# Modeling and Bulk Characterization of 4HSIC Radiation Detector in Sentaurus TCAD Simulation Environment

Garba I. I[1], Nasiru R[2,] Abubakar Y. M[2], Shehu U[3]

[1]Physics with Electronics Department,
Federal University
Birnin Kebbi

[2] Physics Department
Ahmadu Bello University,
Zaria

[3] Metallurgical and Materials Engineering Department,
Ahmadu Bello University,
Zaria

Email: isah.ibrahim@fubk.edu.ng

## Abstract

*This paper gives an insight into the need for radiation detection and the most commonly flexible and efficient radiation detector. It also examines bulk characteristics of 4H-SiC semiconductor radiation detector with Ni and Ti as metals for the contact. Bulk characterization of the device, including: doping concentration, electrons and holes behaviors, space charge and current densities were carried out. The modeling is conducted using Sentaurus Technology Computer Aided Design (TCAD) to examine charge transport in bulk 4HSiC material. Data obtained were further analyzed through Sentaurus visual, sentaurus Techplot and Excel to clearly determine the characteristics of the device. It is observed that when the semiconductor and metal are in contact, the Fermi-level is established where the doping concentration varied with either magnitude of the doping concentration or nature of the dopant. Similarly, Schottky and ohmic contacts and temperature effect were observed from the device characteristics which demonstrate that, the detector can withstand a temperature from the range of 100K to 700K in no fluctuating state.*

**Keywords:** bulk, doping, radiation, detector, Fermi-level, sentaurus TCAD.

## INTRODUCTION

Global challenges due to healthcare management and security as a result of radiation from different sources are very essential to the stability of the entire world. All attempts, to find solution to these global challenges are becoming inadequate as a result of social control competition across the world(IAEA, 2004).

Consequently, advancement in technology has produced steps to tackle some of the challenges through deployment of Physics principles which led to the development of radiation detector (Bell, 2015) which helps in identify the presence of radiation using a system called radiation detector. The detectors can be scintillation, gas or semiconductor radiation detectors (Ouseph, 1975; Ishikawa *et al.*, 2008a; Milbrath *et al.*, 2008).

Radiation detection is efficiently achieved using Helium Three ([3]He) (Agranovich & Maradudin, 1990). However, [3]He proved to be expensive with a limited supply. Alternatively, semiconductor radiation detectors are more available, efficient and cost effective. However, radiation detectors made of semiconductor materials exhibit an unusual behaviour (Ishikawa *et al*., 2008b), thus, affecting the energy resolution of the system, which is observed to arise from metal-semiconductor interface(Owens, 2014).

Semiconductors are materials with conduction ability between an insulator and a conductor (Colinge, 2005). They have very low resistivity to be characterized as an insulator, at the same time, very high resistance to be referred as conductors. They are generally grouped into elemental and the compound semiconductors (Owens, 2012). The elemental semiconductors are silicon (Si) and germanium (Ge) while the compound semiconductors are mostly formed from group II, III, V and VI elements of the Periodic Table. The compound semiconductors are Gallium Arsenide (GaAs), Cadmium Telluride (CdTe), Cadmium Zinc Telluride (CdZnTe), Silicon Carbide (SiC) etc (Owens, 2014).

The operation of semiconductor device is fundamentally based on two energy bands known as valence and conduction bands. The valence band represents a given range of energies made of bounded electrons while the conduction band represents energies due to unbounded electrons (Fiore, 2019). However, between the two, there is what is called forbidden energy (Band gap) (Colinge, 2005). The band gap is a representation of forbidden energy between valence and conduction band, it is the energy required to move an electron from the valence band to the conduction band (freeing electron from the binding energy) as demonstrated in Figure 1.
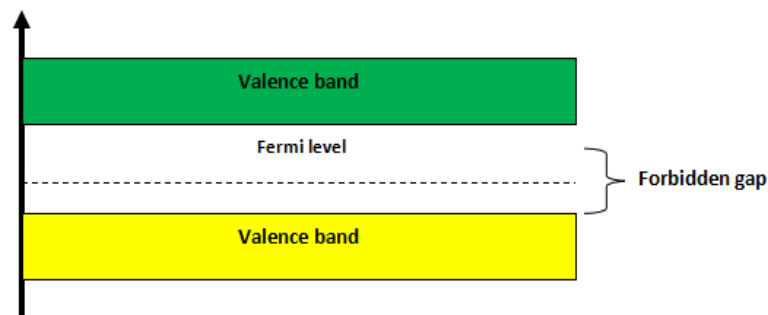


