



Optical and electrical properties of SiC/p-Si heterojunction

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ABSTRACT

In this study, SiC was used to manufacture Al/SiC/p-Si/Al heterojunction structure by thermal evaporation method. X-ray diffractometry (XRD) and field emission scanning electron microscope (FE-SEM) analyses were evaluated for the characterization of semiconductor SiC layers. For the electrical characterization of the heterojunction, current-voltage (I-V), capacitance-voltage (C-V), and conductance-voltage (G-V) parameters were measured at room temperature (RT) and under various illumination conditions. Ideality factor (n) and barrier height (Φ_b) values were calculated as 1.32 and 0.85 eV in the dark and 1.22 and 0.77 eV at 100 mW/cm² illumination at RT, respectively. The results provide information indicating that Al/SiC/p-Si/Al heterojunction structure is promising for photovoltaic devices.

1 Introduction

Photovoltaic devices are mainly based on power electronic devices and Si-based devices are widely used in inverters. However, in recent years, the studies on Si devices have reached a certain intensity and have led to new searches. Silicon carbide (SiC), as a promising technology, is moving toward becoming a strong alternative in semiconductor technology with its high-efficiency applications. The reasons for this are that SiC has higher and lower voltage changes and high thermal conductivity [1]. Recently, SiC-based devices have been used to improve the performance of photovoltaic

inverters [2]. In addition, the use of SiC in the production of diodes has reduced costs. All SiC structures are notable for their properties such as high radiation and chemical tolerance, high thermal conductivity, high hardness, and high critical electric field compared to other semiconductor materials [3].

SiC and Si have a band gap energy of 3.26 and 1.12 eV, respectively [4]. The superior properties of wide band gap semiconductors offer a wide range of applications for many technological devices and enable efficient devices to be manufactured at high temperatures, powers and frequencies [5]. SiC is widely used in micro-electrical-mechanical system (MEMS)-based

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sensors [6], biomedical applications [7], aviation, radar communication, and next-generation energy vehicles [8] due to its ability to be grown on Si wafers.

With the ongoing developments in thin-film growth technology, SiC-based heterojunction photodetector structures have been produced and their results have been reported [9–12]. These heterostructures, those of the isotypes (n-n or p-p), are defined as isotype heterojunctions and those of unisotypes (n-p or p-n) are defined as anisotype heterojunctions [13] and may exhibit advantageous properties compared to metal-semiconductor-metal Schottky barriers [14]. Heterojunction photodetectors can adjust the barrier height in the contact region. Thus, they can effectively increase the charge carriers in the reverse bias region by providing the transport of photogenerated carriers. In addition, the reverse currents of heterojunction photodetectors are smaller in the high reverse bias region. Therefore, the dark currents are lower in this region. Therefore, the expansion of the depletion layer and the decrease in capacitance provide a fast response [15, 16].

Currently, heterostructured device designs composed of SiC and Si are attracting attention for advancements in photovoltaic electronics. The heterojunction structure formed between SiC and Si has better performance compared to traditional Si-based devices [17–19]. However, interest in energy-efficient and high-performance electronic devices is constantly increasing. SiC is attracting attention as an alternative to overcome the difficulties that traditional Si-based devices face at high power, temperature, and frequency [20]. The semiconductor SiC is preferred in power electronics applications due to its properties such as large critical electric field, high thermal conductivity, high electron saturation ratio, chemical inertia, and radiation hardness [21]. Therefore, it is preferred in the production of high-performance and high-efficiency device designs. Si substrates are increasingly used as substrates for SiC due to their large diameters and the necessary thermal and electrical properties [22]. Cicero et al. reported that the SiC/Si interface has a structurally stable structure, and therefore its electronic properties should be investigated [23].

This study investigates the photovoltaic properties of SiC/p-Si heterostructure produced by thermal evaporation. While there are studies on both the photovoltaic properties and the production of SiC via thermal evaporation, research investigating the properties

of photodiodes produced by thermal evaporation is limited.

2 Experimental details

In order to obtain the Al/SiC/p-Si/Al heterojunction structure, commercial p-type silicon (p-Si) wafer was used with thickness, resistance and orientation of 400 μm , 1–10 $\Omega\text{ cm}$, and (100), respectively. Initially, p-Si wafers cut in $1 \times 1\text{ cm}^2$ dimensions were degreased with methanol and acetone in an ultrasonic mixer for 3 min, respectively, according to the RCA1 procedure [24]. In order to create ohmic contact on the matte surface of p-Si, Al metal was coated in a 10^{-6} Torr pressure environment by thermal evaporation method in the NANO-VAK NVTs-400 device. In order to prevent oxidation of the produced p-Si/Al structure, it was annealed at 580 $^{\circ}\text{C}$ for 3 min in nitrogen flow. Thermal evaporation method was used for SiC deposition on the bright surface of the p-Si wafer. In order to make electrical measurements on the SiC layer, Al metal point contacts were coated with the thermal evaporation method in an area of $7.85 \times 10^{-3}\text{ cm}^2$ with the help of a shadow mask. The energy band diagram after contact between Al/SiC/p-Si is in Fig. 1a and the schematic representation of the completed Al/SiC/p-Si/Al heterojunction is in Fig. 1b. Photovoltaic measurements and current-voltage (I-V) measurements were performed with a Keithley 2400 SourceMeter and a COINC-16S-150-002 solar simulator. HP 4192A (50 Hz–13 MHz) LF impedance analyzer was used for capacitance-voltage (C-V) and conductance-voltage (G-V) measurements. Additionally, we have successfully set up a hot probe measurement system using a heating source (soldering iron) and a Keithley 2400 SourceMeter to determine the conductivity type of the synthesized SiC layer. During the measurement, a positive thermoelectric voltage/current was consistently detected at the cold probe relative to the hot probe, which clearly confirms that the thermoelectric majority carriers are holes. Consequently, the conductivity type of the SiC layer has been definitively determined to be p-type.

