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# Modelling of Silicon Carbide (SiC) Schottky Barrier Diode for High-Temperature Terahertz Applications

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**ABSTRACT**

Silicon carbide (SiC) has emerged as a promising semiconductor material due to its wide bandgap and superior thermal conductivity, enabling robust performance in high-temperature and terahertz (THz) frequency applications. This study focuses on optimizing SiC Schottky Barrier Diodes (SBDs) for cutting-edge electronics designed to operate in extreme environments. Using advanced simulation tools like COMSOL Multiphysics and Advanced Design System (ADS), this research explores the intricate relationships between semiconductor properties, device architectures, and manufacturing techniques. Key parameters such as energy band diagrams, electric fields, doping profiles, bandgap, and Schottky barrier height are analyzed under varying conditions, including temperature and doping concentrations. Preliminary computational results demonstrate that SiC SBDs outperform their silicon counterparts, offering superior efficiency, reliability, and stability in high-temperature terahertz applications. This work highlights the potential of SiC-based devices to drive advancements in power electronics and high-frequency technologies, paving the way for their widespread use in aerospace, automotive, and industrial applications.

***Keywords:*** *Schottky barrier diode; terahertz applications; silicon carbide*

## 1. Introduction

The rising demand for dependable and efficient electronic devices that function at elevated temperatures and terahertz (THz) frequencies has propelled the advancement of novel semiconductor technologies. Terahertz technology occupies a distinctive place in the electromagnetic spectrum and is essential for applications including high-speed wireless communication, imaging, spectroscopy, sensing, and security systems. Nevertheless, the severe operational conditions in these applications—such as those seen in aerospace, automotive, and industrial monitoring propose considerable obstacles to conventional semiconductor devices [1]. The unique position of terahertz waves in the electromagnetic spectrum endows them with properties such as orientation, broad bandwidth, penetration capability, and low energy, thereby facilitating extensive research in areas including communication, radar, imaging, sensing, and security inspection. Solid-state Terahertz sources utilizing semiconductor devices have garnered significant interest in Terahertz information technology owing to their attributes, including room temperature operation, compact size, ease of integration, and excellent frequency stability [2-4]. Addressing the pressing need for durable semiconductor devices suitable for use in high-temperature environments

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and terahertz frequency applications, with a specific focus on Silicon Carbide (SiC) Schottky Barrier Diodes. SiC stands out as a promising semiconductor material due to its wide bandgap and excellent thermal conductivity properties, making it well-suited to endure high temperatures and operate efficiently at terahertz frequencies [5,6]. Traditional diodes face challenges such as high leakage currents and limited capacity to handle high reverse voltages, hence the exploration of SiC's unique properties as potential solutions. By optimizing SiC Schottky diode designs, this research aims to develop advanced electronics for heat-intensive settings, with promising implications for various technological applications.

Silicon-Based Schottky Diode are known for their fast-switching speed and low power consumption. However, conventional silicon-based electronics cannot reliably operate at temperatures exceeding 300ºC [7]. This limitation has led to exploring wide bandgap semiconductor materials such as silicon carbide for high-temperature terahertz applications [8]. Schottky diodes have reached a high level of technological maturity and are indispensable in numerous power electronics applications [9]. These diodes have found widespread use across various applications due to their unique characteristics and advantages. However, with technological advancements and the escalating demand for higher-performance diodes, conventional Schottky diodes exhibit limitations [10]. Among various semiconductor devices, the Schottky Barrier Diode (SBD) has garnered considerable attention for its potential in terahertz technology. The emergence of the Schottky Barrier Diode has significantly broadened the capabilities and applications of Schottky diode technology. It has addressed some of the limitations inherent in the standard Schottky diode, particularly concerning reverse voltage rating and leakage current. An in-depth study related to this SBD will become a necessity mainly because this device has great potential for THz applications. Therefore, a preliminary framework is needed to interpret the concepts. In this case, physical modelling is essential to effectively characterize and identify the underlying physical phenomenon demonstrated by these devices. Semiconductor device simulation based on physical models can be helpful in the development of such diodes. The advancement and verification of device simulation tools have become desirable, in comparison to statistically analysed and measured data. Empirical modelling is also required to evaluate and to extract accurate models, aside from determining the performances of linear and nonlinear circuit characteristics. With the aid of modelling, both time and cost of device fabrication and characterization can be substantially minimised [11,12].

