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Determination of temperature dependence of electron effective mass in 4H-SiC from reverse current-voltage characteristics of 4H-SiC Schottky barrier diodes

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Abstract. The current-voltage-temperature profiling method has been used with 4H-SiC Schottky barrier diodes and presented for determining the electron effective mass in 4H-SiC. The extracted electron effective mass has been found to be temperature dependent, it decreases with increasing the temperature. Moreover, a good agreement was found between our obtained values of electron effective mass ($m^* = 0.18m_0$, $0.21m_0$) at room temperature and other values that are obtained by different methods.

Keywords: 4H-SiC, Schottky diode, electron effective mass, I-V method, reverse current, thermionic emission, tunneling current.

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1. Introduction

The wide bandgap semiconductor 4H silicon carbide (4H-SiC) is very promising material for electronic device applications and have attracted much attention, because of its superior material properties for high-temperature, high-power and high-frequency electronics [1, 2]. The electron effective mass in the conduction band and holes in the valance one is important for describing various electrical and optical properties of 4H-SiC material and also for ascertaining the transport properties. The value of effective mass depends on the local curvature of the band near the band extremum [3]. The knowledge of effective mass inherent to electron in the conduction band and hole in the valence band is very necessary for least-squares fits of the experimental electrical characteristics to the temperature dependence of parameters of electronic devices, in particular for Schottky barrier diodes (SBDs) parameters, namely: barrier height and ideality factor. The electron effective mass m^* is the parameter determining the slope of the calculated reverse characteristics [4, 5]. The effective mass, in general, is tensorial, and the more compact information for easy use in device application is the thermal density of states (DOS) effective mass calculated from the effective masses along the principal axes of the ellipsoidal energy surface according to the equation $m^* = \left(m_1^* m_2^* m_3^*\right)^{1/3}$ [6]. The authors always use a single value of effective mass determined at room temperature for determining the temperature dependence of electrical parameters of Schottky barrier diodes. Using the density functional theory (DFT), Wellenhofer and Rossler [7] showed that DOS effective mass for electrons in 4H-SiC increases slightly with increasing temperature, however, it decreases with increasing the temperature for 6H-SiC. The experimental value of electron effective mass in 4H-SiC has been determined by several methods, such as the Hall effect, electron cyclotron resonance, infrared absorption, Raman scattering, and optically detected cyclotron resonance at room temperature. In this study, we investigate the temperature dependence of the electron effective mass in 4H-SiC material from the reverse current-voltage (*I–V–T*) characteristics of 4H-SiC SBDs, then we compare the value of electron effective mass at room temperature with those determined by different measurements and calculated methods.

2. Theory and modeling

Two predominant mechanisms across the Schottky barrier diodes are electron tunneling through the potential barrier and thermionic mechanism over the barrier [8].

The net current density flowing through the Schottky barrier is the algebraic sum of both these currents which are given by [9]

$$J = J_{Tun} + J_{Therm}\,. \tag{1}$$

The reverse tunneling current density component J_{Tun} can be expressed as [10, 11]:

$$J_{Tun} = \frac{A^* T}{k_\mathrm{B}} \int_0^{U_{\max}} T(E_x) \ln\left(\frac{1 + \exp\left(-q\varsigma - E_x\right)/k_\mathrm{B} T}{1 + \exp\left(-q\varsigma - qV_R - E_x\right)/k_\mathrm{B} T} \right) dE_x \tag{2}$$

where ζ denotes a difference between the equilibrium Fermi level and conduction bands, T – temperature, k_B – Boltzmann constant, A^* – effective Richardson constant and $T(E_x)$ is the tunneling probability calculated in this study by using the WKB approximation, because it offers an analytical solution, and it is valid for the Schottky barrier diodes [12]. The parameters ζ, A^* and $T(E_x)$ depend on the effective mass and barrier height as

$$\varsigma\left(m^*\right) = \left(k_\mathrm{B} T/q\right) \ln\left[\frac{N_C\left(m^*\right)}{N_d} \right], \tag{3}$$

$$A^*\left(m^*\right) = \frac{4\pi q k_\mathrm{B}^2 m^*}{h^3}\,, \tag{4}$$

$$T_{WKB}\left(m^*, \phi_b\right) = \exp\left[-2 \int_{x_1}^{x_2} \left(\frac{2m^*}{\hbar^2} \left(U(x) - E_x\right) \right)^{1/2} dx \right], \tag{5}$$

where N_C in Eq. (3) is the effective density of states in the conduction band and is given by

$$N_C\left(m^*\right) = 2\left(\frac{2\pi m^* k_\mathrm{B} T}{h^2} \right)^{3/2}. \tag{6}$$