Figure 1 : Energy band of semiconductor material (Colinge, 2005)

It represents energy threshold for electron mobility whenever semiconductor materials are employed in manufacturing of a radiation detector, depending on the semiconductor material (Lutz, 1999). Most of the electronic devices are products of semiconductor materials and metals (Bell *et al*., 2018). Therefore, the choice of materials for metal contact in the formation of electronic device (radiation detector) largely depends on the characteristics of the semiconductor, the metals and the area where the detector can be deployed.

In this work, Silicon Carbide is chosen as the material for the contact because of its hardness, wide band gap, high displacement threshold energy of 21.8eV and high thermal conductivity (Juvenal & Mendoza, 2013; Gerhardt, 2011). 4H-SiC was chosen because of its high electron mobility that is very essential in radiation detection applications (Juvenal & Mendoza, 2013; Wright & Horsfall, 2007). Titanium (Ti) and Nickel (Ni) are selected as the metals for contact because they are good in formation of reproducible Schottky Barrier Height values, ability to be used at elevated temperatures and excellent resistance to corrosion (Mooch, 1990).

Modeling of semiconductor devices instead of practical growth and development (fabrication) has a greater advantage. Simulation of the devices provide an insight and perspective towards possible errors and other factors that could come over after the development of the device experimentally, regardless of time and cost. Practical implementation of semiconductor device needed a series of engineering processes, wafers, well-equipped laboratory, materials and other consumables to complete the development of the process, which are quite challenging. Moreover, semiconductor device fabrication materials such as: GaN, SiC wafar and so on, that are grossly uncommon and commercially expensive. Therefore, modeling gives an alternative opportunity to implement different ideas and validate the ideas.

Consequently, Sentaurus TCAD is a robust semiconductor device simulation tool that is well-suited for modeling of a semiconductor based electronics device and is chosen for the task(Mohapatra *et al.*, 2020; Nabil *et al.*, 2020).

Accordingly, when a metal and semiconductor materials are in contact, or a p-type and n-type material forming a junction, a barrier is established at the interface (junction) which is essential to the performance of electronics device as a result of transition of holes and electrons from one material to other (Batra, 1989). The potential barrier created at the junction is important in the determination of electrical properties of the semiconductor radiation detector. Applying an external voltage to the junction in the forward biasing mode, the current flows and the Femi-level of the semiconductor pinned in to that of metal as in Figure 2(a and b) with no flow in the reversing mode, the contact is termed Schottky (rectifying in nature) (Batra, 1989; Milnes & Feucht, 1972), and is controlled by bias-dependent changes of the potential barrier height at the interface region. The Schottky current characteristic is given by:

$$I = I_o \left( exp \left( \frac{qV}{nkT} \right) - 1 \right) \tag{1}$$

Where $I_o$ is the reverse bias saturation or leakage current, $T$ is the absolute temperature, $k$ is Boltzmann's constant, $q$ is the electronic charge, $V$ is the bias voltage across the detector, and $n$ is the ideality factor.



