

Temperature dependence of the inhomogeneous parameters of the Mo/4H-SiC Schottky barrier diodes

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Abstract

The inhomogeneous parameters of Mo/4H-SiC Schottky barrier diodes were determined from current–voltage (I – V) characteristics in the temperature range of 303–498 K by using a general approach for the real Schottky diode. In this approach the total series resistances is divided into two resistances; the first one (R_P) is the sum of the series resistances (r) of the particular diodes connected in parallel and the second is the common resistance (R_C) to all particular diodes. The mean barrier height ($\bar{\phi}$) and the standard deviation (σ) decrease linearly with decreasing temperature and they are between the values for the diodes with the two limiting cases; no current spreading and full current spreading. The series resistance R_C increases, while the series resistance R_P slightly decreases with decreasing temperature.

Keywords: Schottky diode, silicon carbide, inhomogeneity, I – V characteristic, mean barrier height, standard deviation, temperature

1. Introduction

The concept of the Schottky barrier height inhomogeneities is relatively well established and their influence on electrical characteristics has been described [1, 2]. According to the majority of the published experimental data the Gaussian distribution seems to be more appropriate for describing the inhomogeneous Schottky diode [3–14]. Several authors [3–14] have used the Werner–Güttler model to fit the theoretical and experimental zero-bias barrier heights and in general there has been very good agreement between these two values. The authors can determine the inhomogeneous parameters; the mean barrier height (ϕ) and the standard deviation (σ) which are independent of temperature. However, analytical studies based on these experimental parameters ($\bar{\phi}$, σ) exhibit several abnormal behaviors. In fact, Chand [15], in his letter, reported an unexpected observation in the current–voltage curves of Schottky diodes, containing barrier inhomogeneities generated using the analytical results based on a Gaussian distribution model of barrier heights. The calculations have shown that the current at lower temperatures may

exceed the current at higher temperatures. Chand [15] found that the origin of these anomalies is the saturation current (I_S), which decreases from its value at room temperature and then starts to increase again below a certain transition temperature. This observation is thus inconsistent with the thermionic emission–diffusion theory. Werner and Güttler [1] did not take into account the influence of the series resistances in their model. Using the thermionic emission expression for the current, the influence of the series resistance can be modeled in three ways [16, 17]. Figure 1 summarizes these three approaches; figures 1(a) and (b) represent the two limiting cases, full current spreading and no lateral current spreading, respectively. In the first case, the current is fully spread in the semiconductor bulk. Consequently, the particular diodes are in parallel, and they are all connected in series with a series resistance. Secondly, it is also possible to assume that each particular diode has its own series resistance. The series resistance is formed by the resistance of a quasineutral part of the semiconductor and by the resistance of the Ohmic contact [16]. In this case the spreading of the current in the substrate is assumed to be negligible. The more general approach of

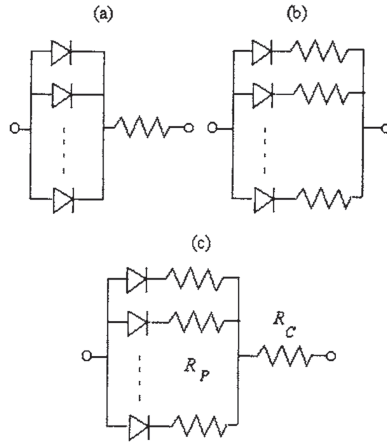


Figure 1. Equivalent scheme of an inhomogeneous Schottky diode with (a) complete current spreading, (b) with no lateral current spreading—the diode is formed by a set of noninteracting particular diodes, and (c) with the partial current spreading in the semiconductor substrate. This figure is reproduced from [16], with the permission of AIP Publishing.