In Eq. (5), $U(x)$ is the potential energy profile, for an arbitrary Schottky diode as measured with respect to the energy of the bottom of the conduction band in the bulk of semiconductor, its expression, when the barrier lowering (second term in Eq. (7)) is included, can be given by [4, 13]:

$$U\left(m^*, \phi_b\right) = \frac{q^2 N_d}{2\varepsilon_S} \left[D\left(m^*, \phi_b\right) - x \right]^2 - \frac{q^2}{16\pi\varepsilon_S x}\,, \tag{7}$$

where ε_S is the semiconductor permittivity, N_d – doping concentration and D is the depletion width that depends on the barrier height and effective mass according to

$$D\left(m^*, \phi_b\right) = \sqrt{\frac{2\varepsilon_S}{qN_d} \left[\phi_b - \varsigma\left(m^*\right) - V_R \right]}\,. \tag{8}$$

The reverse thermionic current density component J_{Therm} can be expressed as [4]

$$J_{Therm} = A^* T^2 e^{-\frac{q}{k_\mathrm{B} T}\left(\phi_b - \Delta\phi_b\right)} \left(e^{\frac{qV_R}{k_\mathrm{B} T}} - 1 \right), \tag{9}$$

where $\Delta\phi_b$ is the barrier lowering due to the image force lowering effect, which is given by [14]:

$$\Delta\phi_b\left(m^*, \phi_b\right) = \left\{ \frac{q^3 N_d \left[\phi_b - \varsigma\left(m^*\right) - V_R \right]}{8\pi^2 \varepsilon_S^3} \right\}^{1/4}. \tag{10}$$

The values of the higher current densities at high reverse bias voltages can spread the lower current density values at low reverse bias voltages by many orders of magnitude. The least squares method that use the sum of the absolute differences between the measured (J_i^{ex}) and theoretical (J_i^{Th}) values is dominated by the higher current densities, and the contribution of lower current densities is very little. So, the least squares method that use the sum of the relative differences is the best choice, because all data will contribute approximately the same amount of relative error S that must be minimal. This new criterion was proposed for the first time by Osvald [15] for determining the Schottky barrier diode parameters from forward *I–V* characteristics.

$$S = \sum_{i=1}^{N} \left(\frac{J_i^{ex} - J_i^{Th}}{J_i^{Th}} \right) = 0\,. \tag{11}$$

Performing the partial derivative of S for two variables (effective mass m^* and barrier height ϕ_b), we can find a system of two nonlinear equations with two variables: m^* and ϕ_b.

$$\begin{cases} f_1\left(m^*, \phi_b\right) = \dfrac{\partial S}{\partial m^*} = -2\displaystyle\sum_{i=1}^{N} \left(\frac{J_i^{ex}}{J_i^{Th}} - 1 \right) \frac{J_i^{ex}}{\left(J_i^{Th}\right)^2} \frac{\partial J_i^{Th}}{\partial m^*} = 0 \\ f_2\left(m^*, \phi_b\right) = \dfrac{\partial S}{\partial \phi_b} = -2\displaystyle\sum_{i=1}^{N} \left(\frac{J_i^{ex}}{J_i^{Th}} - 1 \right) \frac{J_i^{ex}}{\left(J_i^{Th}\right)^2} \frac{\partial J_i^{Th}}{\partial \phi_b} = 0 \end{cases} \tag{12}$$

To extract the parameters of SBDs, namely: the effective mass and barrier height, from the nonlinear system presented by the equation (12), a computer program based on the Newton–Raphson method was applied and well tested using the theoretical data. For more details about this method, please see Ref. [15].