(a)        Metal                interface        semiconductor

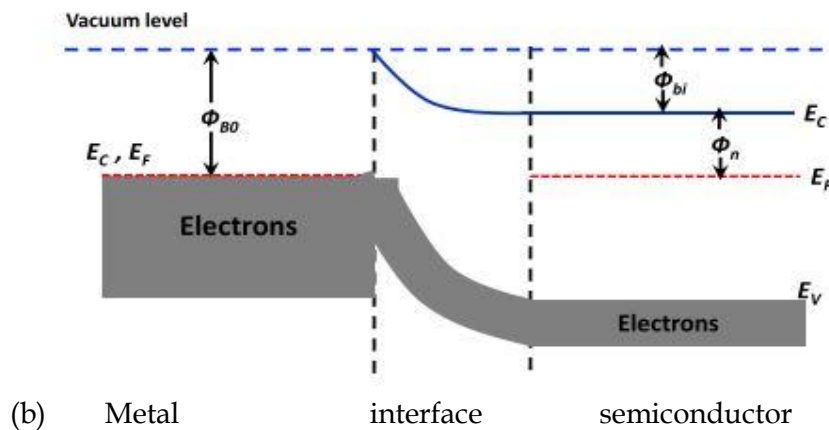(b)        Metal                interface            semiconductor
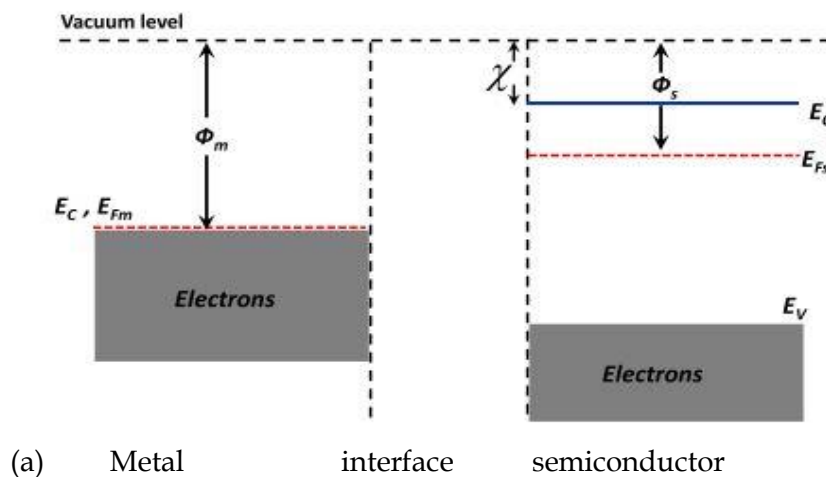
Figure 2 (a and b): Energy band in Metal and Semiconductor (Colinge, 2005)

When the work function of the metal contact matches the work function of the semiconductor, leaving no potential barrier at the interface the contact is referred to as Ohmic (Milnes & Feucht, 1972; Owens, 2012). In this case, the junction exhibits very low resistance that is independent of the applied voltage and is expressed as:

$$R = \frac{v}{I} \qquad (2)$$

The barrier height of metal-semiconductor systems depends on the metal work function ($\emptyset_m$), electron affinity of the semiconductor ($X_s$ ) and the work function of the metal ($\emptyset_s$) (Milnes & Feucht, 1972). The transmission of electron from metal to semiconductor interface that possess a barrier is expressed as

$$\emptyset_B = \emptyset_m - \emptyset_s \qquad (3)$$

If the process is reversed, the barrier becomes:

$$\emptyset_B = \emptyset_m - X_s \qquad (4)$$

Hence, the barrier established at the interface is represented by equation (4).

Furthermore, Semiconductor-Semiconductor junction N-type and P-type regions are created from the same material doped with different doping concentration on the same substrate, especially in the case of a P-N junction diode.

**METHODOLOGY**

The silicon carbide (4H – SiC) of two surfaces; silicon rich face and carbon rich face (c-face) was used. The uniformly doped epitaxial layer was used to create n-type polarity (region) that established the Schottky contact. The donor-concentration on the substrate were nitrogen active concentration of $3 \times 10^{17}$ cm$^{-3}$ and $5 \times 10^{20}$ cm$^{-3}$ in magnitude. Two metals (Ni) and Titanium (Ti) were applied as the contact metals with a rectangular shape geometry.

The Simulations were done with the aid of TCAD which is a physics-based device consisting of models for most of the Physics parameters relevant to electronic device (Nabil *et al*., 2020; synopsis, 2015). The simulations were performed in 2D and It provided surface, electrical and thermal characteristics of the device (Parent, 2014;Folkestad *et al*., 2017).

A rectangular 2D of 4H-SiC detector of dimensions 0.25μm × 0.21μm was modeled in Sentaurus TCAD environment. The device is formed as N-type and doped with Nitrogen Active Concentration of magnitude $3.0 \times 10^{17}$ establishing epitaxial region of $0.25\mu m \times 0.075\mu m$ on the Si face of the substrate with no buffer in between. The part of the substrate region is also doped with Nitrogen Active Concentration of a magnitude $5 \times 10^{20}$ cm$^{-3}$ of a

dimension $0.25\mu m \times 0.2\mu m$. Nickel of $0.25\mu m \times 0.005\mu m$ is deposited on top of the epitaxial layer and titanium at the bottom of $0.25\mu m \times 0.005\mu m$.

