Nigerian Journal of Theoretical and Environmental Physics (NJTEP)
ISSN Print: 3026-9601
ISSN Online: 1597-9849
DOI: https://doi.org/10.62292/njtep.v4i2.2026.128
Volume 4(2), June 2026

Impact of Interfacial Layer Composition and Thickness on Schottky Diode Barrier Height and Ideality Factor

[*1]Dlama Yabwa and [2]Akpevwe Ejiro Ohworho

[1]Department of Physics, Taraba State University, Jalingo, Nigeria.
[2]Department of Physics, Delta State University, Abraka, Nigeria.

[*]Corresponding author's email: yabwa.dlama@tsuniversity.edu.ng

ABSTRACT

This work studies the effect of an interfacial layer on the electrical properties of Schottky diodes contacts formed with three metals - Chromium (Cr), Tungsten (W), and Molybdenum (Mo) - in contact with n-type Germanium (Ge). The electrical parameters studied include the saturation current (I_s), barrier height (Φ_B), ideality factor (n), and series resistance (R_s) at 300 K. Using Cheung's model and the modified Cheung's model, voltage values ranging from 0.09 V to 0.15 V were simulated, consistent with the operational conditions of the models. Results indicate that Cr/n-type Ge and Cr/interfacial-layer/n-type Ge provide the most efficient rectifying contacts, exhibiting optimal barrier heights and low series resistances. These findings highlight the significant role of interfacial layer composition and thickness in tuning Schottky diode performance.

Keywords:
Schottky diode,
Semiconductor,
Modified Cheung model,
Electrical parameters.

INTRODUCTION

Schottky diodes, also known as metal-semiconductor junctions, are formed by the intimate contact between a metal and a semiconductor (Di Bartolomeo *et al.*, 2025; Liu & Tang, 2023). These diodes play a crucial role in modern electronic devices due to their fast-switching characteristics and ability to operate at high frequencies (Somano, 2022). The type of junction formed - ohmic or rectifying - depends primarily on the doping concentration of the semiconductor. High doping levels lead to ohmic contacts, while low doping levels result in rectifying contacts (Di Natale, 2023; Paul et al., 2020). The rectifying behaviour of Schottky diodes underlies their widespread applications in high-speed electronic devices.

The metal-semiconductor interface is also critical for the performance of electronic and optoelectronic devices, as well as for integrated circuit technology (Zhao *et al.*, 2023; Gholami & Khakbaz, 2011). The electrical behaviour at this interface is commonly interpreted using the Schottky barrier concept (Liu *et al.*, 2018). As majority-carrier devices, Schottky diodes have the advantage of fast reverse recovery, as they do not store minority carrier charge, making them suitable for high-frequency applications (Kumar *et al.*, 2025).

Experimentally observed Schottky barrier heights (SBHs) often show weak dependence on the metal work function due to a high density of interface states that pin the Fermi level (Tung, 1993). Interface state models typically assume that the positive and negative charges forming the interface dipole can be individually identified and assigned energy levels (Poli *et al.*, 2020). In this work, we explicitly account for the thickness of the interfacial layer (δ) when calculating electrical parameters.

Here, we study three metals - Chromium (Cr), Tungsten (W), and Molybdenum (Mo) - in contact with an intrinsic n-type Germanium semiconductor. Using thermionic emission theory, Cheung's model, and the modified Cheung's model, we analyse how variations in the interfacial layer affect key electrical parameters: saturation current, barrier height, ideality factor, and series resistance.

Theoretical Background

Basic Thermionic theory

The Schottky barrier diode is a temperature-dependent device, a feature that is evident in its current-voltage relationship as described by thermionic emission. Current transport across the metal-semiconductor interface is activated by temperature (Gholami & Khakbaz, 2011). For a Schottky diode the relationship between the applied forward voltage and current is given by (Tung, 1993),

$$I = I_s \, exp\left(\frac{qV}{nkT}\right)\left[1 - exp\left(\frac{-qV}{kT}\right)\right] \qquad (2)$$

or

$$I = Is\, exp\left[\frac{qV}{kT}\right] \quad (3)$$

where n (=1) is the ideality factor, q is the electronic charge, k is the Boltzmann's constant, T is the absolute temperature in Kelvin, and I_s is the saturation current expressed as