Considering the potential insights offered by computational modelling on the behaviour of Silicon Carbide (SiC) Schottky Barrier Diodes (SBDs) in high-temperature terahertz applications, it is indicated that the analyses provided by such models will highlight the superiority of SiC SBDs over silicon-based diodes. This indication arises from the anticipation that the model will demonstrate greater efficiency and reliability for SiC SBDs, driven by their expected higher reverse voltage tolerance, reduced leakage current, and improved frequency response. These characteristics, reflective of SiC's wide bandgap, excellent thermal conductivity, and stability at elevated temperatures, underscore the significant impact of modelling in elucidating the advantages of SiC SBDs in high-temperature electronic applications.

### *1.1 Literature Review*

Silicon carbide Schottky barrier diodes have garnered considerable attention for their potential in high-temperature terahertz applications, as they exhibit robust performance at elevated temperatures and high frequencies [13]. Kou, W., *et al.,* [14] research showcased the utilization of SiC-based Schottky diodes for terahertz detection, laying the groundwork for advancements in high temperature electronics and terahertz technology. Additionally, Nandi, A., *et al.,* work provided valuable insights into the modelling of SiC Schottky diodes, offering a comprehensive understanding of the device characteristics under extreme operating conditions [15]. Furthermore, Zhang, L., *et al.,* study underscored the potential of SiC Schottky diodes for high-temperature and high frequency applications, highlighting the importance of precise modelling for predicting device performance [16]. The research conducted by various scholars has shed light on the potential applications of silicon carbide Schottky barrier diodes in the field of terahertz technology. The ability of these diodes to operate at high temperatures and frequencies makes them a promising candidate for various high-temperature electronic and terahertz applications [17,18]. Based on the findings from the research conducted by Huang, Maier, and Zhang, it is evident that silicon carbide Schottky barrier diodes hold great potential for use in high-temperature terahertz applications. The ability of these diodes to withstand extreme conditions and operate at high frequencies is a significant advantage for the development of advanced terahertz technology.

The implications of these research findings extend beyond the realm of academic inquiry, as they directly contribute to the advancement of high-temperature electronics and terahertz technology. As such, the continued exploration and refinement of silicon carbide Schottky barrier diodes are essential for unlocking their full potential in high-temperature terahertz applications. To further expand on the potential of silicon carbide Schottky barrier diodes, ongoing research and development efforts have focused on enhancing the material properties and device designs to optimize performance in high-temperature terahertz applications. The work of Huang, et. al., has provided a solid foundation for understanding the fundamental behavior of SiC Schottky diodes under extreme conditions. Building upon this foundation, recent studies have delved into the improvement of material quality, interface engineering, and device geometry to achieve superior electrical and thermal characteristics of SiC Schottky Barrier Diodes.

#### *1.1.1 Schottky barrier diode*

Schottky Barrier Diodes are semiconductor devices known for their fast-switching speed and low forward voltage drop, making them advantageous for high-frequency and power applications. These diodes have a metal-semiconductor junction, and their main advantage lies in their ability to quickly transition between the on and off states. This rapid switching capability makes them ideal for high-frequency rectification and RF applications [19,20]. Additionally, Schottky Barrier Diodes have a lower forward voltage drop compared to conventional diodes, resulting in reduced power losses and higher efficiency in power conversions [21]. However, Schottky Barrier Diodes also have some limitations. One limitation is their relatively low breakdown voltage compared to other diodes, which limit their use in high-voltage applications. Another limitation is their higher reverse leakage current compared to p-n junction diodes, which can affect circuit performance and reliability. Therefore, this study aims to offer a thorough comprehension of the characteristics of this device. Accurate modelling provided by this study is crucial for predicting and optimizing the performance of silicon carbide Schottky barrier diodes in high-temperature environments.

