad (21)$$

Table 1. The n_0 and $\phi_0 + \Delta\phi(0)$ values for different transport mechanisms.

Parameters	Thermionic	Tunnel	Recombination
n_0	1	$1.03 < n_0 < 2$	2
$\phi_0+\Delta\phi(0)$	ϕ_{B0}	$I_0 = I_{02}$	$I_0 = I_{03}$

and

$$Z(V,T)_i = \phi_0(V,T)_i + \frac{V_\mathrm{d}}{n_0(V,T)_i}. \qquad (22)$$

If $Z(V,T)_i$ varies linearly with diode voltage in the ith voltage interval, then $n_0(V,T)_i$ and $\phi_0(V,T)_i$ are constants and they can be found from the slope and the intercept, respectively. Thus, a group of $n_0(V,T)_i$, $\phi_0(V,T)_i$ pairs are obtained for each ith voltage interval where $Z(V,T)_i$ varies linearly with diode voltage.

If all the effects of the transport mechanisms, corresponding to the summatory term, are subtracted from the I–V experimental curves then $\phi_0(V,T)_i$ is the zero barrier height, ϕ_{B0}, and $n_0(V,T)_i$ is close to one.

The method made it possible to identify the dominant transport mechanism in the ith voltage interval by means of $n_0(V,T)_i$ and $\phi_0(V,T)_i$ when these take the values shown in table 1.

3. Discussion

The model was applied to seven I–V experimental curves in the temperature range from 90–350 K reported by Barus and Donoval [21]. These are shown in figure 1. Using equations (1) and (2) and assuming that the thermionic emission is the dominant mechanism of current flow, the barrier height and the ideality factor were determined and these are shown in figures 2 and 3, respectively. The large variation of height barrier and the increase of ideality factor with decreasing temperature are also depicted in figures 2 and 3, respectively. These behaviours cannot be explained satisfactorily on the basis of thermionic emission theory. These results were expected to be due to other transport mechanisms which had been assumed previously.

The Z–V curves are obtained from I–V curves using equation (21). The ith voltage intervals of some curves where the $Z(V,T)_i$ function varies linearly with diode voltage are shown in table 2. The $n_0(V,T)_i$ values are close to one and adding the Schottky effect, $\Delta\phi$, to $\phi_0(V,T)_i$ a barrier height is obtained which is coincident with zero barrier height, ϕ_{B0}, for the temperature range 209–350 K, according to the ideal thermionic emission approach. However, a deterioration of the ideal thermionic emission occurs with the decrease of the temperature. Thus, two voltage intervals are observed in the I–V curves below 209 K. For one, the apparent ideality factor corresponding to the low voltage region is close to two. This means that the current recombination is a dominant transport mechanism for this region. For the other voltage intervals, the apparent ideality factor is slightly larger than one because other mechanisms influence in the moderate voltage region.

A current is obtained using equations (17) and (18) for each new pair of $n_0(V,T)_i$ and $\phi_0(V,T)_i$. By subtracting this current from the total current, we found a new $Z(V,T)_i$ function. Subsequently, new $n_0(V,T)_i$ and $\phi_0(V,T)_i$ are evaluated from the new $Z(V,T)_i$ function. The close

Table 2. The n_0 and ϕ_0 values for voltage intervals of some I–V curves where $Z(V, T)_i$ varies linearly with voltage diode.

Temperature (K)	Voltage interval (V)	$\phi_0 + \Delta\phi(0)$	n_0	Voltage interval (V)	ϕ_0	n_0
350	$V \geqslant 0.02$	0.696	1.020			
305	$V \geqslant 0.02$	0.696	1.021			
270	$V \geqslant 0.02$	0.695	1.033			
209	$V \leqslant 0.13$	0.696	1.000			
140.8	$0.372 \leqslant V \leqslant 0.502$	0.620	1.191	$V \leqslant 0.36$	0.542	1.625
112	$0.382 \leqslant V \leqslant 0.536$	0.575	1.298	$V \leqslant 0.371$	0.521	1.473
90.9	$0.466 \leqslant V \leqslant 0.564$	0.545	1.358	$V \leqslant 0.458$	0.467	1.653

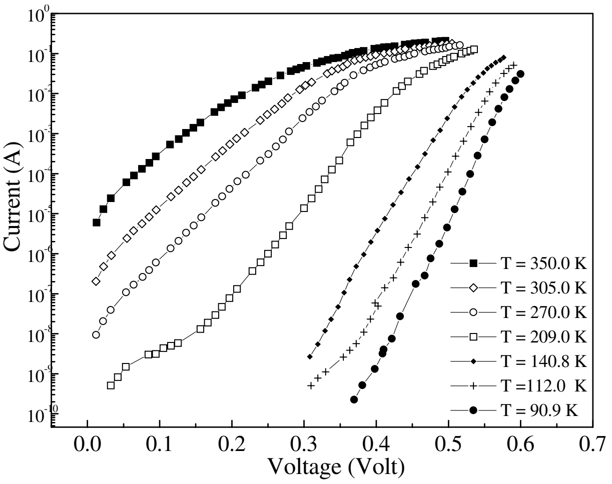

Figure 1. I–V curves reported by Barus and Donoval [21].