3 Result and discussion

3.1 Morphological characterization

SiC nanoparticles with an average diameter of approximately 20 nm were procured from Nanografi

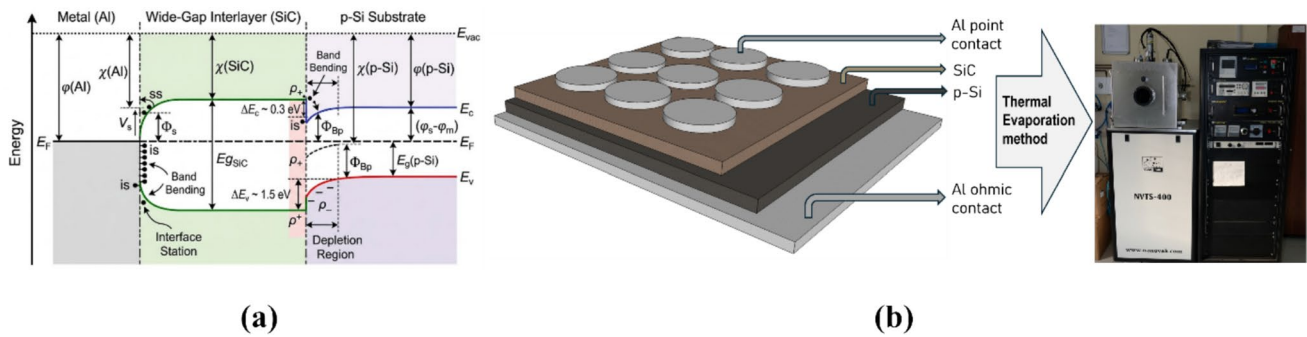


Fig. 1 **a** Energy band diagram and **b** a Schematic diagram of Al/SiC/p-Si/Al heterojunction and thin film coating system

Nanotechnology to produce an Al/SiC/p-Si/Al heterojunction structure. To evaluate the phase composition and degree of crystallinity of the SiC nanoparticles, X-ray diffraction (XRD) analysis was conducted, and the results are presented in Fig. 2. Phase identification was performed by analyzing the XRD pattern using HighScore software, which matched the experimental data with standard patterns available in the software database. The performed analysis revealed that the diffraction peaks of the synthesized SiC nanoparticles matched those of the standard reference pattern (JCPDS Card No. 29-1129) [25, 26]. Furthermore, the matching of the diffraction peaks confirmed that SiC possesses a crystal structure corresponding to the cubic crystal system. In addition, the diffraction pattern of β -SiC is characterized by strong peaks at 2θ values of 35.7° , 41.4° , 60.1° , and 71.9° , which are indexed to the (111), (200), (220),

and (311) planes of its cubic crystal structure, respectively. The existence of small amounts of 6H polytype led to the formation of weak lines [26]. The software analysis enabled finding the two-theta degree that was used to estimate the positions of 6H-SiC. Schematic illustrations of the crystal structure of β -SiC were given in Fig. 2b. These illustrations show that SiC cubic unit cell consists of 46 atoms, 56 bonds, and 14 polyhedra.

Field emission-scanning electron microscopy (FE-SEM) analysis was conducted to characterize the surface morphology of the SiC nanoparticles, providing insights into their structural and morphological properties. FE-SEM images at different magnifications are shown in Fig. 3a, b. From these images, it is understood that SiC particles are in the form of semi-microspheres consisting of nanoparticles. Note that the size of the SiC particles is in the range of 20–50 nm.

