Barrier height inhomogeneities on Pd/n-4*H*-SiC Schottky diodes in a wide temperature range

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Highlights

- Impact of palladium silicidation on barrier height inhomogeneity.
- No correlation between electrically active defects and barrier inhomogeneities.
- Limitation of the Gaussian distribution of barrier heights above 550 K.
- Widest temperature range to be investigated.

Abstract

Barrier height inhomogeneities on Pd/n-type 4*H*-SiC Schottky barrier diodes in the 300–800 K temperature range have been investigated. Palladium is known to form silicide above 673 K. Temperature dependent current-voltage (*I*-*V*) characteristics were analyzed. Barrier height (BH) and ideality factor (*n*) were found to be strongly temperature dependent. Barrier height increased, whilst ideality factor decreased with increasing in temperature and the Richardson plot showed some deviation from linearity. This was attributed to barrier inhomogeneities at the metal-semiconductor interface which resulted in a distribution of barrier heights. From the modified Richardson plot, the modified Richardson constant, A^{**} was found to be 155 $\mathrm{Acm^{-2}K^{-2}}$ and 87 $\mathrm{Acm^{-2}\,K^{-2}}$ in the 300–525 K and the 550–800 K temperature ranges respectively.

Keywords: Barrier height; Richardson constant; 4*H*-SiC; Barrier height inhomogeneities; Schottky Barrier height

1. Introduction

4*H*-SiC has attracted research and commercial interest on electrical device applications due to its exceptional semiconductor properties [1]. The material is superior due to the isotropic nature of its electronic mobility compared to other silicon carbide poly-types [2], [3]. It produces devices that have a breakdown voltage of up to 1000 V and excellent rectifying properties [4]. In addition its excellent physical properties make it ideal for operation under harsh environments like extremely high temperatures and irradiation exposure [5].

When compared to other semiconductors, its large band gap allows device designs which are low on power dissipation and series resistance [6]. The devices can operate with high stability because they are majority carrier devices. They are competitive in high power applications, and complement the evolution of the electronics industry towards high efficiency devices with minimal power loss. Schottky barrier diodes (SBDs) made from the material have been commercially available for a considerable time but their properties and applications are still not thoroughly understood [7], [8], [9], [10].

Of particular research interest are the processing steps involved in device fabrication [11], [12], [13]. Consistent control of metal contact properties on semiconductors is yet to be established so as to optimize reliability [9], [14]. Consistency in structure of the interfacial region and the Schottky barrier height (SBH) contribute significantly to the behavior of metal–semiconductor contacts [6]. A high Schottky barrier is essential for a good rectifying contact whereas low barrier height results in a reverse leakage current which makes the SBDs poor rectifiers [15]. The inability to physically reproduce the SBH is therefore a technologically important concern which is continuously being researched.

In past studies, analysis of current-voltage-temperature, *I-V-T* characteristics of SBDs based on the thermionic emission (TE) model have revealed unexpected variational trends in BH and *n* with temperature [16]. Experimental values of the Richardson constant have also been observed to be significantly lower than expected. These deviations have been ascribed to metal-semiconductor interface inhomogeneties which have been speculated to be due to doping irregularities and surface defects among other reasons [17].

Two well consolidated approaches have been put forward in-order to explain *I-V-T* characteristics of in-homogenous SBDs, based on viewpoints put forward by Tung, Song, Werner and Guttler. In his model Tung assumed that the deviation of device behavior from ideality was due to the interfacial local structure. His model attributed inhomogeneities to the existence of locally uniform regions with lower or higher barriers relative to the mean SBH [18]. Recently he has also speculated that this variation can be accounted for in the chemical bonding picture by the atomic structure of the metal-semiconductor interface [14].

Song followed by Werner and Guttler‘s potential fluctuations model assumes that the metal-semiconductor interface has roughness at atomic level [19]. They assumed a continuous spatial distribution of the Schottky barrier and integrated the TE current with a single barrier height weighted by the Gaussian distribution function to obtain the total current across [20], [21].