real Schottky diode is presented in the figure 1(c) where the first part of the series resistance pertains to the particular small diodes (R_p) and a second part of the resistance (R_c) belongs to the region in which the total current is already homogeneous and is common to all particular diodes [16]. Osvald and Dobrocka in their work [18], extracted the parameters of the barrier height distribution using the no lateral current spreading model for Hg/n-Si, Pb/n-Si and Pb/p-Si Schottky diodes at room temperature. In this work we develop an approach for determining the inhomogeneous parameters such as the mean barrier height, standard deviation, and the two series resistances R_p and R_c directly from the general case presented in figure 1(c) for Mo/4H-SiC at different temperatures. It is known that molybdenum can readily react with the SiC. Molybdenum is known to form a silicide, when it reacts with elemental Si and to form a carbide when it reacts with elemental C. Molybdenum is also known to show little added reaction when performing an annealing up to 800 °C [19]. The evidence thus indicates that reactions and the creation of new phases (Mo_2C , MoSi_2 , Mo_3Si) lead to significant inhomogeneity due to a mixture of different phases at the M–S interface. This is beside the fact that SiC may contain structural and morphological defects that have been identified as micropipes, screw dislocations, grain boundaries, triangular depressions and growth pits. These defects were shown to exist both in the substrates and overgrown epilayers [20].

2. Theory and extraction method of the inhomogeneous parameters

The real Schottky diode can be modeled by the most general approach that consists of particular diodes which are in parallel and each particular diode has its own series resistance $r = R_p A$ (A is the contact area) and they are all connected in

series with a series resistance R_c as shown in figure 1(c) [16]. The expression for the whole current flowing through the inhomogeneous Schottky diode is

$$I = \int A \rho(\phi) j(\phi) d\phi. \quad (1)$$

The current density $j = j(V, \phi)$ depends on the forward bias and on the barrier height (ϕ) and given within the thermionic emission theory as [16]

$$\begin{aligned} j(\phi) &= j_s \{ \exp[q(V - AR_p j(\phi) - R_c I)/kT] - 1 \} \\ &= A^* T^2 \exp(-q\phi/kT) \{ \exp[q(V - AR_p j(\phi) - R_c I)/kT] - 1 \}, \end{aligned} \quad (2)$$

where A , A^* , T , q , and k are the contact area, effective Richardson constant, temperature, electronic charge, and Boltzmann constant, respectively. $\rho(\phi)$ is the normalized distribution function describing the Schottky barrier height (SBH) variations. In the case of a Gaussian distribution of BHs with mean barrier ($\bar{\phi}$) and standard deviation (σ), the distribution function $\rho(\phi)$ is given by

$$\rho(\phi) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(\phi-\bar{\phi})^2}{2\sigma^2}}. \quad (3)$$

Certainly, the limiting cases for $R_p = 0$ or $R_c = 0$ must coincide with the cases for the total current spreading and no current spreading, respectively [16].

In the limiting case of the total current spreading ($R_p = 0$, $R_c \equiv R_s$), substituting $j(\phi)$ and $\rho(\phi)$ in equation (1) and performing integration from $-\infty$ to $+\infty$ for values of ϕ , one obtains [15, 21]

$$I = I_s \left\{ \exp\left(\frac{q(V - R_s I)}{kT}\right) - 1 \right\}. \quad (4)$$

With the saturation current (I_s) and the apparent barrier height (ϕ_{app}) given by

$$I_s = AA^* T^2 \exp\left(-\frac{q\phi_{app}}{kT}\right), \quad (5)$$

$$\phi_{app} = \bar{\phi} - \frac{q\sigma^2}{2kT}. \quad (6)$$

The apparent barrier height (ϕ_{app}) depends on the mean barrier ($\bar{\phi}$), standard deviation (σ), and temperature (T). Equation (6) has been used to find the mean barrier and standard deviation of the distribution. It presents the Werner's model for inhomogeneous Schottky diode. Most of the workers use this equation for extracting the inhomogeneous parameters $\bar{\phi}$ and σ . However, when we apply this method the Schottky diodes exhibit higher currents at low temperatures than at high temperatures [15, 22]. This observation is thus inconsistent with the thermionic emission–diffusion theory. In order To avoid the use of this method for extracting the BH distribution with mean BH and standard deviation, we extract them directly from the most general approach described above and presented by the equations (1)–(3).