$$I_s = AA^{\bullet}T^2\, exp\left(\frac{-q\Phi_B}{kT}\right) \quad (4)$$

where A is the effective diode area, A^* is the effective Richardson constant that varies from one semiconductor to the other, and Φ_B is the barrier height. A modified Equation (2) was referred to as the Richardson equation for Schottky diode given as (Yaganeh and Rahmatollahpur, 2010)

$$I = I_s\left[exp\left(\frac{q(V-IR_s)}{nkT}\right) - 1\right] \quad (5)$$

where IR_s is the voltage across the series resistance of the Schottky diode. Equation (5) was further modified and referred to as the Lieu method (for the values of$V > 3KT/q$) given as (Kudryk, *et al.*, 2014; Ahmad & Sayyad, 2009)

$$I = I_s\left[exp\left(\frac{q(V-IR_s)}{nkT}\right)\right] \quad (6)$$

From equation (4),

$$ln\, I_s = ln\left(AA^*T^2\right) - \frac{q\Phi_B}{kT} \quad (7)$$

or

$$\Phi_B = \frac{kT}{q} ln\left(\frac{AA^*T^2}{I_s}\right) \quad (8)$$

Equation (8) is the expression for the barrier height.

The Cheung – Cheung's Model

The Cheung - Cheung's model also known as Cheung's model is one of the most efficient methods for evaluating the electrical properties of Schottky diode (Gholami & Khakbaz, 2011). Using the I-V characteristics, this model has the advantage of evaluating the ideality factor, series resistance, and the barrier height.

To obtain the Cheung's model, consider equation (6)

$$ln\, I - ln\, I_s = \frac{q(V-IR_s)}{nkT} \quad (9)$$

From equation (9)

$$\frac{nkT}{q}\left(ln\, I - ln\, I_s + \frac{qIR_s}{nkT}\right) = V \quad (10)$$

$$\frac{dV}{d(ln\, I)} = \frac{nkT}{q} + IR_s \quad (11)$$

Equation (10) is the first Cheung's model used for obtaining ideality factor values, and the series resistance.

From equations (4) and (6)

$$I = AA^*T^2\, exp\left(\frac{-q\Phi_B}{kT}\right) exp\left(\frac{q(V-IR_s)}{nkT}\right) \quad (12)$$

Obtaining the natural logarithm of equation (12) gives

$$ln\, I = ln\, A\, A^*T^2 - \frac{q\Phi_B}{kT} + \frac{qV}{nkT} - \frac{qIR_s}{nkT} \quad (13)$$

Equation (13) is further simplified to give

$$V = \frac{nkT}{q} ln\left(\frac{I}{AA^*T^2}\right) + n\Phi_B + IR_s \quad (14)$$

or

$$V - \frac{nkT}{q} ln\left(\frac{I}{AA^*T^2}\right) = n\Phi_B + IR_s \quad (15)$$

One can define a function $H(I)$ such that equation (15) could be written thus

$$H(I) = V - \frac{nkT}{q} ln\left(\frac{I}{AA^*T^2}\right) \quad (16a)$$

and

$$H(I) = n\Phi_B + IR_s \quad (16b)$$

Equations (16a) and (16b) are set of Cheung's models that are used to determine the series resistance and the barrier height.

The Modified Cheung's Model

The Modified Cheung's model is derived from inserting the metal-semiconductor interfacial layer to the Cheung's Model. According to Reddy, *et al.* (2016), the introduction of an interlayer in a Schottky diode leads to an increase in the barrier height. The modified Cheung's model introduces an additional factor as a result of the inserted interfacial layer. This additional term directly impacts the diodes saturation current, I_o. Luongo, *et al.* (2017) obtained the interfacial layer-induced saturation current expression as

$$I_O = AA^*T^2\, exp\left(\chi^{1/2}\delta\right)\left(exp\left(\frac{-q\Phi_B}{KT}\right)\right) \quad (17)$$

or

$$I_O = AA**T^2\, exp\left(\frac{-q\Phi_B}{KT}\right) \quad (18)$$

where $\exp\left(\chi^{1/2}\delta\right)$is the tunneling attenuation factor.$\chi$is the mean barrier height in eV, and δ is the thickness of the interlayer and a new Richardson constant A** is defined as

$$A^{**} = A^*\exp(\chi^{1/2}\delta) \quad (19)$$

From equation (17)

$$\frac{AA^*T^2}{I_O} = exp\left(\chi^{1/2}\delta\right) exp\left(\frac{q\Phi_B}{KT}\right) \quad (20)$$

$$ln\left(\frac{AA^*T^2}{I_O}\right) = \chi^{1/2}\delta + \frac{q\Phi_B}{KT} \quad (21)$$

and $q\frac{\Phi_B}{KT} = ln\left(\frac{AA^*T^2}{I_O}\right) - \chi^{1/2}\delta$ or

$$K_B = \frac{KT}{q}\left\{ln\left(\frac{AA^*T^2}{I_O}\right) - \chi^{1/2}\delta\right\} \quad (22)$$