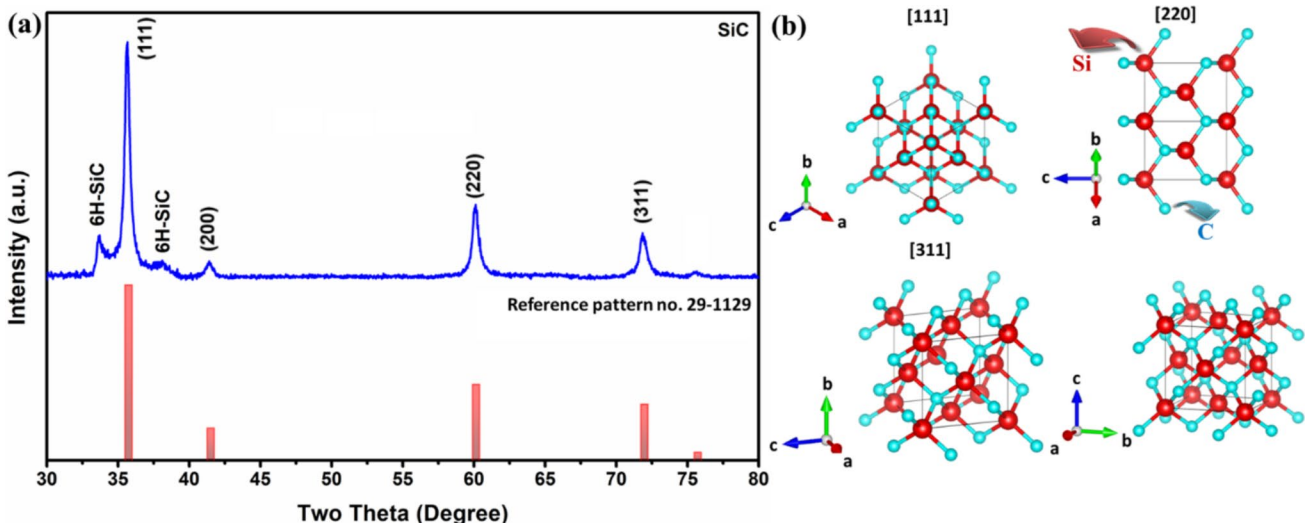


Fig. 2 The X-ray diffraction patterns and corresponding 3D crystal structures of the SiC

3.2 Electrical and optical measurements

The characterization of heterojunction structures can be determined by using I-V measurements based on the thermionic emission (TE) theory. The TE theory is obtained from the linear part of the I-V graphs in the low-voltage region in forward bias and is given by the equations [27–30];

$$I = I_0 \left[\exp\left(\frac{qV}{nkT}\right) - 1 \right] \quad (1)$$

$$I_0 = AA^*T^2 \exp\left(\frac{q\Phi_b}{kT} - 1\right) \quad (2)$$

$$J_n = A_n^*T^2 \exp\left(-\frac{q\Delta E_c}{kT}\right) \left[\exp\left(\frac{qV}{kT}\right) - 1 \right] \quad (3)$$

where q is the electron charge, k is the Boltzmann constant, T is the temperature, n is the ideality factor and I_0 is the reverse saturation current, A is the diode area, A^* is the Richardson constant, ΔE_c conduction band offset, Eq. 3 was not intended to represent a conventional Schottky barrier model. Instead, the equation was employed within the framework of thermionic emission across the heterojunction interface, where the current transport is governed by the conduction band offset (ΔE_c) between SiC and Si. Φ_b is the zero-bias barrier height (BH) [31].

$$n = \frac{q}{kT} \frac{dV}{d(\ln J)} \quad (4)$$

Ideality factor may show deviations from the ideal value of 1 [32–34]. According to TE, Φ_b is calculated as follows with the help of Eq. 2:

$$q\Phi_b = kT \ln\left(\frac{AA^*T^2}{I_0}\right) \quad (5)$$

The semi-logarithmic I-V graphs of the contact structures named as D1, D2, D3, and D4 are given in Fig. 4. In the measurements made in the $-/+2$ V range, it is seen that the D4 device is a better rectifier at room temperature (RT) in the dark. The I-V graphs of the D4 device for photovoltaic catalyzation at 100 mW/cm^2 illumination and in the dark are given in Fig. 5. The n and Φ_b values calculated with the TE equations for the Al/SiC/p-Si/Al heterojunction are 1.32 and 0.85 eV in the dark and 1.22 and 0.77 eV at 100 mW/cm^2 illumination. According to pure TE, n should be equal to 1, which is the ideal value. The deviations from ideality in the calculations can be attributed to the interface

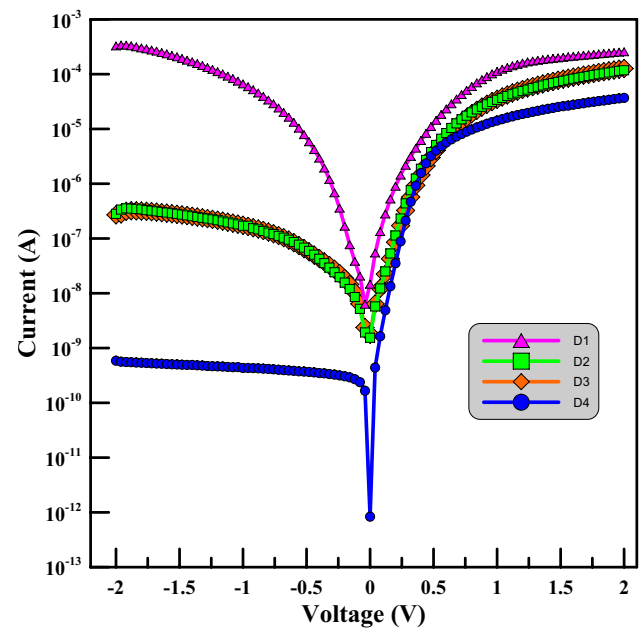
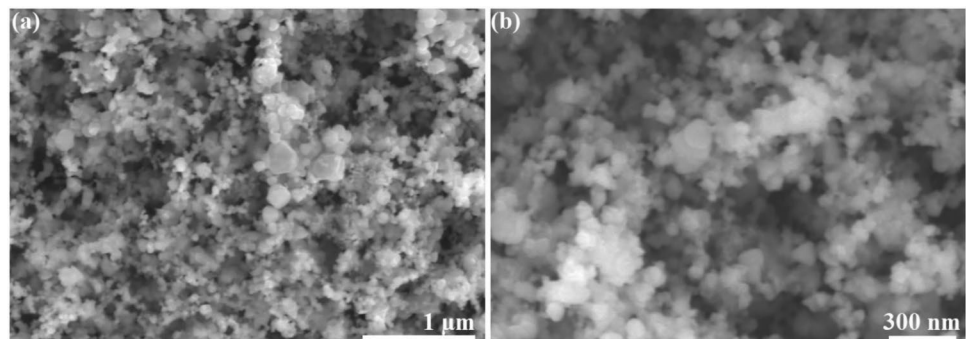