In order to extract the inhomogeneous parameters directly from the most general approach described above we

follow the same method proposed by Osvald [18]. This approach is based on the method of least squares where we sum the squares of the relative differences between the measured and the ideal value

$$S = \sum_{i=1}^N \left(\frac{I_i^{\text{ex}} - I_i^{\text{th}}}{I_i^{\text{th}}} \right)^2, \quad (7)$$

where I_i^{ex} is the j th experimental value, I_i^{th} is the fitting value of the current, i.e. the solution to (1) for $V = V_i$, and N is the number of measuring points. For minimizing the sum of the squares it is necessary to solve the equations

$$F_k = \frac{\partial S}{\partial x_k} = -2 \sum_{i=1}^N \left(\frac{I_i^{\text{ex}} - I_i^{\text{th}}}{I_i^{\text{th}}} \right) \frac{I_i^{\text{ex}}}{(I_i^{\text{th}})^2} \frac{\partial I_i^{\text{th}}}{\partial x_k} = 0$$

$$(k = 1, 2, 3, 4), (x_1 = \bar{\phi}, x_2 = \sigma, x_3 = R_p, x_4 = R_c) \quad (8)$$

From the equation (2) we can obtain the following derivatives

$$\begin{cases} \frac{\partial j}{\partial \bar{\phi}} = \frac{-\beta R_c (j + j_s)}{1 + A\beta R_p (j + j_s)} \frac{\partial I}{\partial \bar{\phi}} \\ \frac{\partial j}{\partial \sigma} = \frac{-\beta R_c (j + j_s)}{1 + A\beta R_p (j + j_s)} \frac{\partial I}{\partial \sigma} \\ \frac{\partial j}{\partial R_p} = \frac{\left(-\beta A j - \beta R_c \frac{\partial I}{\partial R_p} \right) (j + j_s)}{1 + A\beta R_p (j + j_s)} \\ \frac{\partial j}{\partial R_c} = \frac{\left(-\beta I - \beta R_c \frac{\partial I}{\partial R_c} \right) (j + j_s)}{1 + A\beta R_p (j + j_s)}. \end{cases} \quad (9)$$

Using equations (1) and (9), we can obtain the following derivatives

$$\begin{cases} \frac{\partial I}{\partial \bar{\phi}} = \frac{A}{g} \int \frac{(\phi - \bar{\phi})}{\sigma^2} \rho j d\phi \\ \frac{\partial I}{\partial \sigma} = \frac{A}{g} \int \frac{(\phi - \bar{\phi})^2 - \sigma^2}{\sigma^3} \rho j d\phi \\ \frac{\partial I}{\partial R_p} = \frac{-\beta A^2}{g} \int \frac{(j + j_s)}{1 + A\beta R_p (j + j_s)} \rho j d\phi \\ \frac{\partial I}{\partial R_c} = \frac{-\beta A I}{g} \int \frac{(j + j_s)}{1 + A\beta R_p (j + j_s)} \rho d\phi, \end{cases} \quad (10)$$

where

$$g = 1 + A\beta R_c \int \frac{\rho (j + j_s)}{1 + A\beta R_p (j + j_s)} d\phi, \quad \beta = q/kT.$$

Inserting the expression of derivatives $\frac{\partial I_i^{\text{th}}}{\partial x_k}$ into (8) we arrive at four normal equations for the parameter $\bar{\phi}$, σ , R_p and R_c . We use Newton–Raphson’s method for solving the non-linear equation system. The model described above was implemented in a FORTRAN program for extracting the inhomogeneous parameters of the SBDs, namely the mean barrier ($\bar{\phi}$), standard deviation (σ), and the tow resistances R_p and R_c . The program was successfully tested with theoretical

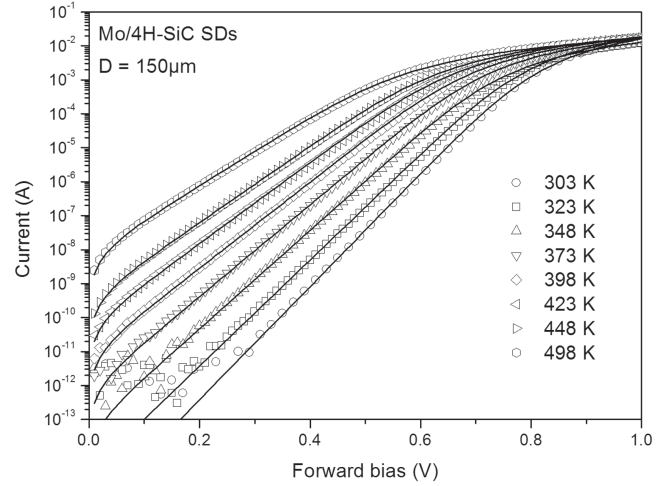


Figure 2. Forward experimental I - V - T curves (symbols) and fitted I - V - T curves (lines) of Mo/4H-SiC diode at different temperatures, diameter $D = 150 \mu\text{m}$, dose $= 1.75 \times 10^{14} \text{ cm}^{-2}$.