Equation (22) is the expression of the modified/new barrier height as a result of the introduction of interlayer. To obtain the modified series resistance in the presence of an interlayer let us consider equations (2) and (17) such that $I = AA^*T^2\, exp(\chi^{1/2}\delta)\left(exp\frac{-q\Phi_B}{KT}\right) exp\left\{\frac{q(V-IR_S)}{nKT}\right\}$

(23)

From equation (21)

$$ln\, I = ln\, A\, A^*T^2 - \chi^{1/2}\delta - \frac{q\Phi_B}{KT} + \frac{qV}{nKT} - \frac{qIR_S}{nKT} \quad (24)$$

$$\frac{qV}{nKT} = ln\, I - ln\, A\, A^*T^2 + \chi^{1/2}\delta + \frac{q}{KT}\left(\Phi_B + \frac{IR_S}{n}\right) \quad (25)$$

$$V = \frac{nKT}{q} ln\left(\frac{I}{AA^*T^2}\right) + \frac{nKT}{q}\chi^{1/2}\delta + n\Phi_B + IR_S \quad (26)$$

One can define a function F(I) such that equation (26) can be written as

$$F(I) = n\left(\frac{KT\chi^{1/2}\delta}{q} + \Phi_B\right) + IR_S \quad (27)$$

This is the modified Cheung's model equation. In this modified model, the condition that led to equation (25) still holds, and hence

$$\frac{dV}{d\ln I} = \frac{nKT}{q} + IR_S \qquad (28)$$

MATERIALS AND METHODS

This study is entirely computational, and is aimed at investigating the variation of electrical properties in Schottky diodes. Measured values of key parameters were obtained from literature, and fundamental thermionic emission equations, Cheung's model, and the modified Cheung's model were applied throughout the computational process. The methodology is structured as follows:

Procedure for Selection of Materials and Values

Choice of Metals

Selecting an appropriate metal and semi-conductor is essential for forming a good metal-semiconductor contact. Chromium (Cr), Tungsten (W), and Molybdenum (Mo) were chosen based on their work functions relative to the electron affinity of n-type Germanium. These choices ensured measured values of barrier height consistent with a rectifying Schottky contact. Values for the measured work functions of the metals and the electron affinity were obtained from relevant references. Saturation current values were in the range of microamperes (μA), suitable for evaluating diode behaviour.

Choice of Semiconductor

While most Schottky diode research focuses on extrinsic semiconductors, this study uses an intrinsic n-type Germanium (Ge). In intrinsic semiconductors, electrons and holes are generated solely by thermal excitation, providing a clear platform to investigate interfacial layer effects (Gaur & Gupta, 2011).

Selection of Temperature

Schottky diodes are thermally stable at room temperature, and all simulations were conducted at 300 K.

Choice of Voltage Range

Cheung's model is valid for voltages that satisfy its operational conditions $V > \frac{3kT}{q}$ (Kudryk *et al.*, 2014). At 300 K, voltages between 0.09 V and 0.15 V were used for all simulations.

Materials and Constants Used

The materials and constants employed in the computational process are summarized in Table 1.

Table 1: Materials and Constants Used

Metal	Work Function Φ_m(eV)	Semiconductor	Electron Affinity χ(eV)	Richardson's Constant; A^* (A cm^{-2} K^{-2})	Effective Area A(cm^2)
Chromium (Cr)	4.50	n-type Ge	4.05	112	2×10^{-4}
Tungsten (W)	4.55	-	-	-	-
Molybdenum (Mo)	4.60	-	-	-	-

Other constants:

Boltzmann's constant, $k = 1.38 \times 10^{-23}$ J K^{-1}

Electronic charge, $q = 1.602 \times 10^{-19}$ C

Computational Procedure

Barrier Height Calculation

The barrier heights were calculated using Equation (1), with measured work functions obtained from Lee *et al.* (2006) and effective diode areas from Ahmad & Sayyad (2009). Richardson constants for n-type Si from Guler, *et al.* (2009) and for n-type Ge from Mikhelashvili *et al.* (2001).