Some notable research outcomes from investigating inhomogeneities in 4*H*-SiC devices are from Bolen et al. who investigated barrier height in homogeneity in Ti/4*H*-SiC SBDs in the 293–390 K temperature range and showed that barrier height inhomogeneity is highly influenced by device area [22]. They concluded that threading screw dislocations affect the electrical characteristics of 4*H*-SiC SBDs to an insignificant extent. Another important result was from Ma et al. who etched the surface of 4*H*-SIC using reactive ions and hydrogen. They demonstrated that barrier height inhomogeneities can be manipulated and proposed that sharp apex pits control barrier height inhomogeneities [23] Also Rocafforte et al. attributed underestimation of the Richardson‘s constant in the 98–483 K range in silicon carbide to the active area in current transport which is lower than the total contact area. They singled out contact quality as a highly contributing factor [24].

In this article the forward bias *I-V* characteristics of Pd/n-4*H*-SiC SBD were studied on the basis of Werner‘s model. The data was analyzed assuming a Gaussian distribution of BHs to yield information on the temperature dependence of Schottky diode parameters in the 300–800 K range. This temperature range is the widest to be investigated when compared to previous studies. Information on the operation of 4*H*-SiC at high temperatures is very important because it gives insights on the stability of the contacts at such temperatures. Furthermore, palladium is known to form silicides in the 673–873 K temperature range [25]. Therefore we set out to observe if the reaction phase had an impact on the *I-V* characteristics as temperature increased.

Palladium is a preferred metal contact on electronic devices because it has superior material weight to thickness ratio.

2. Experimental procedure

Nitrogen doped n-type 4*H*-SiC wafers consisting of an epi-layer of net doping density $7 \times 10^{15}\text{cm}^{-3}$ grown on a highly doped substrate of doping density of $10^{18}\ \text{cm}^{-3}$ as specified by the supplier Cree Inc were used. Smaller samples of the wafers were cut and cleaned in a two-step procedure. The wafers were first degreased by boiling consecutively in three different organic solvents namely tetrachloro-ethylene, acetone and methanol. They were then rinsed in deionized water with a resistivity of 18.2 MΩcm. Thereafter, the samples were etched by dipping in 2% hydrofluoric acid solution for 60 s, rinsing in deionized water.

Immediately afterwards an ohmic contact was formed by resistively depositing 3000 Angstroms of nickel on the sample backside ($10^{18}\ \text{cm}^{-3}$) in an Edwards Auto 306 vacuum system followed by thermal annealing at 950 °C for 10 min in argon flowing at a rate of approximately $3\ \text{dm}^3/\text{min}$. After annealing, the degreasing procedure was repeated but instead of boiling the samples were rinsed in an ultrasonic bath and dried using nitrogen gas.

500 Å thick, circular palladium Schottky contacts, 0.6 mm in diameter were thermally evaporated through a metal mask. Contact quality was evaluated using *I-V* and *C-V* measurements. An HP 4140B pA meter /DC voltage source was used for *I-V* measurements and an HP 4192A LF impedance analyzer was used for *C-V* measurements.

Temperature dependent *I-V* and *C-V* measurements were carried out at 25 K intervals continuously in the 300 K–800 K temperature range in a HFS600E-PB4 temperature controlled stage made by Likam scientific instruments.

3. Results and discussion

3.1. Forward I-V characteristics.

Assuming pure thermionic emission, the *I-V* relationship across a Schottky barrier for ($V > 3kT/q$) can be given by [26].

$$I = AA^{*}T^{2}\exp\left(-\frac{q\phi_{ap}}{kT}\right)\left[\exp\left(\frac{q(V-IR_{s})}{nkT}\right)-1\right] \qquad (1)$$

where q is elementary charge, A is the diode area, A^* is the Richardson constant ($=146\ \text{Acm}^{-2}\ \text{K}^{-2}$), V is bias voltage, n is ideality factor, Φ_{ap} is the apparent BH and T is temperature, k is the Boltzmann constant.