data. Note here, when $R_c = 0$ (no current spreading, $R_p \equiv R$) we obtain the same equations of the three parameters ($\bar{\phi}$, σ , R) obtained by Osvald [18].

3. Results and discussion

In this section, the model is validated against measurements on silicon carbide SBDs. The device under examination in this work is a Mo/4H-SiC Schottky barrier diode with high-resistivity guard rings manufactured on an n-type 4H-SiC (0 0 1) substrate. The wafers had an n-type epitaxial layer with a donor concentration in the range of 8.0×10^{15} – $1.3 \times 10^{16} \text{ cm}^{-3}$. The high-resistivity layer forming the guard ring was generated by carbon ion implantation using a Varian 350D ion implanter. The ion implantation was performed at room temperature and at different energies and doses ranging from 1.2×10^{12} to $1.75 \times 10^{14} \text{ cm}^{-2}$. Schottky diode diameters ranging from 150 to 300 μm were used. The electrical I - V - T measurements of the Schottky diodes were made in the temperature range of 303–473 K with a step of 25 K. The details concerning fabrication, optimization, and electrical characterization of the devices are reported elsewhere [9, 23]. Figure 2 shows the forward I - V - T characteristics of the Mo/4H-SiC SBD measured at temperatures 303–498 K range (symbols) and the fitted curves (lines) calculated with the extracted inhomogeneous parameters using equation (1). It can be seen from this figure that the experimental I - V curves totally coincide with the simulated I - V plots over the entire bias range which indicates that the temperature-dependent I - V characteristics of the Mo/4H-SiC Schottky diodes can be explained on the basis of thermionic emission mechanism with the Gaussian distribution of the barrier heights.

In figure 3, the extracted mean barrier height ($\bar{\phi}$) in the case of the Mo/4H-SiC diodes at different temperatures and for various implantation doses are shown. It is clear from this figure that the mean barrier height depends on the temperature and increases with increasing temperature and doses of ion

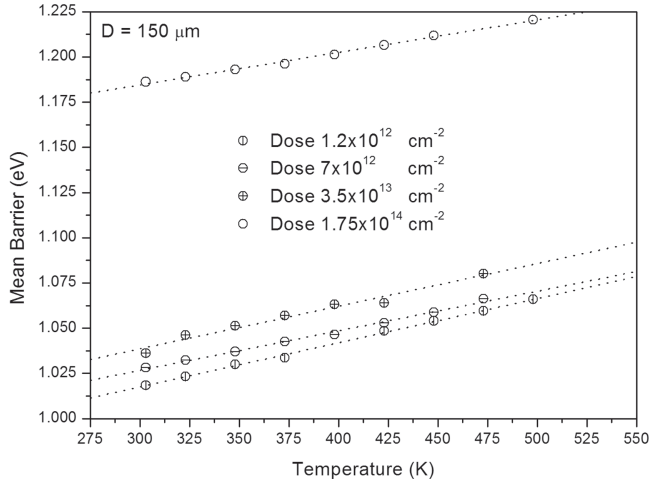


Figure 3. Extracted mean barrier height of Mo/4H-SiC diodes at different temperatures for different doses with diameter $D = 150 \mu\text{m}$.

Table 1. The extracted zero temperature mean barrier height $\bar{\phi}_0(T = 0\text{K})$ and the temperature coefficient $\alpha_{\bar{\phi}}$ for Mo/4H-SiC diodes at various doses and different diameters.