Saturation Current Calculation

Using Equation (4), saturation currents were simulated over the voltage range 0.09-0.15 V at 300 K.

Cheung's Model Analysis

i. Using Equation (11), plots of H(I) versus I were generated.
ii. Curved points were approximated with least-squares fitted straight lines Kudryk, *et al.* (2014) and Gholami & Khakbaz (2011).
iii. Series resistance (R_s) was obtained from the slope, and the ideality factor (n) from the intercept.
iv. Using Equations (16a) and (16b), barrier heightΦ_B(intercept) and another set of series R_s (slope) values were calculated similarly from a plot of H(*I*) against (*I*).

Modified Cheung's Model Analysis

i. The electrical parameters of the modified Cheung's model were obtained by considering the effects of the interfacial layer on the Cheung model using Equations (27) and (28).
ii. Plots of H(I) versus I and F(I) versus I were fitted with straight lines with $R_S(=a)$and $b\left(=\frac{KT\chi^{1/2}\delta}{q} + \Phi_B\right)$.

iii. Barrier height (Φ_B), ideality factor (n), and series resistance (R_s) were extracted from the respective equations (22, 27, and 28).

This procedure allowed a direct comparison of electrical parameters with and without the interfacial layer for all three metals in contact with n-type Ge.

RESULTS AND DISCUSSION

Eighteen graphs were generated to extract the series resistance, barrier height, and ideality factor for the three metals in contact with n-type Germanium. These included:

i. Three plots for each metal using conventional I-V characteristics and the modified I-V model.
ii. Six plots for each metal using Cheung's and modified Cheung's models.

For conciseness, six representative plots are presented here: Cr/I/n-type Ge, W/I/n-type Ge, and Mo/I/n-type Ge at 300 K (Figures 1-6).