I_s, the saturation current which is the intercept of the ln I versus V curve given by [27]

$$I_s = AA^*T^2\exp\left(\frac{q\phi_{Bo}}{kT}\right) \qquad (2)$$

where ϕ_{Bo} is the zero bias barrier height. Fig. 1 shows the semi-log characteristics obtained from the Pd/*n*-4*H*-SiC SBDs in the 300–800 K temperature range. The curves have linear regions in the intermediate bias regions where linear fits of Equation (1) have been performed. In the 600–800 K range there is evidence of generation-recombination current at low bias ($V < 0.5$). The deviation from linearity observed at $V > 1.25$ V has been attributed to series resistance [28]. As predicted by Eq. (1) the *I-V* plots shift towards high bias voltage with decreasing temperature.

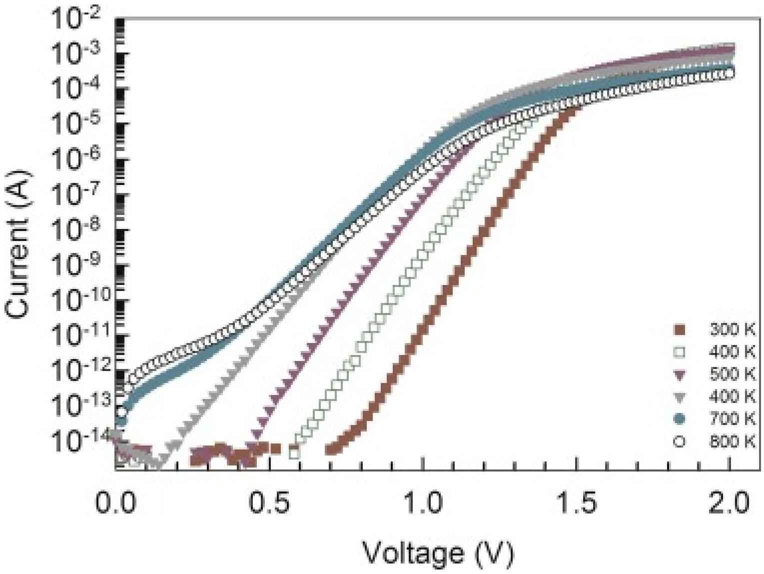


Fig. 1. Semi-logarithmic forward bias *I-V* curves as a function of temperature for Pd/*n*-4HSic Schottky barrier diodes.

The zero bias barrier height, $\Phi_{\text{I-V}}$, is calculated from the relationship [29].

$$\Phi_{Bo} = \frac{kT}{q} ln\frac{AA^*T^2}{I_S} \qquad (3)$$

The calculated bias barrier heights from Eq. (3) are plotted in Fig. 2. From the graph increase in barrier height is noted with increasing temperature which contradicts the negative temperature coefficient of *n*-4*H*-SiC. Similar results have also been observed by other researchers in different compound semiconductors [30], [31]. $\Phi_{I\text{-}V}$ increased from 1.42 eV at 300 K to 2.27 eV at 800 K. The temperature dependence of the BH is to be expected since the current transport is thermally activated. However, the negative temperature coefficient suggests that the barrier height should be higher at low temperatures as at such the electrons will have lesser energy to surmount the barrier.

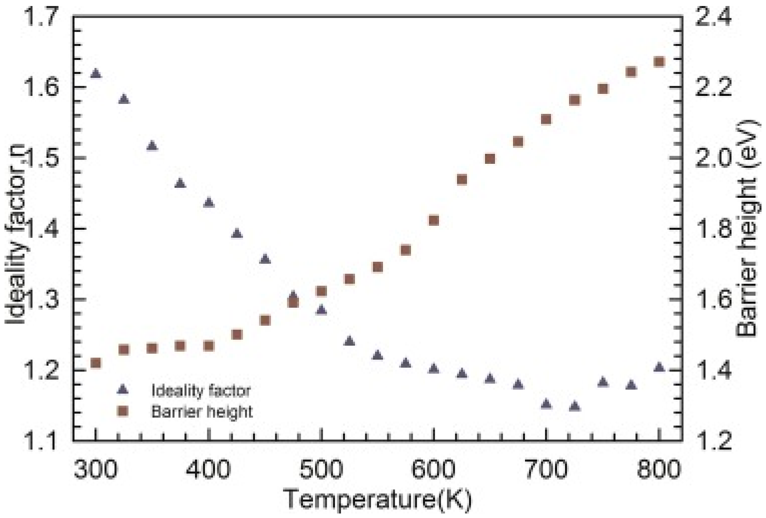


Fig. 2. Ideality factor and *I-V* barrier height as a function of temperature for Pd/*n*-4HSiC Schottky barrier diodes in the 300–800 K temperature range.