3. Results and discussion

In order to extract the effective mass and barrier height from the reverse *I–V–T* characteristics obtained for *n*-4H-SiC SBDs, we used the experimental data previously published in the literature by two authors [16, 17]. The doping concentration N_D, temperatures and types of diodes are summarized in Table 1.

As we showed in our previous works [18, 19], the barrier height depends strongly on reverse bias voltage, especially for low reverse bias at low temperatures. In order to obtain the best results, we will omit to use the data that exhibit the reverse bias dependence of barrier height.

Fig. 1 shows the reverse *I–V–T* characteristics of the metal/4H-SiC SBDs (diodes D_1 and D_2) measured at different temperatures (symbols) and the fitted curves (lines) calculated by using the equation (1) with the two characterized parameters $\left(m^*, \phi_b\right)$ extracted using the optimization process.

These two extracted parameters are listed in Table 2 for two diodes D_1 and D_2. It can be seen from Fig. 1 that the experimental *I–V–T* curves totally coincide with the simulated *I–V–T* plots over the entire bias range.

Fig. 2 shows the temperature dependence of electron effective mass for both diodes D_1 and D_2. As shown in this figure, the electron effective mass tends to decrease with increasing the temperature for both diodes. This new result is in contradiction with that obtained by Wellenhofer and Rossler [7] using DFT theory for *n*-4H-SiC material.

Table 1. Some properties of SiC diodes taken from two works.

Type	Symbol	Concentration N_d (cm^{-3})	Temperature T(K)	Reference
Ni/4H-SiC	D_1	2×10^{15}	298–522	[16]
Ni_2Si/4H-SiC	D_2	3×10^{15}	302–517	[17]

Table 2. The obtained values of effective mass and barrier height for two diodes D_1 and D_2 at various temperatures.

Diode	Temperature T(K)	Effective mass (m^*/m_0)	Barrier height (eV)
D1	298	0.211	0.962
	359	0.121	1.129
	407	0.130	1.204
	465	0.090	1.321
	496	0.086	1.371
	522	0.084	1.408
D2	301	0.179	0.863
	346	0.228	0.885
	436	0.114	1.079
	476	0.112	1.104
	517	0.129	1.143

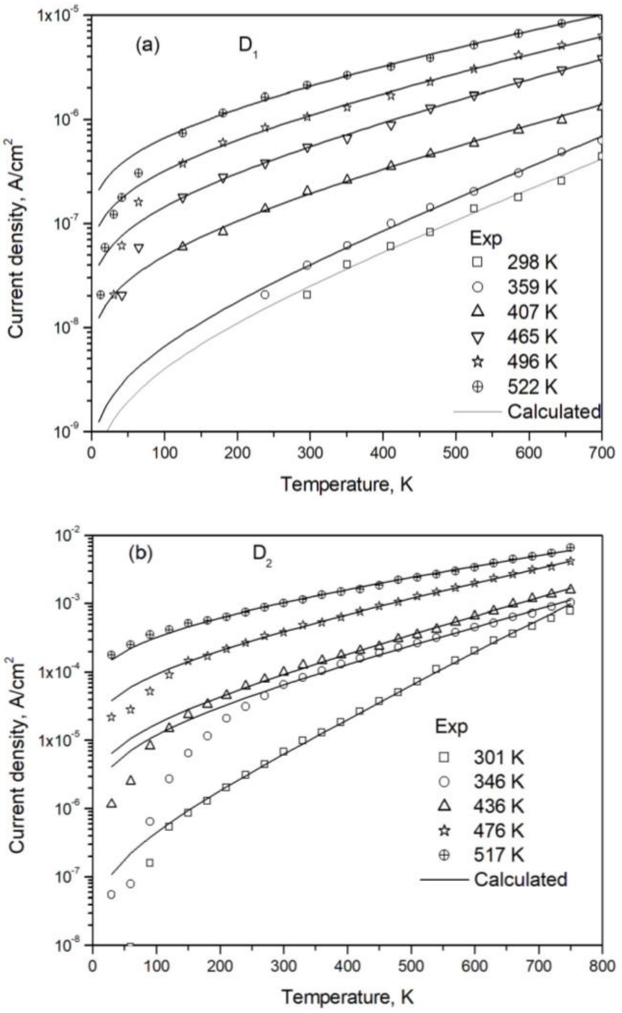

Fig. 1. Experimental reverse *I–V–T* characteristics of metal/4H-SiC Schottky diodes (symbols) and the theoretical reverse *I–V–T* characteristics (continuous lines) calculated using the extracted parameters listed in Table 1: (a) for the diode D_1 and (b) for the diode D_2.