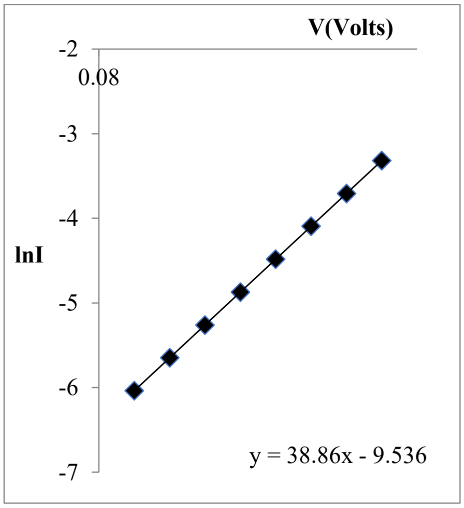

Figure 1: Graph of dv/dlnI vs I(A) for Cr/I/n-type Ge at T=300K

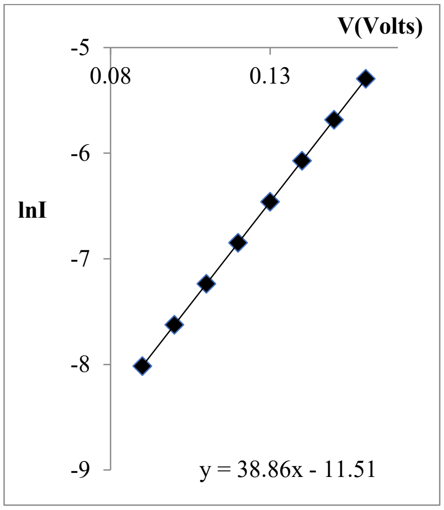

Figure 2: Graph of dv/dlnI vs I(A) for W/I/n-type Ge at T=300K

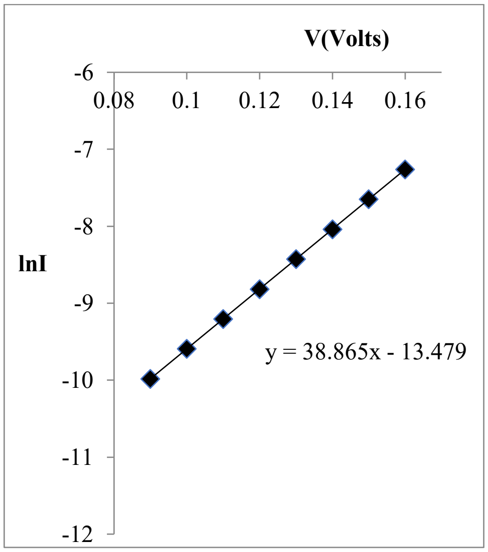

Figure 3: Graph of dv/dlnI vs I(A) for Mo/I/n-type Ge at T=300K

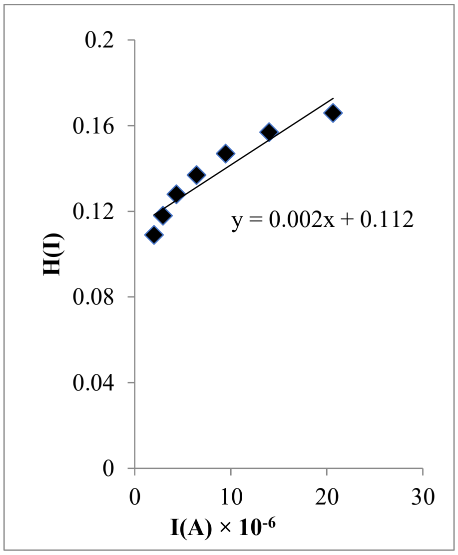

Figure 4: Graph of H(I) vs I(A) for Cr/I/n-type Ge at T=300K

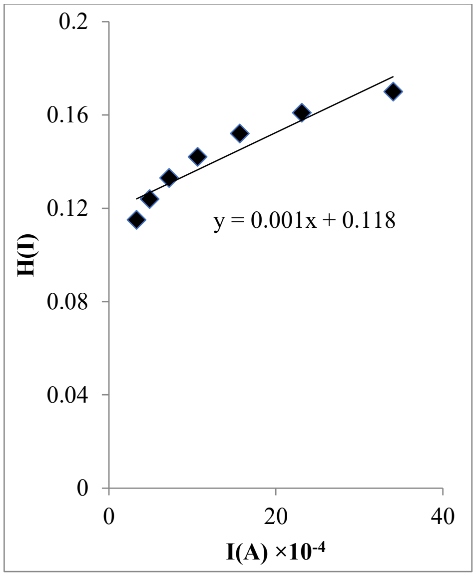

Figure 5: Graph of H(I) vs I(A) for W/I/n-type Ge at T=300K

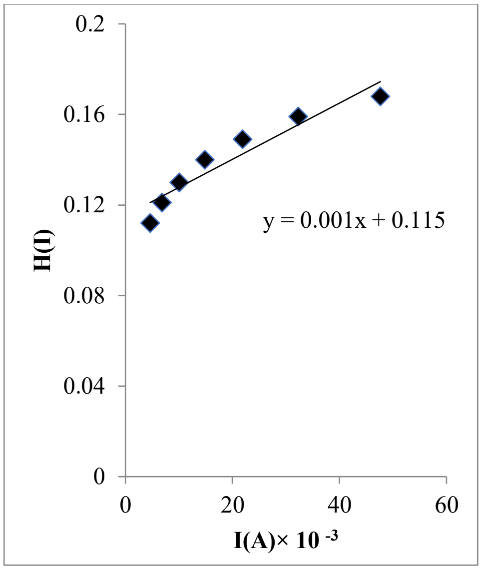

Figure 6: Graph of H(I) vs I(A) for Mo/I/n-type Ge at T=300K

Figures 1–3: dv/dlnI versus I(A) for Cr/I/n-type Ge, W/I/n-type Ge, and Mo/I/n-type Ge.
Figures 4–6: H(I) versus I(A) for the same contacts.

Electrical Parameters without Interfacial Layer

Table 2: Electrical parameters of Schottky diode without interfacial layer

Metal-Semiconductor Contact	I-V Model		Cheung's Model		
	I_o×10^{-5} (A)	Φ_B(eV)	n	R_s(Ω)	Φ_B(eV)
Cr/n-type Ge	13.090	0.6709	0.104	0.18	1.16
W/n-type Ge	1.9020	0.7857	0.078	0.43	1.53
Mo/n-type Ge	0.2733	0.9013	0.059	1.46	1.99

Saturation current (I_o) values ranged from microamperes to nanoamperes, consistent with nearly ideal rectifying behaviour (Gholami & Khakbaz, 2011).