From the gradient of the least squares fits on the linear regions of *I-V* plots, *n* was obtained as [32]

$$n = \frac{q}{kT}\frac{dV}{d(\ln(I))} \tag{4}$$

The value of *n* decreased with increasing temperature from 1.62 at 300 K to 1.15 at 700 K to 1.20 at 800 K. Such a variation of ideality factor is unexpected since the variation of *n* and $\Phi_{I\text{-}V}$ has shown linear correlation behavior in past studies [33]. This result was observed repeatedly and might be attributed to the formation of the Pd_3Si phase during silicidation of silicon carbide in the 673–873 K range might be responsible [25]. The variation if ideality factor in the 300–700 K range can result from increase in series resistance and the influence of other current transport mechanisms as displayed in Fig. 1 [34], [35]. Ideality factor is mainly a measure of deviation from pure thermionic emission theory [30]. Several defect states exist in 4*H*-SiC in this temperature range including the Z1/Z2 observable around 300 K and the EH6/EH7 observable around 500 K using DLTS [36], [37]

3.1.1. The Richardson constant

The Richardson plot is shown in Fig. 3.The plot is obtained after linearizing Eq. (2) yielding the equation

$$\ln\left(\frac{I_S}{T^2}\right) = \ln(AA^*) - \frac{q\Phi_{Bo}}{kT} \tag{5}$$

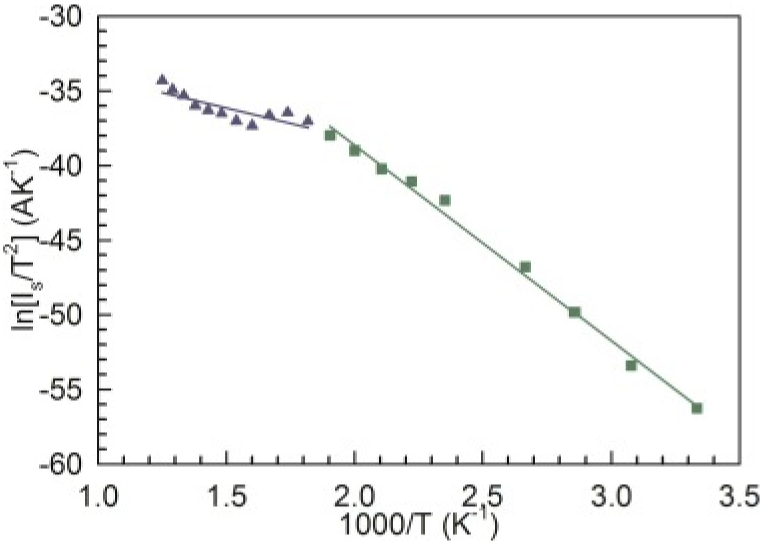


Fig. 3. Richardson plot for Pd/*n*-4*H*-SiC Schottky barrier diodes in the 300–800 K temperature range.

Two linear regions with different slopes are shown. This splitting of the Richardson plot into two linear regions has also been observed by other researchers in 4*H*-SiC and other semiconductors and has been explained as due to two distinct conduction mechanisms, spatial in-homogenous BHs and interfacial potential fluctuations that consist of irregular barrier areas [26], [38], [39], [40]. At high temperatures there will be enough energy for the current to flow through high barriers whilst at low temperatures it will preferentially flow through low barriers, in the potential distribution. The presence of extended defects in 4*H*-SiC has been also shown as one of the contributing factors to the inhomogeneities [41].