## Result and discussion

The characteristics of the detector is defined by mesh build in it. Hence, the mesh inside the device as shown in Figure 3 where the size of the mesh exhibit uniform and fine nature responsible for the accuracy of the detector surface structure resolution and the results as a whole. Hence, it is also observed that, the better the mesh the longer the simulation time and the better, the resolution. Therefore, the behaviour of the mesh is determined by the exchange between the simulation duration and simulation accuracy.
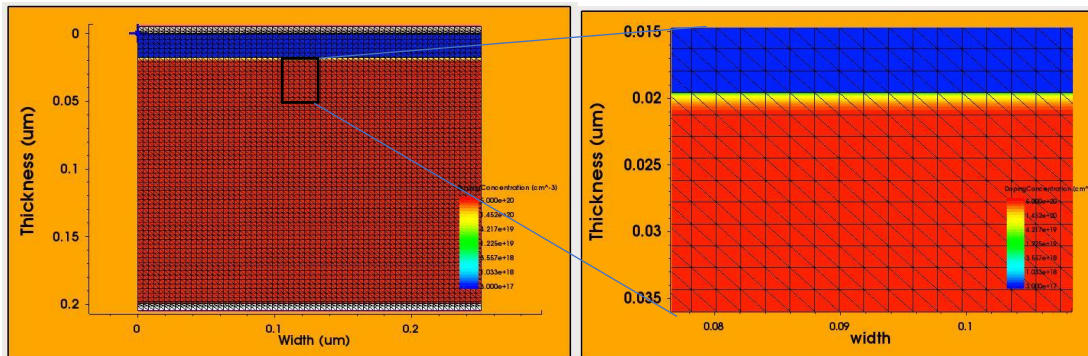


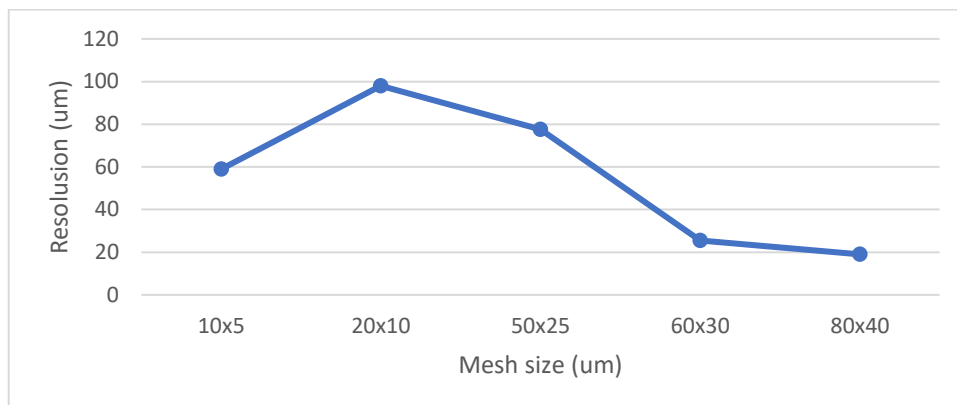Figure 3: Structure of 4HSiC device indicating the meshing