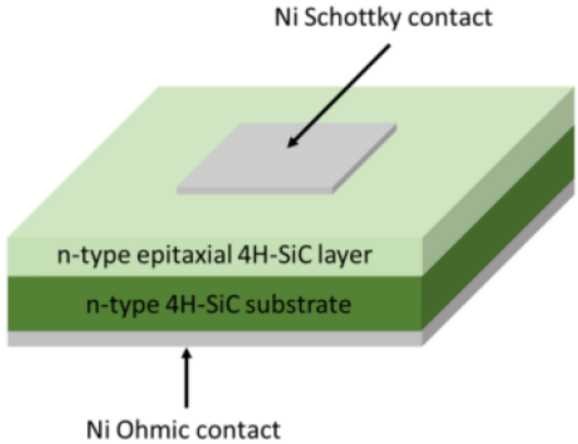


**Fig. 1.** SiC Schottky Barrier Diode Structure [19]

### *1.1.2 Physical modelling*

Physical modelling is a fundamental platform that offers insight into underlying device phenomena that are concealed beneath the device structures and fabrication processes. Trial and experimental methods are rarely used in semiconductor technology since it is expensive and time-consuming. For this reason, precise and realistic device simulations are crucial. A key component of a successful device production process is device modelling or simulation.

Device simulation allows for a thorough exploration of a device's intrinsic physical structure, including the energy band diagram, electric field, and 2-DEG density. Utilizing semiconductor device modelling, a device has been built for the model whose electronic behavior I grounded in fundamental physics. Examples of this include the thickness of the different layers that comprise the device, doping profiles, and compositions of epitaxial layers. Device simulation and device structure definition may precisely reproduce DC and RF output characteristics when the right materials are used. This makes it possible to predict device performance further, which could lead to higher-quality devices. This is especially true for THz applications, where even a tiny change in a parameter's value might harm the circuit design. For this reason, it is crucial to use device simulation while examining tunnel diode device behavior. Precise material properties in the model statement are necessary for physical modelling to give a true understanding of the behavior of the device. This study made use of the COMSOL Multiphysics and Advanced Design System (ADS) software tools, two robust semiconductor simulators, and microwave design systems that are available commercially.

The physical modelling of Schottky Barrier Diodes involves a complex interplay of semiconductor properties, device structures, and manufacturing processes. Recent advancements in the development of MOS Schottky diodes have focused on aspects such as insulating materials, doping effects, and novel manufacturing techniques, leading to improved device performance and expanding the range of potential applications [23]. The incorporation of oxide semiconductor thin-film materials, both p-type and n-type, has further broadened the design space, enabling the exploration of optoelectronic applications.At the core of the physical modelling of diodes lies the understanding of semiconductor dopability, a critical factor in determining the practical viability of semiconductor materials. A comprehensive model that describes semiconductor dopability and its governing material properties is essential for guiding the development of efficient and reliable diode devices.

#### *1.1.3 SiC bandgap modelling*

The accurate modelling of the bandgap of Silicon Carbide (SiC) is a critical aspect of the physical modelling of SiC-based Schottky Barrier Diodes. The wide bandgap of SiC, ranging from 2.3 eV for 3C-SiC to 3.2 eV for 4H-SiC, is a key enabler for the device's high temperature and high-voltage capabilities. Several models have been proposed to describe the bandgap of SiC as a function of various parameters, such as temperature and doping concentration. One widely used model is the Varshni equation, which expresses the temperature dependence of the bandgap:

$$E_g = E_g(0) - \frac{\alpha T^2}{\beta + T} \tag{1}$$

Where Eg is the bandgap energy, T is the absolute temperature, and α and β are material-specific parameters. Another model, the Shi-Singh model, considers the effect of doping concentration on the bandgap:

$$E_g = E_g(0) - \Gamma N^{\frac{1}{3}} \tag{2}$$

where Eg is the intrinsic bandgap, N is the doping concentration, and Γ is a material-dependent constant. These models, combined with experimental data and numerical simulations, enable researchers to accurately predict the bandgap of SiC under various operating conditions, which is essential for the design and optimization of SiC-based Schottky Barrier Diodes.