Activation energy (E_a) and A* were deduced from the slope and intercept of these straight lines. From Fig. 4, in the first region i.e 300–525 K, E_a and A* were obtained as 1.13 eV and 1.5×10^{-3} Acm^{-2} K^{-2} and for the 550–800 K region they were 0.35 eV and 3.4×10^{-11} Acm^{-2} K^{-2} respectively. The magnitudes of A* in both regions are lower than the theoretical value of 146 Acm^{-2} K^{-2}. Zaman et al. have shown that the value of the Richardson constant can be affected by fabrication conditions after evaluating it for three different metals on 4*H*-SiC SBDs [42]. Pirri et al. found an average value of 1.16 eV for 20 Ti/4*H*-SiC devices and A* of 17 Acm^{-2} K^{-2}. They argued on the inadequacies of the model used in the calculation of the widely accepted theoretical value of 146 Acm^{-2} K^{-2} which disregards crystallographic anisotropy and the exact position of the conduction band minima [43]. The barrier height (E_a) is lower than the theoretically expected by about two orders of magnitude. Hamida et al. attributed this to the effective diode area being smaller than the actual geometric device area [27].

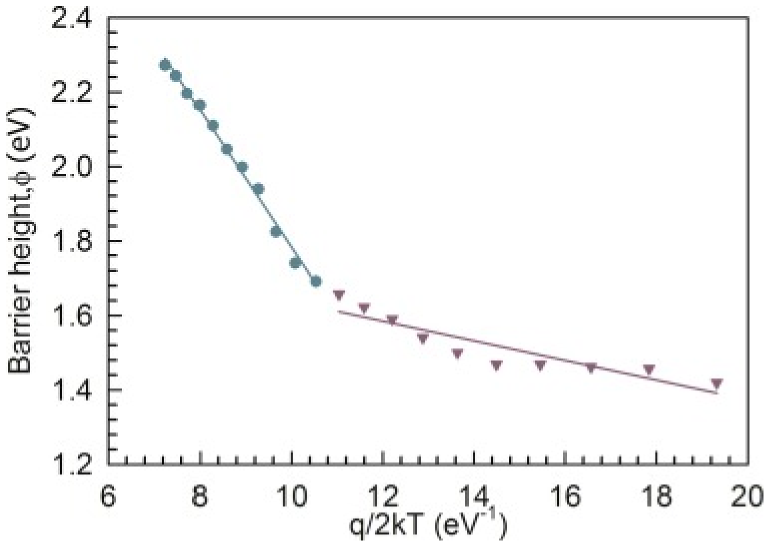


Fig. 4. Zero bias apparent barrier height versus *q/2kT* for Pd/*n*-4*H*-SiC Schottky barrier diodes according to the Gaussian distribution of barrier heights.

3.2. Barrier height inhomogeneity analysis.

To account for barrier height inhomogeneities, the model of Werner and Guttler was adopted by introducing a Gaussian distribution of BHs with an average

and standard deviation σ_S as [20].

$$P(\Phi_B) = \frac{1}{\sigma_s\sqrt{2\pi}}\exp\left[-\frac{(\Phi_B - \bar{\Phi}_B)^2}{2\sigma_s^2}\right] \qquad (6)$$

where $1/\sigma_S\sqrt{2\pi}$ is the normalization constant. The current across the barrier $I(\Phi_B,V)$ is the current at a bias *V* becomes [44]

$$\int_{-\infty}^{+\infty} I(\Phi_B, V)P(\Phi_B)d\Phi_B \qquad (7)$$

for a BH given by Eq. (1) and $P(\Phi_B)$ is the normalized distribution function giving the probability of occurrence of Φ_B. Integrating Eq. (6) from -from $-\infty$ to ∞ the current *I* through the barrier is obtained as $I(V)$

$$= AA{*}T^2\exp\left[\left(\frac{-q}{kT}\right)\left(\bar{\Phi}_{Bo} - \frac{q\sigma_s^2}{2kT}\right)\right] \times \exp\left(\frac{qV}{n_{ap}kT}\right)$$
$$\left[1 - \exp\left(\frac{-qV - IR_s}{kT}\right)\right] \qquad (8)$$