Figure 4: Meshing size ant time take for the mesh building

## Space Charge

Metal semiconductor interface formation initiate Fermi level pining which in turn initiates charge transfer of electrons from the semiconductor to the metal that led to the formation of space charge within the semiconductor. It is observed in Figure 5 that, the space charge is formed at the interface between the bulk and epitaxial regions (i.e at the region with high doping concentration and the region of lower doping concentration). This is because at these regions with two dissimilar magnitudes of doping concentration close to one another, form an important concentration gradient which leads to difference in charge carrier concentration sideways to the spatial dimension as shown in Figure 5. This reaffirms that, the more the impurities the more the space charge and vice-versa which give rise or fall of drift current across the entire detector as supported by Kwon *et al.* (2019).
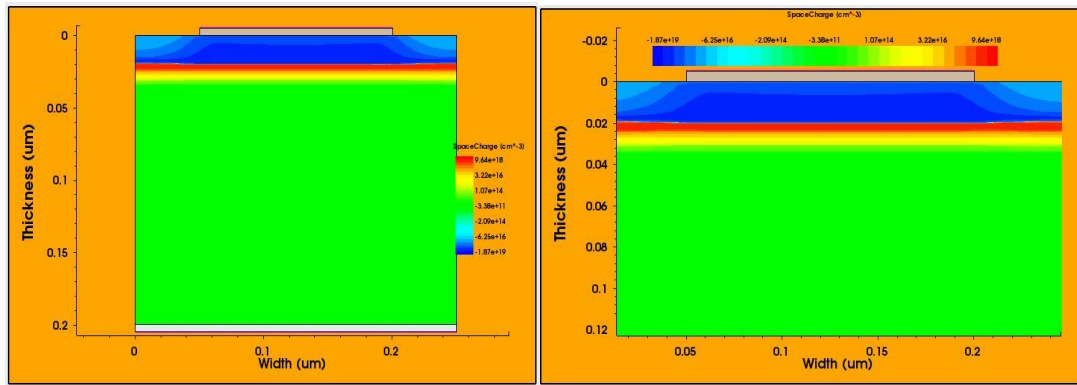
Figure 5: Detector characteristics in terms of space charge

Hence, it can also be established that, epitaxial region appeared to be schottky due to the low magnitude of spaced charge at the region. On the other hand, the high space charge region appeared to be ohmic. Therefore, the modelled device demonstrates schottky contact at the region where Ni is the contact metal due to the epi-nature of the region and ohmic at the region where Ti is the contact metal because of higher magnitude of the space charge.

Subsequently, the impact of the metal contact is visible particularly at the epitaxial region showing the field distribution from where the metal end, down to the heavily space charge presence, thus proving the presence of the metal at the top of epitaxial region as the basic component of the detector manufacturing.
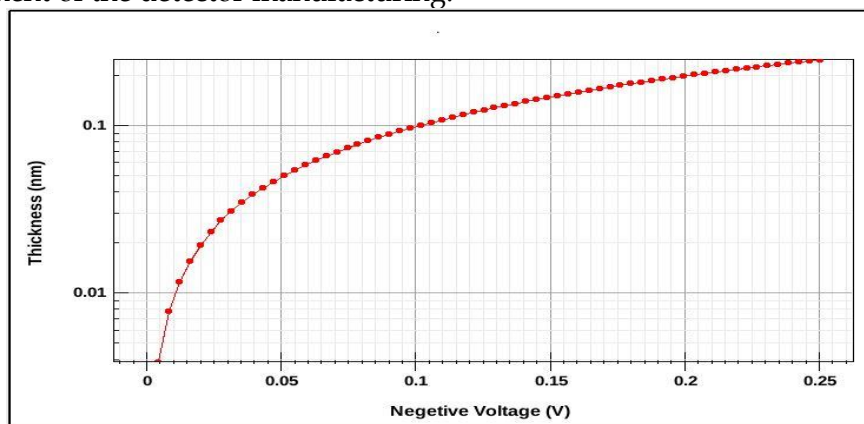


Figure 6: Space charge thickness to breakdown voltage

Similarly, it can be seen in Figure 6 that increase in the thickness of the epitaxial-layer results to increase in the breakdown voltage. This is as a result of rise in the thickness of the depletion region which in turned gives rise to the increase in electric field.

**Barrier height ideality factor and temperature**
The whole result in Figure 7 reveals that, as the temperature is increased from 100K to 700K at the interval of 50K there was a corresponding decrease in schottky barrier height and an increase in ideality factor.

The barrier height and ideality factor are very key to the current voltage characteristic that give optimum account on electrical behaviour of the device. Equation 1 and .2 clearly establish the role of ideality factor and barrier height to electrical properties of the device respectively.

$$I = I_o \left( exp \left( \frac{qV}{nkT} \right) - 1 \right) \tag{5}$$

Where $I$ is the schottky current, $I_o$ is the reverse bias saturation or leakage current, $T$ is the absolute temperature, $k$ is Boltzmann's constant, $q$ is the electronic charge, $V$ is the bias across the detector, and $n$ is the ideality factor.