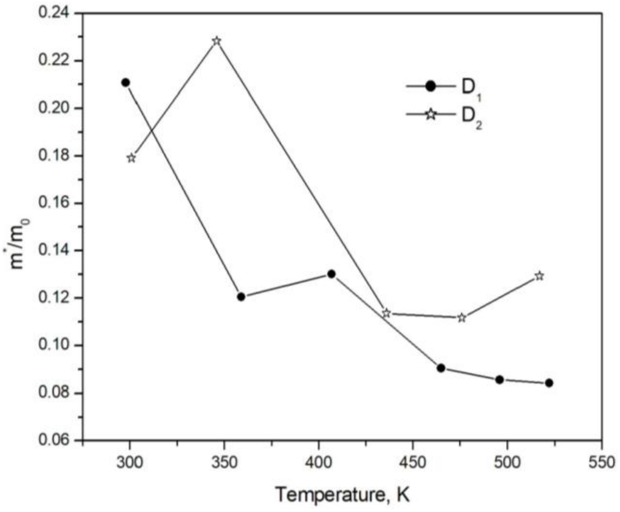

Fig. 2. Effective mass as a function of temperature for *n*-4H-SiC.

Table 3. The electron effective mass values obtained in this work with the *I–V* method and other experimental and theoretical values published previously in the literature.

$m_{\parallel}/m_0$	$m_{\perp}/m_0$ or $m_{\perp 1}/m_0$, $m_{\perp 2}/m_0$	DOS effective mass (m^*/m_0)	Reference
0.22	0.18	0.19	[20]
0.19	0.21	0.20	[21]
0.48	0.30	0.351	[22]
0.29	0.42	0.37	[23]
0.33	0.58, 0.31	0.39	[24]
0.31	0.57, 0.28	0.37	[24]
0.62	0.39, 0.13	0.31	[25]
0.31	0.62, 0.27	0.37	[26]
0.31	0.58, 0.28	0.37	[27]
		0.21, 0.18	This work

In Table 3, we summarized the values of electron effective mass extracted using the developed method at room temperature with those determined in several experiments [20-24] and calculated [24-27]. The values of $0.21m_0$ (diode D_1) and $0.18m_0$ (diode D_2) extracted using our method well agree with the experimental ones obtained by Gotz *et al.* $0.19m_0$ [20] and Lomakina *et al.* $0.20m_0$ [21].

4. Conclusions

In conclusion, we have directly determined the electron effective mass in 4H-SiC by applying the *I–V–T* technique to 4H-SiC Schottky barrier diodes. The effective mass has been found to decrease with the increase in temperature. Two values of the electron effective masses at room temperature have been experimentally determined as $m^* = 0.21m_0$ and $m^* = 0.18m_0$. Very good agreement has been found between our experimental results and the other experimental electron effective mass values $m^* = 0.19m_0$ and $m^* = 0.20m_0$ obtained using other methods.

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Визначення температурної залежності ефективної маси електрона в 4H-SiC від зворотних вольт-амперних характеристик діодів з бар’єром Шотткі на основі 4H-SiC

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Анотація. Метод профілювання струму, напруги та температури було використано для діодів з бар’єром Шотткі на основі 4H-SiC і представлено для визначення ефективної маси електрона у 4H-SiC. Виявлена ефективна маса електрона залежала від температури, вона зменшується зі збільшенням температури. Крім того, було знайдено хорошу узгодженість між отриманими нами значеннями ефективної маси електрона ($m^* = 0{,}18m_0$, $0{,}21m_0$) при кімнатній температурі та іншими значеннями, отриманими різними методами.

Ключові слова: 4H-SiC, діод Шотткі, ефективна маса електрона, I-V метод, зворотний струм, терміонна емісія, тунельний струм.