Diameter (μm)	Dose (cm^{-2})	$\bar{\phi}_0(T = 0\text{K})$ (eV)	$\alpha_{\bar{\phi}} \times 10^{-4}$ (eV K^{-1})
300	1.2×10^{12}	0.915	2.835
	7×10^{12}	0.971	2.263
	3.5×10^{13}	0.973	2.325
	1.75×10^{14}	1.120	1.969
200	1.2×10^{12}	0.953	3.627
	7×10^{12}	0.964	2.502
	3.5×10^{13}	0.966	2.487
150	1.2×10^{12}	0.944	2.438
	7×10^{12}	0.961	2.187
	3.5×10^{13}	0.968	2.357
	1.75×10^{14}	1.130	1.797

implantation. The decreasing of mean barrier height with decreasing temperature clearly indicates that the current at low temperatures is predominantly contributed by low barrier heights in the distribution. The mean barrier heights extracted from equation (6) which correspond to the full spreading case are independent of temperature.

The mean barrier height ($\bar{\phi}$) varies linearly with temperature according to equation (11)

$$\bar{\phi} = \bar{\phi}_0(T = 0\text{K}) + \alpha_{\bar{\phi}}T, \quad (11)$$

where $\bar{\phi}_0(T = 0\text{K})$ is the zero temperature mean barrier height and $\alpha_{\bar{\phi}}$ is the temperature coefficient of the mean barrier height determined from the y-axis intercept and the slope of the straight line, respectively. The linearity of the mean barrier was observed by ballistic electron emission microscopy studies (BEEM) with temperature coefficients ($\alpha_{\bar{\phi}}$) equal to -1.3×10^{-4} and $-2.3 \times 10^{-4} \text{ eV K}^{-1}$ for

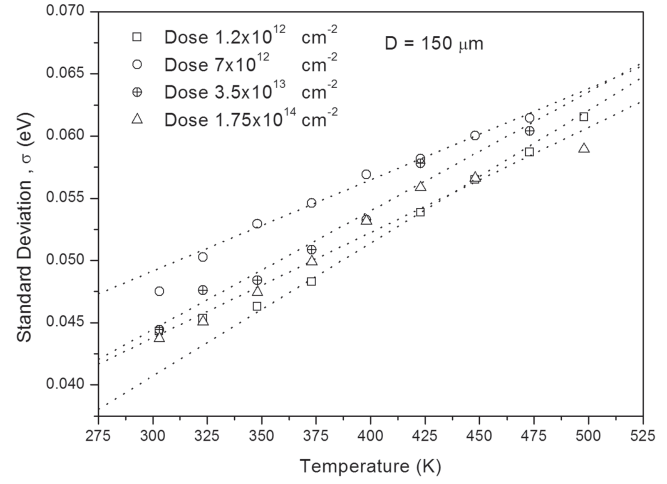


Figure 4. Extracted standard deviation of Mo/4H-SiC diodes at different temperatures for different doses with diameter $D = 150 \mu\text{m}$.

Table 2. The extracted zero temperature standard deviation $\sigma(T = 0\text{K})$ and the temperature coefficient α_{σ} for Mo/4H-SiC diodes at various doses and different diameters.

Diameter (μm)	Dose (cm^{-2})	$\sigma(T = 0\text{K})$ (eV)	$\alpha_{\sigma} \times 10^{-5}$ (eV K^{-1})
300	1.2×10^{12}	0.0114	9.159
	7×10^{12}	0.0262	6.815
	3.5×10^{13}	0.0197	8.013
	1.75×10^{14}	0.0129	9.219
200	1.2×10^{12}	0.0215	8.601
	7×10^{12}	0.0168	9.312
	3.5×10^{13}	0.0277	6.263
150	1.2×10^{12}	0.0087	10.682
	7×10^{12}	0.0271	7.330
	3.5×10^{13}	0.0158	9.547
	1.75×10^{14}	0.0184	8.458

silicon Schottky diodes [24]. Table 1 summarizes the different obtained values of the mean barrier $\bar{\phi}_0(T = 0\text{K})$ and the temperature coefficient ($\alpha_{\bar{\phi}}$) for the different structures Mo/4H-SiC.