$$I_o = T^2 A^0 A \exp\left(\frac{q\phi}{kT}\right) \quad\quad\quad (6)$$

Where $\phi$ is the Schottky barrier height, $A$ and $A^0$ are rectifier and Richardson constants respectively.
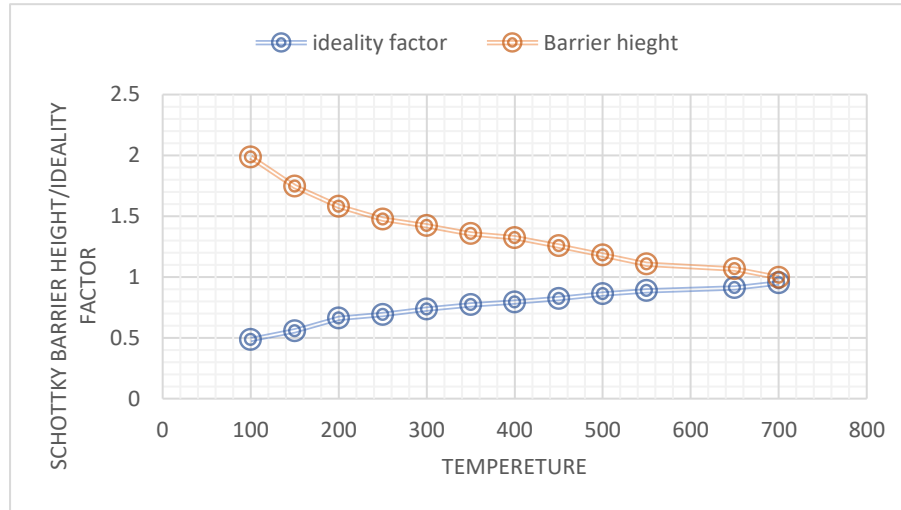


Figure 7: Characteristics of schottky barrier height and ideality factor with change in temperature

The decrease in barrier height and upswing in ideality factor with temperature is in agreement with thermionic emission theory as corroborated by Abubakar (2016) but contrary to the findings of (Bekaddour *et al*. 2023;Adoun *et al*. 2019) where they signify abnormal characteristic in the barrier height and ideality factor with increase in temperature according to their findings, the deviation from the thermionic is as a result of atomic interaction and homogeneous nature of the metal semiconductor interface.

The deviation from the thermionic emission is as a result of atomic interaction and inhomogeneous nature of the metal semiconductor interface (Bekaddour *et al*., 2023; Adoun *et al*., 2019).

**Current Voltage Characteristic**

The current voltage characteristics show the behaviors for both Ni/4H-SiC/Ti interfaces. We can observe that, the relationship proved to be ohmic at the heavily doped region as depicted in Figure 5, revealing the impact of temperature. A schottky characteristics at the lightly doped region is noticed in Figure 5 also revealing the effect of temperature. This finding has supported the claim made by Rama, *et al* (2018) where he posited that "the presence of heavily doped semiconductor layer under the metal makes the contact more ohmic".

We can now conclude that, contact between semiconductor material always prove to be schottky unless the device is subjected to another scientific or engineering process to make it ohmic. The result further demonstrated that, the current voltage behaviour depends on the generation and recombination rates in relation to the inter facial defect as earlier stated by (Karsthof *et al*., 2020).
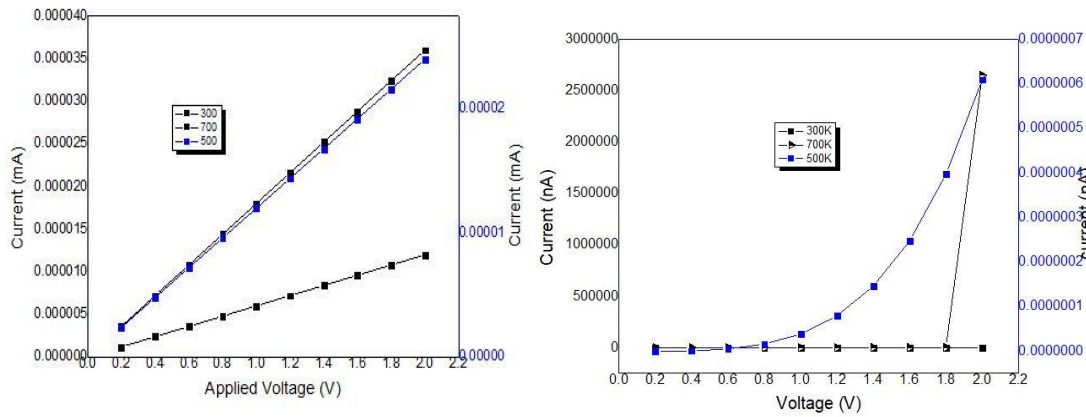
Figure 8: Current voltage characteristics.