Fig. 4 Semi-logarithmic I-V plots of the Al/SiC/p-Si/Al heterojunction measured from various point contacts at RT in the dark

Fig. 3 The FE-SEM images of SiC at various magnifications



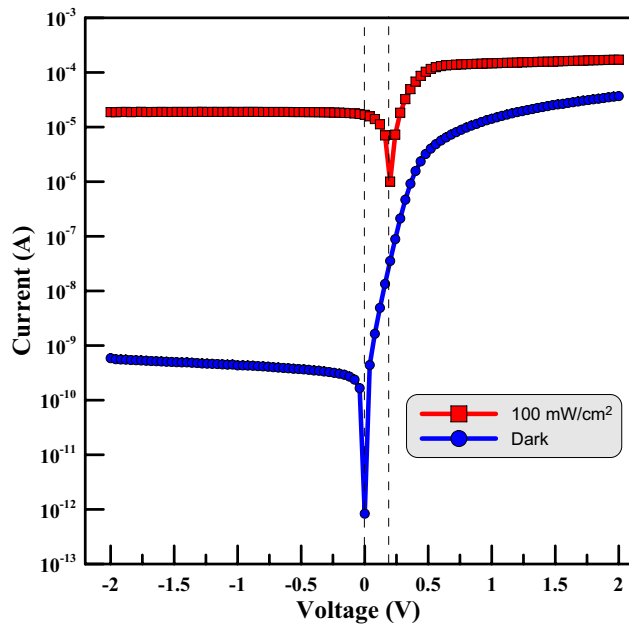


Fig. 5 Semi-logarithmic I–V plots of the Al/SiC/p-Si/Al heterojunctions under dark and illuminated conditions at room temperature

states [35], barrier inhomogeneity [36], series resistance (R_s) effect [37], and irregular distribution of interface charges [38]. It can also be related to the existence of interface states in the forbidden gap of the SiC/p-Si heterostructure. Various results obtained in the calculations may be due to the interface conditions of the SiC/p-Si heterojunction, heterointerface inhomogeneities, series resistance effect, tunneling factor, and inhomogeneities of carrier charges at the interface [36]. However, in highly mismatched systems, a dense network of mismatched dislocations can be found in the SiC/p-Si interface layers depending on the thickness. The interactions between the interface and dislocations should be taken into account [39]. High lattice mismatch between covalent materials at semiconductor device interfaces can also be decisive [40].

Figure 5 shows the changes in the semi-logarithmic I–V plots of the Al/SiC/p-Si/Al heterojunction in the dark and at 100 mW/cm² illumination. The response in illumination has given a very good response as a photodiode or photodetector. The low current in reverse bias offers high detection and high BH of high-performance photodetectors. The effect of the photodetector on the photocurrent can be explained by the internal or built-in electric field formed in the SiC/p-Si heterojunction [9]. The device behaved as a rectifier in the reverse bias region and

gave a clear and good response to the light intensity. Electron-hole pairs, which act as extra free carriers in the illuminated device, are formed and increase the current in reverse bias. The current value measured at -2 V and in darkness was 5.86×10^{-10} A, while it was measured at 1.88×10^{-5} A in the illumination. This high difference in reverse bias can be explained by the high resistance generated after illumination [41]. When the SiC/p-Si heterojunction structure is illuminated, more electrons and holes are produced and contribute to the photocurrent of the photodetector by passing through the barrier with the electric field. Therefore, the experimental data obtained by the photoelectric effect are consistent with TE [42]. It can be explained by the increase of electron-hole pairs in the SiC/p-Si hetero-interface region with increasing density and shifting toward opposite ends of the heterojunction with the applied bias [43, 44].

Moreover, as shown in Fig. 6a, the current density showed changes consistent with the TE theory, which suggests that photodiodes are affected by illumination. The semi-logarithmic I–V characteristic changes depending on the interface states or excited charge carriers at the SiC/p-Si hetero-interface. When the SiC/p-Si heterostructure is illuminated, the absorption of photons falling on the SiC/p-Si hetero interface and the p-Si substrate, depending on the light intensity, causes the formation of electron-hole pairs. [11, 45–47]. The photoresponse change (I_{on}/I_{off}) of reverse bias currents at -2 V is presented in the current–time (I–t) plot for 100 mW/cm² illumination in Fig. 6b. As can be seen, it shows stable and reproducible responses in the dark and in the illumination. The photocurrent value, which varies depending on the on and off state, is approximately in the range of 5×10^{-7} A to 1×10^{-3} A. The current remains constant as the population of free charge carriers increases with the light turn on. When the light is turned off, the current decreases and becomes fixed at a certain value. [47, 48].