#### *1.1.4 Schottky barrier height modelling*

The Schottky barrier height is a crucial parameter in the physical modelling of Schottky Barrier Diodes, as it determines the device's key characteristics, such as forward voltage drop, reverse leakage current, and switching performance. The Schottky barrier height, ΦBn, is defined as the energy difference between the metalwork function and the semiconductor's electron affinity. It can be expressed as:

$$\Phi B = \Phi_m - X \tag{3}$$

where $\Phi_m$ is the metalwork function and X is the semiconductor electron affinity. Several models have been developed to describe the Schottky barrier height, considering various factors, such as interface states, metal-semiconductor interactions, and the image-force effect.

#### *1.1.5 Significant of modelling studies for SiC Schottky barrier diodes*

Modelling studies serve as a fundamental tool in understanding the complex behaviors of SiC SBDs. These studies employ various computational techniques, such as finite element analysis, device simulation, and material characterization, to predict device performance accurately. According to Xia *et al.,* these techniques are crucial for providing a comprehensive understanding of the electrical and thermal dynamics of SiC SBDs, which is essential for optimizing device design and performance under different operational scenarios [12]. The predictive capabilities of modelling studies are invaluable for the design and optimization of SiC SBD structures. By simulating different conditions and configurations, researchers can identify the optimal design parameters that maximize performance and efficiency. Modelling studies also allow for virtual prototyping, which significantly accelerates the development cycle and reduces the time-to-market for new SBD designs. Siddaiah *et al.,* emphasize that these approaches are critical for pushing the boundaries of SiC SBD technology and fostering innovation within the field [12].

Modelling studies also facilitate the exploration of advanced device concepts and novel material combinations. By utilizing computational models, researchers can investigate new materials and structures that could potentially enhance performance and reliability of SiC SBDs. This innovative approach not only drives technological advancements but also supports the development of more efficient and reliable power electronic systems. While modelling studies provide significant insights, their predictions must be validated with empirical data and experimental testing. This combination ensures the accuracy of the models and the practical applicability of the findings. Experimental validation is crucial for confirming the reliability and performance of the modelled devices under real-world conditions. This research will work closely with the Malaysia Nuclear Agency, which the agency will focus on the fabrication and experimentation of SiC Schottky Barrier Diodes. This collaboration will ensure that the theoretical models are thoroughly tested and validated, bridging the gap between computational predictions and practical applications.

## 2. Methodology

This study aims to investigate the correlation between the properties of Silicon Carbide (SiC) in Schottky Barrier Diodes (SBDs) and their performance in High-Temperature Terahertz (THz) applications. Specifically, the study will focus on key SiC properties, including thickness and transport mechanisms, which are crucial for optimizing the performance of SBDs in such applications.

To achieve the objectives, a comprehensive approach combining 2D/3D device modelling, simulation of the device fabrication process, and characterization of the current-voltage (I-V) and radio-frequency (RF) characteristics is employed. These tools will be used for model optimization, analysis, and validation of the device performance.

Device modelling serves as a fundamental platform for gaining insights into the underlying physical phenomena of semiconductor devices, which are often obscured by complex device structures and fabrication processes. Given the high costs and time demands associated with experimental techniques, experimental approaches are not always feasible. Therefore, accurate and reliable device simulations are essential for predicting device behavior and guiding design decisions. Device modelling plays a critical role in optimizing fabrication outcomes and ensuring the successful development of high-performance devices.

Through simulation, key internal parameters such as the energy band diagram, electric field distribution, and two-dimensional electron gas (2-DEG) density can be analyzed in detail. The device model incorporates fundamental physical principles, including the composition of the epitaxial layers, doping profiles, and layer thicknesses, to capture the electronic behavior of the device. With a well-defined device structure and proper materials input, simulations can accurately reproduce both DC and RF output characteristics, which are essential for predicting device performance and quality. This approach is particularly critical for THz applications, where even small deviations in parameter values can significantly influence the design of THz circuits. Consequently, the use of advanced device simulations is pivotal in understanding and optimizing the behavior of SiC Schottky Barrier Diodes for such high-frequency applications.