## CONCLUSION

An electronics device (4H-SiC based Radiation Detector) is modeled using Sentaurus TCAD. Bulk characterization was conducted based on physics parameters namely: doping concentration, electrons and holes mobility, space charge, electrons and holes velocities and electric field. From the bulk characterization it is noticed that, schottky nature of the contact is formed at epitaxial region of the detector and as the doping concentration increase the space charge increased. The increase in doping concentration also leads to hole and electron mobility decreasing due to frequent carrier collisions with impurity. It also confirms that, motion of electron toward one direction and holes in the opposite direction leads to the inducement of charge to transverse within the device.

At 700K temperature the total current density exhibits abnormal behaviour which is believed to be a product of high temperature adverse effect on device.

## REFERENCES

Abubakar, Y. M. (2016). *Silicon and silicon carbide radiation detectors for alpha and neutron detection at elevated temperatures* (Issue November). University of Surrey.

Adoun, A. S., Ansouri, S. M., Hellali, M. C., Akhdar, N. L., Ima, A. H., & Enamara, Z. B. (2019). *Investigation , analysis and comparison of current-voltage characteristics for Au / Ni / GaN Schottky structure using I-V-T simulation. 37*(3), 496–502. https://doi.org/10.2478/msp-2019-0041

Agranovich, V. M., & Maradudin, A. A. (1990). *Modern Problems in Condensed Matter Sciences* (V. Editors, U. W.P. HALPERIN Evanston, Illinois, & U. L.P. PITAEVSKII Moscow (eds.); Vol. 26). Elsevier Science Publishers.

Batra, I. P. (1989). *Metallization and Interfaces NA TO ASI Series*. Plenum Press New York and London Published in cooperation with NATO Scientific Affairs Division. https://doi.org/10.1007/978-1-4613-0795-2

Bekaddour, A., Rabehi, A., & Tizi, S. (2023). Micro and Nanostructures Effect of the contact area on the electrical characteristics of the Ti / 6H – SiC ( n ) Schottky diode. *Micro and Nanostructures, 173*(August 2022), 207464. https://doi.org/10.1016/j.micrna.2022.207464

Bell, Steven J., Baker, M. A., Duarte, D. D., Schneider, A., Seller, P., Sellin, P. J., Veale, M. C., & Wilson, M. D. (2018). Comparison of the surfaces and interfaces formed for sputter and electroless deposited gold contacts on CdZnTe. *Applied Surface Science, 427*, 1257–1270. https://doi.org/10.1016/j.apsusc.2017.08.077

Bell, Steven James. (2015). *Fabrication and Characterisation of Gold Contacts on CdZnTe Radiation Detectors by* (Issue March). University of Surrey, Guildford, GU2 7XH [2] Rutherford

Appleton Laboratory, Harwell, OX11 OQX.

Colinge, J.-P. C. and C. A. C. (2005). *Physics of semicondutor devicees*. Kluwer Academic Publishers.

Fiore, J. M. (2019). *Semiconductor Devices: Theory and Application*. Mohawk Valley Community College.

Folkestad, Å., Akiba, K., Beuzekom, M. Van, Buchanan, E., Collins, P., Occo, E. D., Canto, A. Di, Evans, T., Lima, V. F., Pardiñas, J. G., Schindler, H., Vicente, M., Diaz, M. V., & Williams, M. (2017). *Nuclear Inst . and Methods in Physics Research , A Development of a silicon bulk radiation damage model for Sentaurus TCAD*. *874*(September), 94–102. https://doi.org/10.1016/j.nima.2017.08.042

Gerhardt, R. (2011). *Properties and Applications of Silicon Carbide Edited by Rosario Gerhardt*. intech. www.intechopen.com

IAEA. (2004). *Radiation , People and the enviroment*.