The effect of the change in the semi-logarithmic I–V characteristic on the electrical parameters provides important information. Especially with the increase in the voltage in the forward bias, a bending away from linearity is observed in the graph following the linear region. The most obvious parameter of this change because of the rise in voltage is the R_s effect. Cheung functions are used for the calculations of the electrical parameters in this region [49–51]. Cheung functions are given as follows:

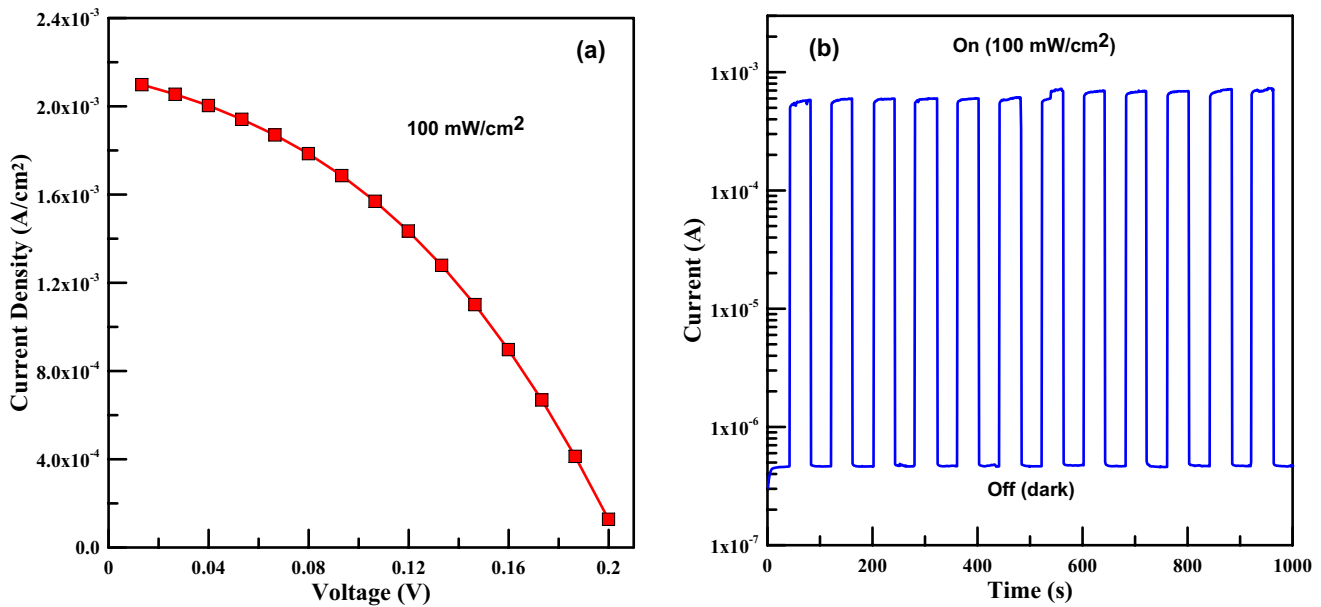


Fig. 6 **a** The current density–voltage (J–V) plot and **b** The current–time (I–t) variation of the Al/SiC/p-Si/Al heterojunction at RT in the dark

$$\frac{dV}{d(\ln I)} = \frac{nkT}{q} + IR_s \quad (6)$$

$$H(I) = n\Phi_b + IR_s \quad (7)$$

In Fig. 7, the $dV/d(\ln I)$ -I and $H(I)$ -I characteristics of the experimental Cheung functions are shown for the Al/SiC/p-Si/Al heterojunction at RT, respectively. According to Eq. 6, a straight line should be formed for the bending region deviating from linearity in the forward bias I–V plot. Therefore, R_s and n values are calculated from the slope of the $dV/d(\ln I)$ -I plot. The calculated n value is 1.28 and the R_s value is 42.03 kΩ. Using the n value calculated by Eq. 6 and the same region of the semi-logarithmic I–V plot, the $H(I)$ -I plot also gives a straight line. The Φ_b value is calculated from the point where the $H(I)$ -I plot intersects the y-axis. Also, from the slope of the graph, the second R_s value is calculated, which allows us to evaluate the consistency of the Cheung functions. The Φ_b value obtained from the second equation is 1.58 eV and the R_s value is 40.41 kΩ.

Thus, the three basic parameters that we use to evaluate the electrical characterization of photodiodes are calculated [52]. The main reason for the difference between the n and Φ_b values calculated from the TE and Cheung methods is that they are obtained from different regions of the semi-logarithmic I–V

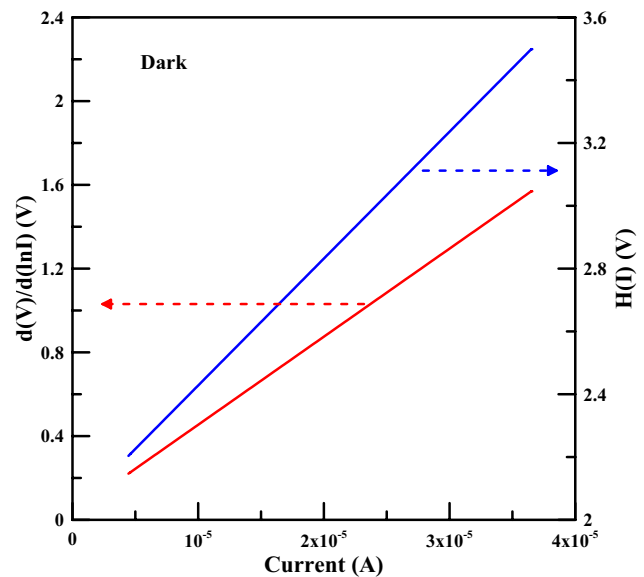


Fig. 7 Semi-logarithmic I–V plots of the Al/SiC/p-Si/Al heterojunction device obtained using Cheung functions at RT in the dark