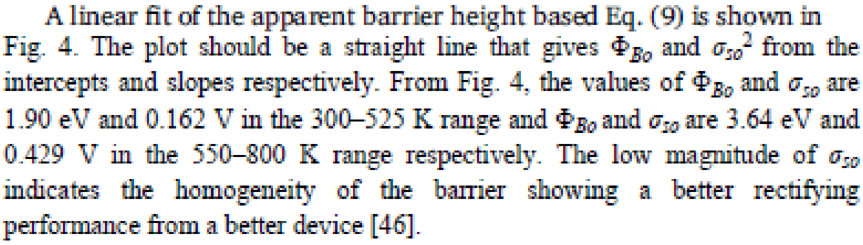
where Φ_{Bo} and n_{ap} are the apparent barrier height and ideality factor, respectively given by

$$\Phi_a p = \Phi_{Bo} - \frac{q\sigma_s^2}{2kT} \qquad (9)$$

$$\left(\frac{1}{n_{ap}} - 1\right) = \rho_{2-}\frac{q\rho_3}{2kT} \qquad (10)$$

assuming that the modified SBH (Φ_{Bo}) and σ_S are linearly bias dependent on Gaussian parameters such as $\Phi_B = \Phi_{ap} + \rho_2 V$ and $\sigma_s = \sigma_{so} + \rho_3 V$ where ρ_2 and ρ_3 are temperature dependent voltage coefficients which express the voltage deformation of the BH [19], [45]. The temperature dependence of σ_s is negligible.

Fig. 4 shows two distinct straight lines with transition happening at 525 K. The current transport mechanism across the barrier is influenced by barrier inhomogeneities. At temperatures close to room temperature TE becomes the dominant current transport mechanism. At higher temperatures generation-recombination causes deviation of the barrier height from the value obtained from a homogeneous barrier [16].



A linear fit of the apparent barrier height based Eq. (9) is shown in Fig. 4. The plot should be a straight line that gives Φ_{Bo} and σ_{so}^2 from the intercepts and slopes respectively. From Fig. 4, the values of Φ_{Bo} and σ_{so} are 1.90 eV and 0.162 V in the 300–525 K range and Φ_{Bo} and σ_{so} are 3.64 eV and 0.429 V in the 550–800 K range respectively. The low magnitude of σ_{so} indicates the homogeneity of the barrier showing a better rectifying performance from a better device [46].

3.3. The modified Richardson plot

The modified Richardson plot was put forward by Hackam and Harrop inorder to consider deviation from the pure thermionic emission which assumes a uniform barrier [47]. The Richardson plot of Pd/*n*-4*H*-SiC SBDs was not entirely linear. To correct for this discrepancy, and yield an improved value of the Richardson constant closer to the theoretical value of 146 $AK^{-2}\,cm^{-2}$, Eq. (2) can be rewritten according to a Gaussian distribution of barrier heights as [48].

$$I_s = AA^{**}\exp\left[-\frac{q\Phi_{ap}}{kT} + \frac{q^2\sigma_{so}^2}{2k^2T^2}\right] \qquad (11)$$

Based on Eq. (9) the modified Richardson plot of

$$\ln\left(\frac{I_s}{T^2}\right) - \left(\frac{q^2{\sigma_{so}}^2}{2k^2T^2}\right) = \ln(AA^*) - \frac{q\Phi_{ap}}{kT} \qquad (12)$$

has been plotted in Fig. 5.