Ishikawa, I., Kada, W., Sato, F., Kato, Y., Tanaka, T., & Iida, T. (2008a). Development of a radiation detector based on silicon carbide. *Journal of Nuclear Science and Technology*, *45*, 489–491. https://doi.org/10.1080/00223131.2008.10875897

Ishikawa, I., Kada, W., Sato, F., Kato, Y., Tanaka, T., & Iida, T. (2008b). Development of a radiation detector based on silicon carbide. *Journal of Nuclear Science and Technology*, *45*(3), 489–491. https://doi.org/10.1080/00223131.2008.10875897

Juvenal, K., & Mendoza, Z. (2013). Fabrication and Characterization of Compact High Resolution Radiation Detectors Based On 4H-SIC N-Type Epilayer and CDZNTE. In *University of South Carolina Scholar Commons Theses and Dissertations 1-1-2013*. http://scholarcommons.sc.edu/etd/2476%0A

Karsthof, R., Wenckstern, H. Von, Zú, J., Deparis, C., & Grundmann, M. (2020). *Nickel Oxide – Based Heterostructures with Large Band Offsets*. https://doi.org/10.1002/pssb.201900639

Kwon, I. S., Kim, S. J., Asif, M., & Lee, B. W. (2019). Evaluation of electric field and space charge dynamics in dielectric under dc voltage with superimposed switching impulse. *Energies*, *12*(10). https://doi.org/10.3390/en12101836

Lutz, G. (1999). *Semiconductor Radiation Detectors Device Physics* (2nd ed.). Springer Berlin Heidelberg New York This.

Milbrath, B. D., Peurrung, A. J., Bliss, M., & Weber, W. J. (2008). Radiation detector materials: An overview. *Journal of Materials Research*, *23*(10), 2561–2581. https://doi.org/10.1557/JMR.2008.0319

Milnes, A. G., & Feucht, D. L. (1972). *Metal-Semiconductor Junctions*.

Mohapatra, S., Sahu, P. K., Rath, S., & Murty, N. V. L. N. (2020). Defect characterization and numerical modelling of single-crystal ultra-pure intrinsic -diamond. *Diamond and Related Materials*, *106*(December 2019), 107822. https://doi.org/10.1016/j.diamond.2020.107822

Mooch, W. (1990). *Electronic structure of metal-semiconductor contacts*. Kluwer Academic Publishers.

Nabil, A., Shaker, A., Abouelatta, M., Ragai, H., & Gontrand, C. (2020). *Tunneling FET Calibration Issues : Sentaurus vs . Silvaco TCAD Tunneling FET Calibration Issues : Sentaurus vs . Silvaco TCAD. November*. https://doi.org/10.1088/1742-6596/1710/1/012003

Owens, A. (2012). *Compound semiconductor series in sensors*. CRC Press Taylor & Francis Group 6000 Broken Sound Parkway NW, Suite 300 Boca Raton, FL 33487-2742 ©.

Owens, A. (2014). *Semiconductor materials and radiation detection. April 2006*. https://doi.org/10.1107/S0909049505033339

P.J.Ouseph. (1975). *Introduction to Nuclear Radiation Detectors* (G. W. Ewing (ed.)). Plenum Press • New York and London. https://doi.org/10.1007/978·1-4684-0835-5

Parent, D. (2014). Introducing TCAD Tools in a Graduate Level Device Physics Course. *IEEE TRANSACTIONS ON EDUCATION, VOL. 51, NO. 3, September 2008*, 1–6. https://doi.org/10.1109/TE.2008.916765

Rama, S., Ayyagari, U., Guido, L. J., Burgos, R. P., & Ball, A. H. (2018). *Modeling and Electrical Characterization of Ohmic Contacts on n-type GaN Master of Science Electrical Engineering Modeling and Electrical Characterization of Ohmic Contacts on n-type GaN*. Virginia Polytechnic Institute and State University.

synopsis. (2015). *Sentaurus™ Device User Guide version K* (Issue June).

Wright, N. G., & Horsfall, A. B. (2007). SiC sensors: A review. *Journal of Physics D: Applied Physics*, *40*(20), 6345–6354. https://doi.org/10.1088/0022-3727/40/20/S17