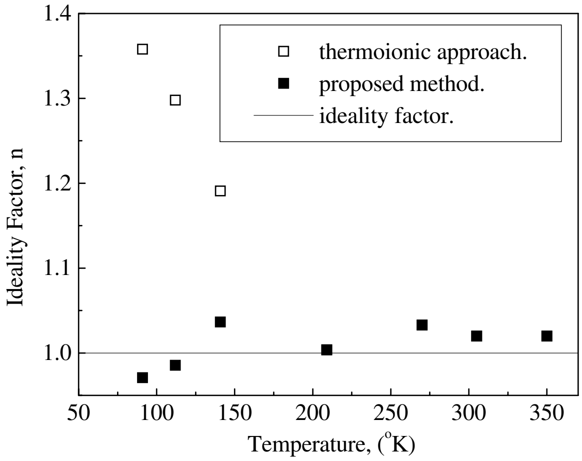

Figure 3. Comparison between the ideality factor determined by the thermionic emission approach and using the proposed method.

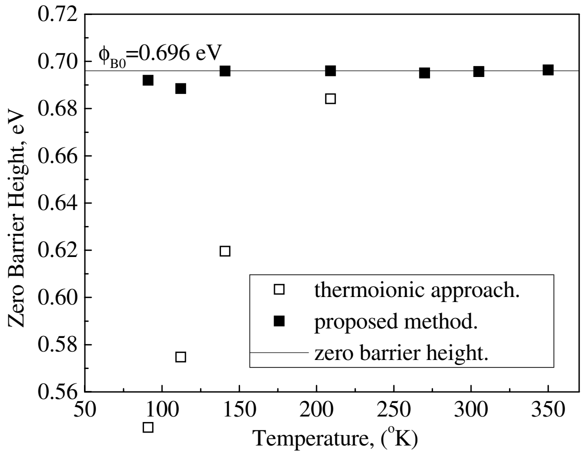

Figure 2. Comparison between the barrier heights determined by the thermionic emission approach and using the proposed method.

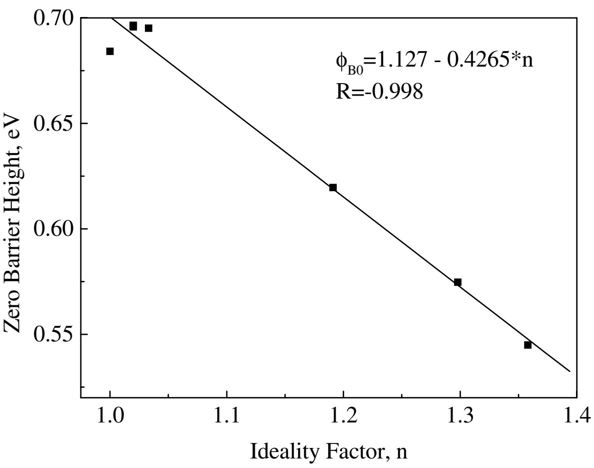

Figure 4. Zero barrier height as a function of the ideality factor.

proximity of $\phi_0(V, T)_i$ and $n_0(V, T)_i$ values to 0.696 eV and 1, respectively, are also easily seen in figures 2 and 3. The new parameters are almost temperature independent.

The value of $\phi_0(V, T)_i$ reached is close to 0.696 eV and is in very good agreement with the value of ϕ_{B0} reported by Barus and Donoval [21].

Figure 4 shows that there is a pronounced correlation between the zero barrier heights and the ideality factors that were calculated by the thermionic emission approach. The straight line is a least-squares fit of the experimental data. This behaviour has been reported by other authors [27] and it is also observed in the laterally inhomogeneous barrier height [16–18].

The cause of the ideal behaviour deviation of the Schottky contact requires a careful study where all effects must be considered. The transport mechanisms and laterally inhomogeneous barrier height must be specially treated because both effects present a large decrease of ϕ_{B0}, an increase of n with decreasing temperature, and a linear variation of ϕ_{B0} with the ideality factor.

4. Conclusions

We have developed a new method to determine the barrier height of the Schottky contacts with very promising results. If at least one transport mechanism is dominant on voltage intervals, then it is possible to quantify the influence of those effects that produce a deviation of thermionic mechanism behaviour on the I–V curves. The evaluation of barrier height and the ideality factor from I–V curves in a wide temperature range, using the thermionic emission approach, leads us to physically unacceptable values. The nonideal behaviours caused by the presence of different transport mechanisms or the laterally inhomogeneous barrier heights are similar.

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