graph in the forward bias. The TE method is calculated in the low-voltage region of the semi-logarithmic I–V graph, while the Cheung functions are calculated in the high-voltage region [33]. In addition, irrespective of how advanced the vacuum techniques

are, it is not possible to completely prevent the oxide layer at the interface [53, 54]. The high R_s values calculated from the Cheung functions can be attributed to the presence of the SiC/p-Si hetero-interface [55]. The p-type trap layer introduced by charge carriers at the hetero-interface between SiC and p-Si increases the internal electric field and changes the distribution of the electric field. [56].

Another method used in calculating electrical parameters is Norde functions [57, 58]. In this proposed method to determine the R_s value, the minimum value of the connection point in the Norde functions is used to evaluate the electrical properties associated with the device and is calculated with the following equations [59, 60]:

$$F(V) = \frac{V}{\gamma} - \left(\frac{kT}{2} \right) \ln \left(\frac{I(V)}{AA * T^2} \right) \quad (8)$$

where γ and $I(V)$ represent the smallest integer exceeding the n parameter and the current calculated from semi-logarithmic I–V measurements, respectively. The $F(V)$ – V graph of the Al/SiC/p-Si/Al heterojunction structure is given in Fig. 8. The equations Φ_b and R_s determined by the minimum of this graph are, respectively;

$$\varphi_b = F(V_0) + \frac{V_0}{\gamma} - \frac{kT}{q} \quad (9)$$

$$R_s = \frac{kT(\gamma - n)}{qI_{min}} \quad (10)$$

The calculated Φ_b value using Norde functions is 0.85 eV and R_s value is 205.8 k Ω . Cheung functions are calculated for the region where semi-logarithmic I–V graphs deviate from linearity in the forward-bias region and provide information about the series resistance effect. Norde functions, on the other hand, examine the entire forward-bias region. Therefore, the differences in calculations stem from the region in which the functions are used [51, 61, 62].

SiC has solved the problems experienced in materials such as UV single photon counting avalanche photodiodes [63] and it has been reported that the UV photodiode has a stable response property at high temperatures [18]. As a radiation detection material, its electrical and capacitance properties have improved its performance [64, 65]. In addition to the literature, our research shows that the SiC/p-Si heterostructure improves the photovoltaic characteristics in lighting.

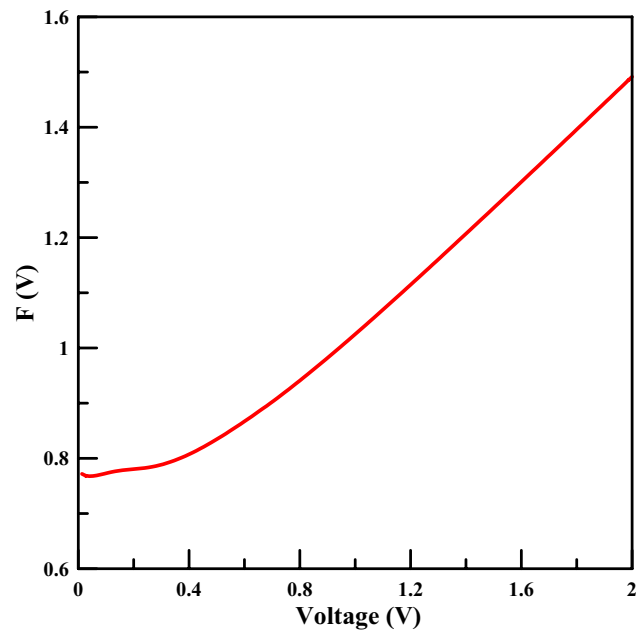


Fig. 8 The obtained Norde functions plot of the Al/SiC/p-Si/Al heterojunction device at RT in the dark

The change of C–V characteristic of Al/SiC/p-Si/Al heterojunction structure with respect to frequency is shown in Fig. 9. The C–V characteristic was performed in the range of $-/+3$ V from 1 to 5 MHz at RT in the dark. The evaluation of the capacitance and conductance status of the charge carriers at the SiC/p-Si hetero-interface provides important information for the electrical characterization of the device [66]. According to the C–V measurements in Fig. 9, the capacitance increased with increasing voltage and this increase is more evident in the forward bias region. In the reverse bias case of heterojunctions, the depletion region expands and the ionized charges decrease, increasing the rectification capacity [67]. The C–V characteristic decreased with increasing frequency. While a certain peak first occurred with the increasing voltage, it decreased afterwards. At high frequencies, it showed an almost constant character after the peak at low voltage. In Fig. 9, the capacitance value peaked in the low forward bias region for low frequencies, while it was almost constant for high frequencies. The increase in frequency caused the capacitance to decrease together with the R_s effect. The fact that a more significant decrease occurred especially between 0.5 and 3 V is due to the R_s effect being more decisive in the depletion region. While the capacitance characteristic in the contact becomes more ideal as the frequency increases, the