The plots of the extracted standard deviation (σ) as a function of temperature for different doses are given in figure 4. The plots are straight lines according to equation (12)

$$\sigma = \sigma(T = 0\text{K}) + \alpha_{\sigma}T \quad (12)$$

Equation (12) gives temperature coefficients $\sigma(T = 0\text{K})$ and α_{σ} from the intercept and slope, respectively. The values of $\sigma(T = 0\text{K})$ and α_{σ} were obtained and listed in table 2 for different structures. The obtained values for standard deviation appear to be reasonable and decrease with decreasing temperature. The smaller values for standard deviation at low temperatures do not lead to any excess of the saturation

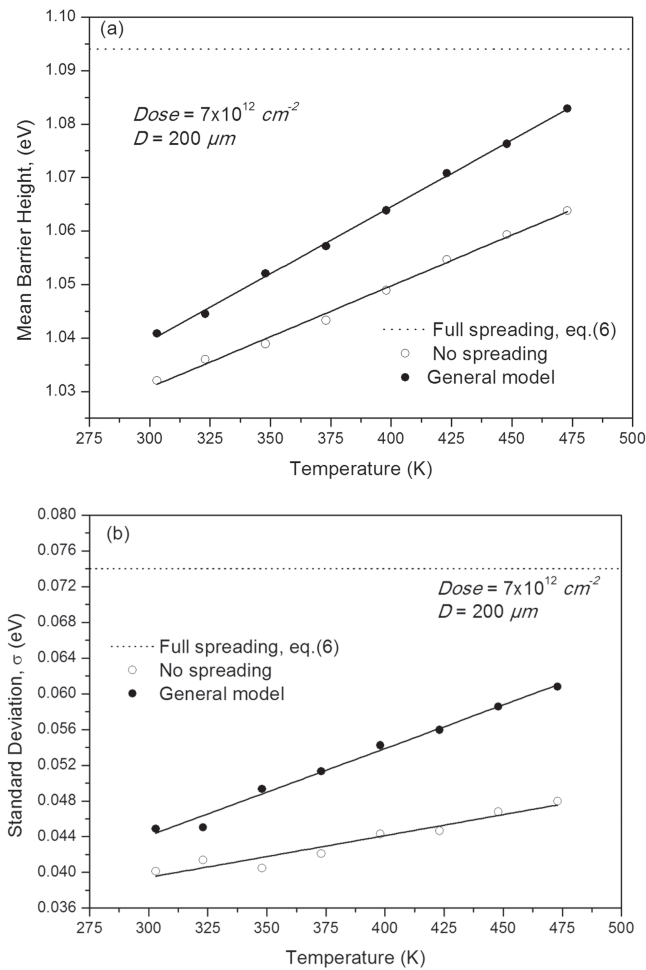


Figure 5. Comparison between the extracted values of $\bar{\phi}$ and σ obtained by different three approaches. (a) The mean barrier height $\bar{\phi}$, (b) the standard deviation σ .

current at low temperatures when compared to the saturation current at high temperatures [22]. The BEEM studies have reported the low values of the standard deviation; 0.03, 0.04 [25], 0.02 [26], and 0.013–0.022 V [27] at room temperature and ~ 0.011 – 0.021 V [24] in the temperature range of 129–252 K.

It is clear from tables 2 and 1 that the zero temperature mean barrier height is practically independent of the contact area and remained unchangeable despite the varied implantation doses. However, no such trend is observed for zero temperature standard deviation. This is due to the fact that the width of the Gaussian barrier distribution (i.e., its standard deviation) is not only dependent on intrinsic properties of the contacts, but also dependent on the implantation doses of the guard ring.

The mean barrier heights and standard deviations for the general model are between the values for the diodes with the two limiting cases (no current spreading and full current spreading) as shown in figure 5. The apparent barrier heights and ideality factors extracted from simulated I - V curves of general model are between the values for the diodes with the series resistance concentrated in R_C and R_P [16].