Series resistance (R_s) increased with decreasing metal work function, from 0.18 Ω for Cr/n-type Ge to 1.46 Ω for Mo/n-type Ge.

Electrical Parameters with Interfacial Layer

Table 3: Electrical Parameters of Schottky Diode with Interfacial Layer

	Cheung's Modified Model		
Metal-Semiconductor Contact	**n**	**R_s(Ω)**	**Φ_B(eV)**
Cr/I/n-type Ge	0.051	4.40	2.2091
W/I/n-type Ge	0.071	0.62	1.6573
Mo/I/n-type Ge	0.054	2.30	2.1179

A look at Tables 2 and 3 shows that the barrier heights increased with the introduction of the interfacial layer, which is consistent with literature reports (Reddy *et al.*, 2016; Seven *et al.*, 2024; Bala, 2012).
Ideality factors remained largely constant, reflecting the constant simulation temperature of 300 K (Islam & Efeoglu, 2025).
Series resistance increased in all cases when an interfacial layer was present, most notably in Cr/I/n-type Ge (4.40 Ω). This aligns with experimental findings that interfacial layers add resistance to carrier transport.

Comparison and Interpretation

Cr/n-type Ge and Cr/I/n-type Ge consistently exhibited the best rectifying behaviour, with high barrier heights and relatively low series resistance.
The presence of an interfacial layer significantly increased the barrier height while moderately affecting the ideality factor.
W/I/n-type Ge showed a smaller increase in series resistance compared to Cr/I/n-type Ge and Mo/I/n-type Ge, indicating that the effect of the interfacial layer depends on the specific metal used.

These results confirm that the composition and thickness of the interfacial layer are key factors in tuning the electrical properties of Schottky diodes.

CONCLUSION

The study demonstrates that the presence of an interfacial layer significantly influences the electrical parameters of Schottky diodes. Using the modified Cheung's model, the barrier height and series resistance increased for all three metals (Cr, W, Mo) when in contact with n-type Germanium, thus confirming the key role of the interfacial layer in modulating diode performance.

Among the metals studied, Cr/n-type Ge and Cr/I/n-type Ge consistently exhibited the most favourable rectifying behaviour, with high barrier heights and relatively low series resistance. This indicates that Chromium, both with and without an interfacial layer, forms the best metal-semiconductor contact under the simulated conditions.

Overall, these results highlight that careful selection of metal and consideration of interfacial layer composition and thickness are crucial for optimizing Schottky diode performance, particularly in applications requiring low series resistance and high rectification efficiency.

REFERENCES

Ahmad, Z; and Sayyad, H. M (2009). Extraction of Electronic Parameters of Schottky Diode based on an Organic Semiconductor Methyl – red. *Elsevier Physica E. 41: 631 – 634.*

Bala, S. (2012), The role of interface state density in I-V characteristics of metal-semiconductor contact with interfacial layer. *International Journal of Emerging Technology and Advanced Engineering, 21(12).*

Di Bartolomeo, A., Intonti, K., Peluso, L., Di Marco, R., Vocca, G., Romeo, F., and Orhan, E. (2025). Metal-semiconductor Schottky diode with Landauer's formalism. *Nano Express*, *6(2): 1-20.*

Di Natale, C. (2023). The Metal-Semiconductor Junction. In *Introduction to Electronic Devices.* Cham: Springer Nature Switzerland - 49-82.

Gaur, K. R; and Gupta, L. S (2011). *Engineering Physics.* Dhanpat Rai Publications Ltd. New Delhi, India.

Gholami, S. and Khakbaz, M (2011). Measurement of I-V characteristics of a PtSi/p - Si Schottky diode at low temperatures. *International Journal of Electronics and Communication Engineering, 5(9): 1280-1283*.

Guler, G., Gullu, O. Karatas, S., and Bakkaloglu, O. F. (2009) Analysis of the series resistance and interface state densities in metal semiconductor structures. *Journal of Physics: Conference Series 153(2009) 012054*. https://doi.org/10.1088/1742-6596/153/1/012054

Islam, M. T., and Efeoglu, H. (2025). Temperature-Dependent I–V Characteristics of Schottky Diodes: A Comprehensive Review of Barrier Height, Ideality Factor, and Series Resistance. *Journal of Electronic Materials, 54(12):1-34*.