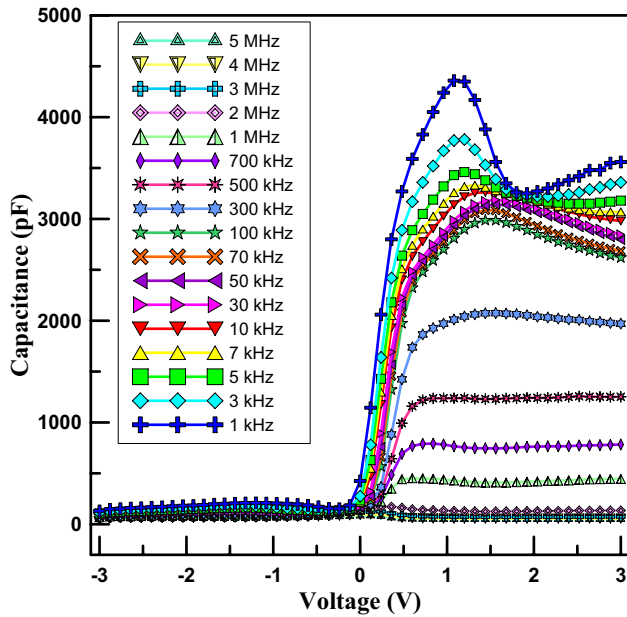


Fig. 9 Frequency-dependent capacitance–voltage (C–V) plot of Al/SiC/p-Si/Al heterojunction device at RT in the dark

difference at low frequencies can be attributed to the surface conditions and inhomogeneities in the barrier [30, 68, 69].

The G–V characteristic given in Fig. 10 increased with increasing frequency in the reverse bias region. While it increased with increasing frequency at low frequencies in the forward bias region, there were fluctuations at high frequencies. The change of the $1/C^2$ –V graph of the Al/SiC/p-Si/Al heterojunction structure in reverse bias is given in Fig. 11 for each frequency. It is seen that they have almost parallel lines at high frequencies. Diffusion potential (V_d), acceptor concentration (N_a), Fermi energy level (E_f), and barrier height ($\Phi_{b(C-V)}$) can be calculated by evaluating the change of the $1/C^2$ –V graph from the C–V characteristic measured with frequency. The electrical characterization of hetero-interfaces is calculated by the following equations: [47, 70]:

$$C^{-2} = \frac{2(V_0 + V)}{\epsilon_s \epsilon_0 q A^2 N_a} \quad (11)$$

where ϵ_s is the dielectric constant of Si, ϵ_0 is the dielectric constant of vacuum, q is the electron charge, and N_a is the acceptor concentration [71]. V_d is the diffusion potential and is calculated by the following equation:

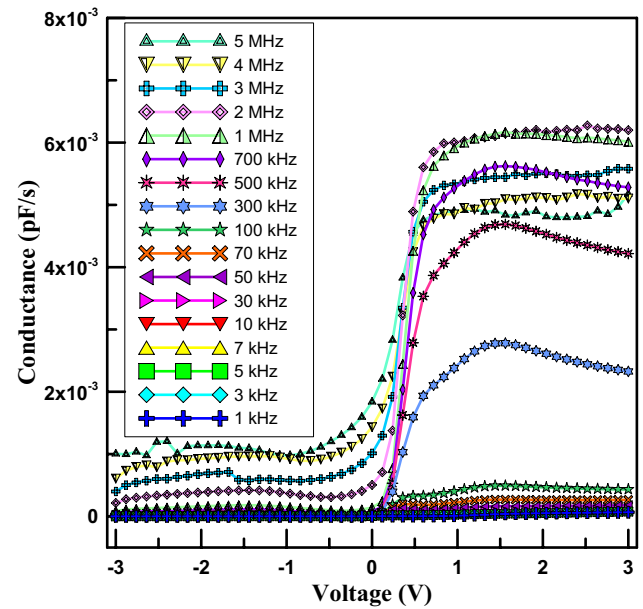


Fig. 10 Frequency-dependent conductance–voltage (G–V) plot of Al/SiC/p-Si/Al heterojunction device at RT in the dark

$$V_d = V_0 + \frac{kT}{q} \quad (12)$$

The equations for calculating other parameters obtained from the $1/C^2$ –V characteristic are as follows:

$$N_a = N_v \exp\left(\frac{E_f - E_v}{kT}\right) \quad (13)$$

$$E_f = kT \ln\left(\frac{N_a}{N_v}\right) \quad (14)$$

$$(\Phi_b)_{C-V} = \frac{V_d}{n} + E_f \quad (15)$$

The electrical parameters obtained from the C–V characteristic are given in Table 1. As can be seen from the table, the $\Phi_{b(C-V)}$ value increases with increasing frequency. The difference between the Φ_b values calculated from I–V and the $\Phi_{b(C-V)}$ values calculated from C–V is primarily explained by the difference in these measurement techniques [47, 72]. C–V calculations are an important parameter in the electrical characterization of SiC/p-Si heterojunctions. They provide useful information about changes in barrier distribution in the heterojunction.