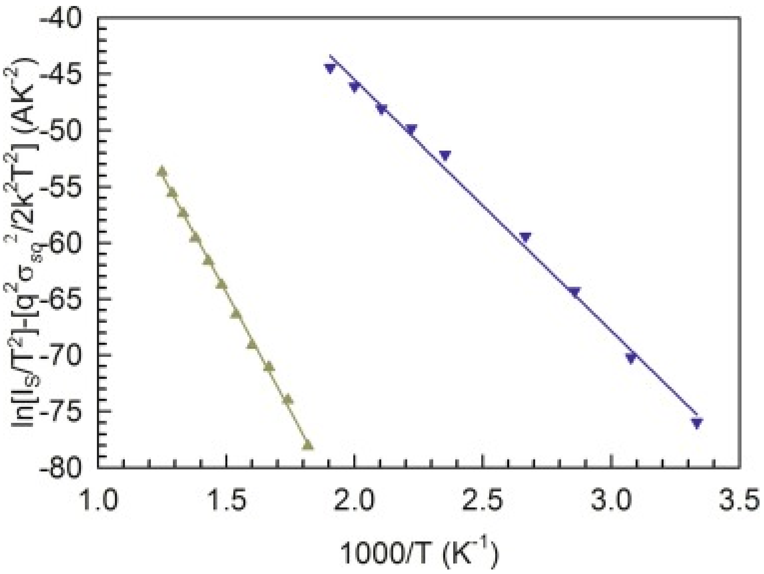


Fig. 5. Modified Richardson plot for the Pd/*n*-4*H*-SiC Schottky barrier diodes according to the Gaussian distribution of barrier heights.

This plot accounts for deviations of the BH and is expected to be a straight line with a slope and *y*- intercept which yield a mean BH and a modified Richardson constant. The two values of σ_{so} were calculated from Fig. 4 in the 300–525 K temperature range and 550–800 K temperature range. The mean zero bias BHs were calculated to be 1.92 eV and 3.22 eV in the 300–525 K range and the 550–800 K ranges respectively. Also from the intercepts the corresponding modified Richardson constants were obtained to be 155 A cm^{-2} K^{-2} and 87 A cm^{-2} K^{-2} between 300 and 525 K and 550–800 K respectively. These values are within a reasonable range with the theoretically expected value of 146 A cm^{-2} K^{-2}.

The nature of the inhomogeneities contributes largely to these results and they may involve interface properties like composition and charge amongst others [49]. The value obtained in the 300–525 K range is a better approximation of the widely accepted theoretical value than the one in the 550–800 K range. The model that was used to calculate the 146 Acm^{-2}K^{-2} value has limitations. It is obtained from a simple calculation that does not take into account quantum mechanical tunneling unlike the one by Crowel et al. [43], [50], [51]. As suggested by Pirri et al. an accurate Richardson constant must be calculated from a model that takes into account crystallographic anisotropy like the presence of extended defects in the material [43]. The effects of these could manifest more as the temperature increases providing activation energy thus affecting the Richardson‘s constant at higher temperatures.

Close to 300 K current transport would be preferably through lower barriers in the potential distribution. The results indicate the dominance of TE whilst anomalies can be attributed to other current transport mechanisms.

4. Conclusion

Current-voltage characteristics of Pd/n-4*H*-SiC Schottky barrier diodes were analyzed from 300 to 800 K. BH increased with increasing temperature contradicting the negative temperature coefficient of n-4*H*-SiC. *n* decreased with an increase in temperature and an irregular trend was observed in the 700–800 K range. The discrepancy we speculated as due to silicidation to form Pd_3Si in the 673–873 K range. Deviations from the TE theory were accounted for by assuming a Gaussian distribution of inhomogeneities at the metal-semiconductor interface. The mean values and standard deviation were determined to be 1.90 eV and 0.162 V in the 300–525 K range and 3.63 eV and 0.430 V in the 550–800 K range. The modified Richardson constant for the 300–525 K range was found to be 155 A K^{-2} cm^{-2} [52]. Proximity of the calculated modified Richardson constant to the theoretical one is a satisfactory proof of the success of the Gaussian distribution in explaining temperature dependence of *I-V* characteristics in the 300–525 K temperature range of Pd/4*H*-SiC Schottky diodes. The lower value of the modified Richardson‘s constant in between 550 K and 800 K was attributed to the limitations in this temperature range of the model used for calculation of the widely accepted value of the Richardson constant. No correlation was observed between the electrically active defect states and the barrier height inhomogeneities.

Acknowledgements

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