Jang, M. and Lee, J (2002). Analysis of Schottky Barrier Height in small contacts using a Thermionic – field Emission Model. *ETRI Journal. 24(6); 455 – 461*

Kudryk, Ya. Ya.; Shynkarenko, V. V.; Slipokurov, V. S.; Bigun, R. I.; Kudryk, R. Ya. (2014). Determination of the Schottky Barrie Height in diodes based on Au-TiB_2- n-SiC 6H from the current-voltage and capacitance-voltage characteristics

Kumar, A., Paswan, M. K., Panda, P., and Agarwal, A. (2025). A Comprehensive Study on Schottky Diode for High-Speed Application. *Proceedings of the National Academy of Sciences, India Section A: Physical Sciences*, *1-10*.

Lee, L; Sheu, K; and Lin, W; (2006): Schottky Barrier Height of metal contacts to N-type gallium nitride with low temperature grown cap layer. *Applied Physics Letters. 88. 032103: 1-3.*

Liu, Y., Guo, J., Zhu, E., Liao, L., Lee, S. J., Ding, M., and Duan, X. (2018). Approaching the Schottky–Mott limit in van der Waals metal–semiconductor junctions. *Nature*, *557(7707), 696-700.*

Liu, Z., and Tang, W. (2023). A review of Ga2O3 deep-ultraviolet metal–semiconductor Schottky photodiodes. *Journal of Physics D: Applied Physics*, *56*(9), 093002.

Luongo, G; Guibileo, F; Genorese, L; Lemmo L; Martucceillo, N; and Bartolomeo, D. A. (2017) I-V and C-V characterization of a High-Responsibility Graphene/Silicon Photodiode with Embedded MOS capacity. *Nanomaterials 7:158*

Mikhelashvili, V; Eisenstein, G. and Uzdin, R. (2001). Extraction of Schotky diodes Parameters with a bias dependent barrier height. Solid State Electronics: *45:143-148.*

Murugeshan, R; and Sivaprasath, E. (2012). Modern Physics. 16th Edition. S, Chand and Company LTD. New Delhi, India.

Nawar, A. M. (2025). Schottky diodes. In *Electric and Electronic Applications of Metal Oxides*: *207-227*. *Elsevier*.

Paul, F., Manjunatha, K. N., Govindarajan, S., and Paul, S. (2020). Single step ohmic contact for heavily doped n-type silicon. *Applied Surface Science*, *506*, 144686.

Pipings, P. and Lapeika, V. (2010). Analysis of Reverse – Bias leakage current Mechanisms in Metal/GaN Schottky diode. *Advances in Condensed Matter Physics*; 1 -7

Poli, E., Jong, K. H., and Hassanali, A. (2020). Charge transfer as a ubiquitous mechanism in determining the negative charge at hydrophobic interfaces. *Nature communications*, *11(1), 901*.

Reddy, S.; Jyoth, J.; Yuks, I; Rajagopol R; Jeong, J; Lee, S; and Choic, C. (2016) Modification of Schottky Barrier Properties of T/P-type Inp Schottky Diode by Polyniline (PANI) organic outer layer. *Journal of S/C Technology and Science. 16():1598-1657.*

Seven, E., Akay, D., Ocak, S. B., and Orhan, E. Ö. (2024). Characterization of electrical parameters in PbO/SnO2 double layer semiconductor (DLS) diodes. *Materials Science in Semiconductor Processing*, *169*, 107913.

Somano, T. T. (2022). Characteristics of Semiconductor Diode and Its Application. *International Journal of Engineering*, *6(2): 20-29*.

Tung, T. R (1993). Schottky barrier height – do we really understand what we measure? *J. Vacuum Science Technology B. 11(4): 1546 - 1552.*

Yaganeh, A. M. and Rahmatollapher, H. S. (2011). Barrier Height and Ideality Factor Dependency on identically produced small Au/P-Si Schottky Barrier Diodes. *Journals of Semiconductors, 31(7): 1-6*.

Yang, H. M; Teo, K. B. K; and Milne, I. W. (2005). Carbon nanotube Schottky diode and directionally dependent Field – effect transistor using asymmetrical Contacts. *Applied Physics Letters*. 87; 253166 (1 – 3).

Zhao, Q., Chen, P., Zheng, D., Wang, T., Castellanos-Gomez, A., and Frisenda, R. (2023). Multifunctional indium selenide devices based on van der Waals contacts: High-quality Schottky diodes and optoelectronic memories. *Nano Energy*, *108*, 108238.