Fig. 11 Frequency-dependent $1/C^2$ -V plot of Al/SiC/p-Si/Al heterojunction device at RT in the dark

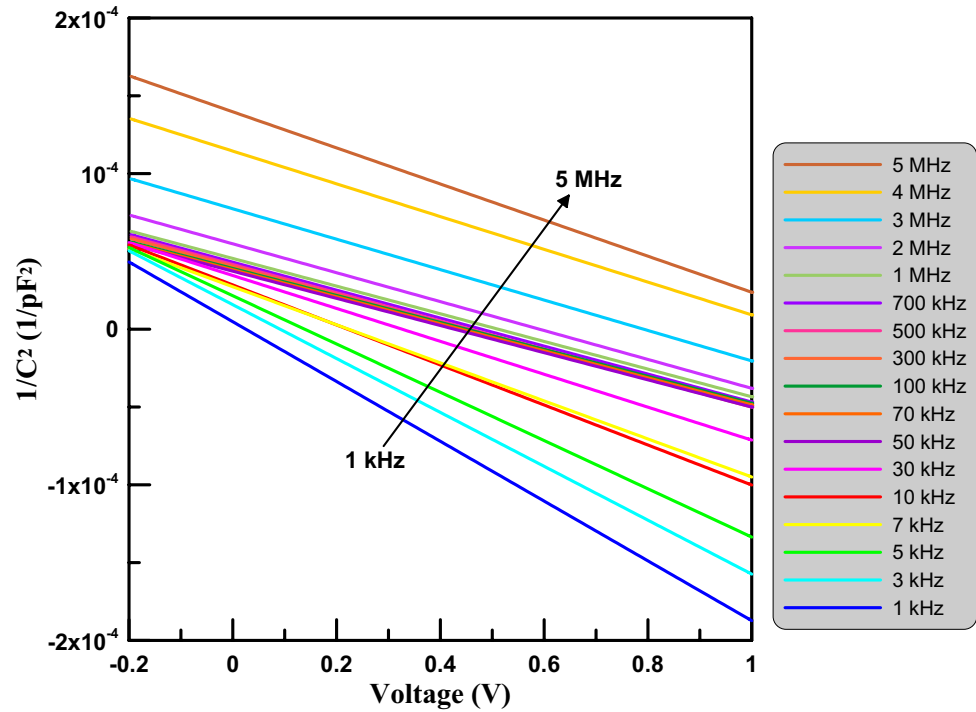


Table 1 Electrical parameters calculated from the $1/C^2$ -V characteristic of the Al/SiC/p-Si/Al heterojunction structure at various frequencies

f (kHz)	V_d (V)	N_a ($\text{cm}^{-3} \cdot 10^{15}$)	E_f (eV)	$(\Delta\Phi_b)_{C,V}(\text{eV})$ $V_d + E_f$	$(\Delta\Phi_b)_{C,V}(\text{eV})$ $(V_d/n) + E_f$
1	0.08	1.53	0.25	0.33	0.31
3	0.09	1.12	0.26	0.35	0.33
5	0.14	1.25	0.26	0.40	0.36
7	0.22	1.59	0.25	0.48	0.42
10	0.22	1.52	0.25	0.48	0.42
30	0.33	1.85	0.25	0.58	0.50
50	0.43	2.23	0.24	0.67	0.57
70	0.44	2.24	0.24	0.68	0.58
100	0.45	2.24	0.24	0.69	0.59
300	0.45	2.15	0.25	0.69	0.58
500	0.46	2.14	0.25	0.70	0.59
700	0.48	2.16	0.25	0.72	0.61
1000	0.51	2.19	0.24	0.76	0.63
2000	0.59	2.09	0.25	0.84	0.69
3000	0.79	1.99	0.25	1.04	0.85
4000	1.09	1.85	0.25	1.33	1.07
5000	1.21	1.69	0.25	1.46	1.17

The increase in N_a value with increasing frequency indicates that the interface charges of SiC/p-Si heterostructure are distributed uniformly in the band gaps of the layers at the interface states. Since the charge carriers at the hetero-interface are in thermal

equilibrium, they are at the same level as the Fermi energy in the contact region. The fact that the E_f values in the table do not change with increasing frequency also supports this situation. While the charge distribution in the Si layer is determined locally, the

charge of the SiC layer in the depletion region is determined by the space charge [73, 74]. The capacitance increases with voltage. As the depletion region in the contact increases, the ionized charge decreases and the diode capacitance increases. The decrease in capacitance as the frequency increases is due to the overcapacitance caused by the hetero-interface which can follow the alternating current signal [72, 75].

4 Conclusion

- The thermal evaporation method was used to produce Al/SiC/p-Si/Al heterojunction structure.
- For the electrical characterization of heterojunction, the results obtained from I-V characteristics were evaluated with TE, Cheung, and Norde functions. The ideality factor and barrier height obtained at RT and in the dark were calculated as 1.32 and 0.85 eV.
- In order to better understand the photoresponse properties, I-V properties were taken in the dark and at 100 mW/cm². The ideality factor and barrier height in the light and at RT were 1.22 and 0.77 eV, respectively. The current saturation of the device is quite suitable for photovoltaic applications.
- Electrical parameters obtained by taking frequency-dependent C-V measurements at RT and in the dark were evaluated. The obtained results show that the SiC/p-Si hetero-interface is promising.
- As a result, SiC/p-Si hetero-interface can be considered as an alternative model to the high lattice mismatch between covalent materials at semiconductor device interfaces where only silicon is used.

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Author contributions

Lutfi Bilal Tasyurek and Ikram Orak wrote main manuscript text Ikram Orak made measurements Adem Sarilmaz and Faruk Ozal made experimental preparations All authors reviewed manuscript.

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Data availability

No datasets were generated or analysed during the current study.

Declarations

Competing interests The authors declare no competing interests.

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