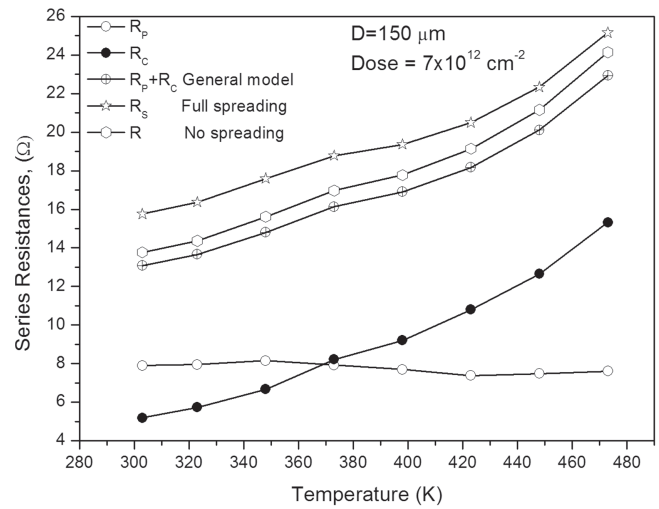


Figure 6. The extracted series resistances by different approaches for Mo/4H-SiC Schottky diodes at various temperatures, with diameter $D = 150 \mu\text{m}$ and dose $= 7 \times 10^{12} \text{ cm}^{-2}$.

Figure 6 shows the variation of the extracted series resistances R_P and R_C as a function of temperature for the structure Mo/4H-SiC with diameter $D = 150 \mu\text{m}$ and Dose $= 7 \times 10^{12} \text{ cm}^{-2}$ (almost of our diodes follow the same behavior of this example diode). The sum of the two series resistances ($R_P + R_C$) is also compared with the two others resistances R_S and R obtained by applying the two limiting cases; full current spreading and no current spreading, respectively. From this figure we can observe several remarks: first, the series resistance R_C increases, while the series resistance R_P slightly decreases with increasing temperature. Second, the magnitude of the resistance R_C is large compared to the resistance R_P at high temperatures, while they have the same orders of magnitude at low temperatures. Third, the sum of R_P and R_C has the same shape as the series resistance R_S (full spreading) and R (no spreading) and the value of sum ($R_P + R_C$) remains below R_S and R . This small difference between the values of the series resistances for all the three approaches may be a result of the inhomogeneous models that consider the same elementary resistance (r) of each diode. However, but actually, these resistances may different from each other at the inhomogeneous Schottky contacts because the roughness of the interface is non-uniform. When considering the fluctuation of the elementary resistance (r) in the inhomogeneous models the equations will be more complicated. The existence of the resistance R_P may be responsible for the deviation of the ideality factor of the diode from unity [16].

The temperature dependence of the ideality factor n has often been accredited to current transport mechanisms not following the ideal thermionic emission theory. Various studies have cited different reasons for this nonideal dependence. Werner and Güttler [1] proposed that such dependence originates from Schottky barrier inhomogeneity, which could be due to different interface qualities which depend on several factors such as surface defect density, surface treatment, deposition processes. Werner and Güttler [1] concluded that

the ideality factor n of Schottky contacts reflects the deformation of the barrier distribution under applied bias. Tung [2] in his work reported that the dependence of the potential barrier (effective SBH) on the applied bias leads to an ideality factor that is greater than 1. Osvald [16] in his work made some numerical experiments to explore the influence of the resistance components (R_P and R_C) on the I - V curves of the structure. He concluded that if the current is spread unevenly (R_P is non null) in the semiconductor bulk of a diode, its ideality factor deviates from unity. By contrast, if the current is fully spread (R_P is null) in the semiconductor bulk of a diode, its ideality factor remains unity regardless of the value of the standard deviation. Unfortunately, our samples showed smaller variations in the both values of the series resistance R_P and ideality. Factor n (n vary from 1.06 to 1.03 in the range of 303–473 K) which is why we cannot identify a clear dependence between them.

4. Conclusion

In conclusion, we have established an approach for determining the barrier heights distribution from a general model of the Schottky diode. This general approach allows us to divide the whole series resistance of the Schottky diode into two parts R_P and R_C which almost have the same orders of magnitude. This approach enables us to explain the electrical characteristics of Schottky diodes without using the ideality factor n which can be substituted by the Gaussian barrier height diode with the mean barrier height ($\bar{\phi}$) and the standard deviation (σ). The temperature dependence of the mean barrier height and standard deviation for the Mo/4H-SiC Schottky diodes has been found. The mean barrier height ($\bar{\phi}$) and the standard deviation (σ) decrease with decreasing temperature and the low values of the standard deviation do not lead to any abnormal behaviors of the current at low temperatures.

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