For this study, three commercial semiconductor simulation tools—SILVACO, COMSOL, and Advanced Design System (ADS)—will be employed to model, simulate, and analyze the device's performance in both DC and RF regimes.

### *2.1 Objective I: To Design and Model The SiC Schottky Barrier Diode in COMSOL MultiPhysics and/or Analytical Model in MATLAB*

In this study, the Schottky Barrier Diode (SBD) structure, incorporating the properties of Silicon Carbide (SiC) such as thickness and transport mechanisms, will be modeled and simulated. The physical modelling of these structures will be carried out using COMSOL Multiphysics and/or MATLAB, depending on the specific requirements of the simulation.

The barrier layer thickness will be systematically varied over a range from a few nanometers to several hundred nanometers to explore its influence on device performance. COMSOL Multiphysics will be employed to solve the structural, numerical, and physical models governing the SBD. This includes the resolution of key physical mechanisms associated with the device's operation.

The simulation will focus on optimizing models for various physical processes such as generation-recombination, charge transport, trapping mechanisms, and surface density effects. These optimized models will enable accurate predictions of the Schottky Barrier Diode's performance characteristics, including its electrical and thermal behaviors, under different operating conditions.

Concurrently, the electrical, optical, and thermal characteristics such as wavelength, current density, and efficiency of the Schottky Barrier Diode can be obtained. The SiC Schottky Barrier Diode material and structure, physical model and device operation will be investigated based on the fabricated studies by Abdullah *et al.,* 2018 and Ariffin, K. N. Z., 2019. Figure 2 and 3 shown the expected SiC Schottky Barrier Diode Epitaxial Layer.

EPITAXIAL LAYERS FOR SCHOTTKY BARRIER DIODE

| | |
|---|---|
| 750 nm | SiC $5.0 \times 10^{15}$ cm$^{-3}$ |
| 750 nm | SiC $3.0 \times 10^{16}$ cm$^{-3}$ |
| 750 nm | SiC $1.0 \times 10^{17}$ cm$^{-3}$ |
| 750 nm | SiC $5.0 \times 10^{17}$ cm$^{-3}$ |
| 750 nm | SiC $3.0 \times 10^{17}$ cm$^{-3}$ |
| | Si |

Epitaxial layer structures for SBDs with doping and layer thickness profiles

**Fig. 2.** SiC Schottky barrier diode epitaxial layer

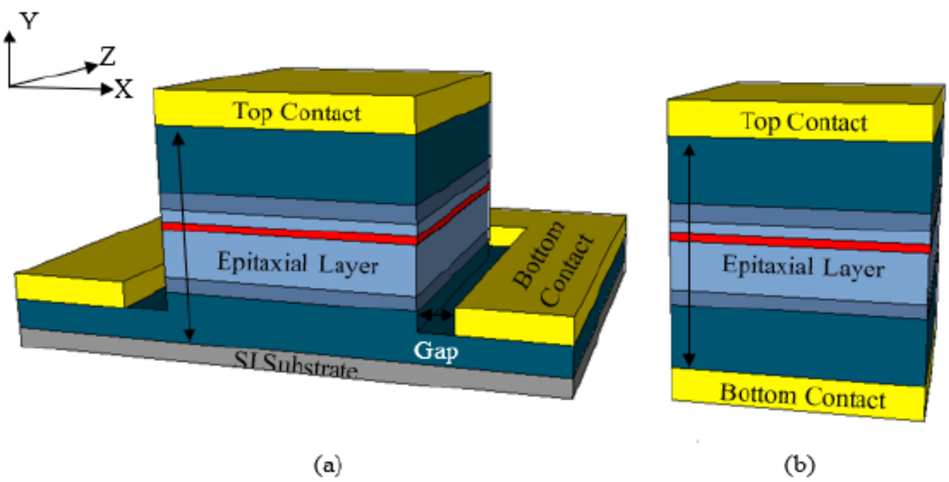


**Fig. 3.** Expected Schottky barrier diode structure (a) planar structure, and (b) back-contacted structure

### *2.2 Objective II: To Simulate The Fabrication Process of The Optimised SiC Schottky Barrier Diode Structure in COMSOL/Silvaco*

At this stage, the simulation of the SiC Schottky Barrier Diode (SBD) will be performed using COMSOL and SILVACO modelling tools. The simulation will encompass two different device structures: a planar design and a back-contacted design. The fabrication process of each structure will be modeled to assess the impact of design variations on device performance.

The output current will be measured under direct current (DC) conditions, with a voltage applied to the top contact. This will allow for the analysis of the input voltage versus leakage current characteristics, providing valuable insights into the electrical behavior and efficiency of the Schottky Barrier Diode under different structural configurations.

### *2.3 Objective III: To Analyse the Radio Frequency (RF) Performance of the SiC Schottky Barrier Diode in an Advanced Design System (ADS)*

For high-frequency applications, the performance of the SiC Schottky Barrier Diode (SBD) will be predicted through RF simulation. This approach serves as a valuable tool for extracting key parameters that are essential for the design of subsequent circuit applications.

Empirical modelling of the SiC Schottky Barrier Diode will be conducted to investigate the device's performance, focusing on both intrinsic and extrinsic parameters derived from high-frequency S-parameter data. The model will be utilized for data validation by comparing the simulated S-parameters with those extracted from the device.

Intrinsic and extrinsic parameters of the SiC Schottky Barrier Diode will be obtained from S-parameters simulated using SILVACO. These simulated results will then be compared with theoretical parameters derived from experimental studies, allowing for a thorough evaluation of the model’s accuracy and predictive capability.

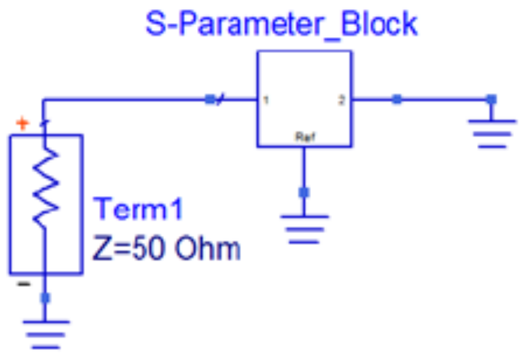


**Fig. 4.** Topology of COMSOL S-parameter dataset in ADS

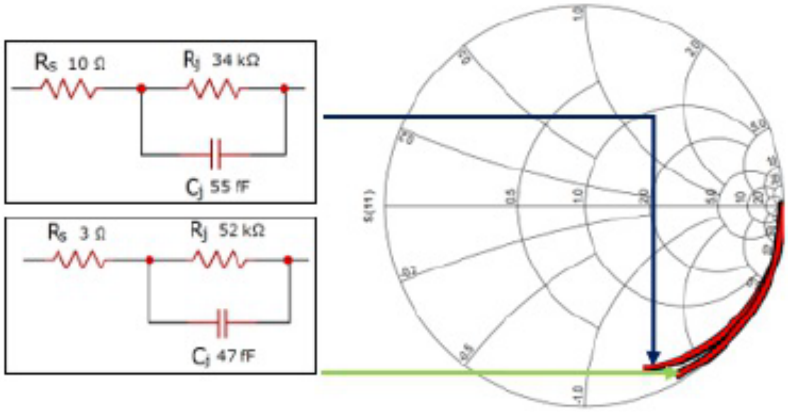


**Fig. 5.** Expected S-parameters from Smith-charts for the intrinsic parameters of SiC Schottky barrier diode

In this phase, the performance and reliability of the SiC Schottky Barrier Diode will be evaluated through extensive material characterization and the analysis of device characteristics, including DC, capacitance-voltage (C-V), and RF measurements. These analyses will enable a deeper understanding of the correlation between the device's physical properties and its output characteristics.

## 3. Conclusions

To achieve this, advanced modelling tools, including COMSOL Multiphysics and Advanced Design System (ADS), will be employed. These sophisticated simulation platforms are integrated into the study to facilitate a comprehensive understanding of the underlying device physics and their influence on the device's output performance. By utilizing these tools, the research aims to establish a clear link between the physical behavior of the device and its measured characteristics.

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