A method of determining the parameters in systems with serialized Current-Voltage characteristics

R.O. Ocaya\textsuperscript{1}, F. Yakuphanoglu\textsuperscript{2}

\textsuperscript{1} Department of Physics, University of the Free State (Qwaqwa), South Africa.
\textsuperscript{2} Department of Physics, Faculty of Science, Firat University, Elazig, Turkey.

E-mail: ocayaro@ufs.ac.za

Abstract. We propose a method of determining the parameters of systems with serialized characteristics, which may suggest the existence of symmetry in the system. The method is demonstrated in extracting the parameters of a metal-semiconductor in the presence of significant series resistance, which is itself important but limits the accuracy of the existing methods in the determination of the other calculated parameters such as barrier height and ideality factor. We show the steps involved in establishing whether symmetry exists, and show that some functional interrelations between the parameters and the independent variables can readily be established. We use actual measurement data from an experimental diode and show that the results outperform the popular Cheung-Cheung approach. This general approach, therefore, represents a significant advancement in the analysis of serialized empirical data.

1. Introduction

The interface between a semiconductor and a metal interface can be a junction that is either Ohmic, or rectifying. The resulting two terminal device, termed a Schottky diode, has many constructions and applications. The electrical characteristics of Schottky diodes are described by the thermionic emission (TE) model. Over the years, methods have been developed to implicitly extract the intrinsic properties of the innate materials of the diode using the TE model [1, 2, 3, 4]. However, the results exhibit variance between methods even on the same device for two main reasons. Firstly, the parameters are interdependent, and secondly, the TE diode current is dependent on itself and on series resistance, $R_s$. The manipulation of the TE equation to extract important device parameters is generally a non-trivial exercise [5, 6]. Most methods downplays the role of the series resistance, or restrict the calculation bias range, or make restrictive simplifying assumptions, albeit with generally limited success [7, 8, 9, 10, 11, 12].

In this article, we use Lie group theory [13] to show that the extraction of important device parameters such as $R_s$ can be simplified by introducing a canonical system. Although the symmetry analysis is not new [13] it is considered by most experimental scientists to be complex and not directly applicable to aid their work. Thus it has largely remained in abstract mathematics. In short, Lie groups describe special sets of manifolds that are differentiable and have specific operators that make up what are referred to as their admissible algebras. Yet despite the fact that these groups have been studied vigorously over the years they have remained obscure to empirical fields due to their perceived high degree of abstraction. In this article we show that contrary to this general hostile view, symmetry analysis indeed has provides methods through which deep insights into practical systems can be gleaned. We propound the idea that the TE equation is a differentiable solution of some ordinary differential equation (ODE) $y'$ such that through an infinitesimal parameter, $\varepsilon$, generates any other solution, $y'$. In this article, we will use the
Figure 1. Apparent symmetry between two typical curves in an I–V characteristic. There is translation action along both axes [14].

Schottky diode to provide pragmatic examples. However, the general approach of the method will be applicable to other device I–V device characteristics. We attempt to show that the mappings between any two solutions depends on $R_s$, and trace an unique solution orbits. Finally, we suggest that the method is directly applicable to real diode data. However, in order to be pragmatic we shall follow an approach that is more illustrative than deeply theoretical. The interested reader can refer to a more rigorous discussion in our recent article [14].

2. Theory
The TE Schottky diode current $I$ can be written as [8, 15, 16]

\[ I = AA^*T^2 \exp \left( -\frac{q\phi}{kT} \right) \exp \left( \frac{qV - IR_s}{nkT} \right) \left[ 1 - \exp \left( -\frac{qV - IR_s}{nkT} \right) \right], \tag{1} \]

where $V$=applied bias, $T$=absolute temperature, $\phi$=barrier height, $n$=ideality factor, $q$=electronic charge, $k$=Boltzmann constant, $A$=diode area, and $A^*$=Richardson constant. If we set $V=x$, $I=y$, $q/kT=b$, $b/n=c$, $R_s=r$, and $AA^*T^2=(1/s)$, then Eq.1 becomes:

\[ y = \left( \frac{1}{s} \right)e^{-b\phi(x)+c(x-y)} \left[ 1 - e^{-b(x-y)} \right]. \tag{2} \]

Recently, we showed for the first time that I–V Schottky diode characteristics meet the necessary conditions of a symmetry group [14]. The first condition is the existence of a set of continuously differentiable solutions, clearly represented by each characteristic of the device. The second condition is closure, since the allowed group action, such as differentiation, on one solution gives another characteristic that is still in the group. The existence of the group action (operator) meets the third condition. We summarize these observations in the theorems that follow.

**Theorem 1** The Schottky diode I–V characteristics form a continuously differentiable group that has a unique translational, series resistance-dependent symmetry.
Proof: The body of Schottky diode literature suggest that barrier height varies almost linearly with bias \( x \) \([15, 17]\) i.e. \( \phi(x) = \Phi_0 + \alpha x \), where \( \Phi_0 \) is the zero-bias barrier height, and \( \alpha \) is a bias-coefficient. Differentiating Eq. 2 w.r.t \( x \) with \( \phi' = \alpha \) gives:

\[
y' = \frac{[(b + \alpha b - c)e^{-b(x-\gamma)} - (\alpha b - c)]e^{(x-\gamma)}}{se^{b\Phi_0} + r[c + (b - c)e^{-b(x-\gamma)}]e^{(x-\gamma)}}
\]

\[
= \frac{\theta(x,y)}{p + r\xi(x,y)},
\]

(3)

where \( p = \exp(b\Phi_0) \). A differentiable symmetry exists if the mapping \((x, y) \mapsto (\hat{x}, \hat{y})\) implies that

\[
\hat{y}' = \frac{\hat{\theta}(\hat{x}, \hat{y})}{p + r\xi(\hat{x}, \hat{y})}.
\]

(4)

This property is met only by the transformations of the form:

\[
\hat{x} = x + \delta r e, \quad \text{and} \quad \hat{y} = y + \delta e.
\]

(5)

in terms of the infinitesimal parameter \( \epsilon \). The transformations in Eq. 5 are unique if for an arbitrary tangent vector field e.g. \((\xi(x,y), \eta(x,y))\) we arrive at same symmetry in each case. The linearized symmetry condition \([18, 13, 19]\) of the ODE in Eq. 3 (i.e. \( y' = \omega(x,y) \)) is

\[
\eta_x + (\eta - \xi_x)\omega - \xi_\omega \omega^2 = \xi_\omega + \eta \omega_x,
\]

(6)

To illustrate, we choose the arbitrary but broadly applicable ansatze \((\xi, \eta) = (\alpha(x), \Gamma(y) + \gamma(x))\) and \((c_1x + c_2y + c_3, c_4x + c_5y + c_6)\) both separately result in the transformations in Eq. 5, implying the uniqueness of the transformations above. One could then consider two mappings given the two points \((x, y)\) (on Curve 1) and \((\hat{x}, \hat{y})\) (on Curve 2). In the first case, Curve 1=Curve 2. In the second case Curve 1\neq Curve 2. Consider the linearizing near-identity transformations on the \((x,y)\) plane by varying the small parameter \( \epsilon \):

\[
\hat{x} = x + \epsilon \xi(x,y) + \mathcal{O}(\epsilon^2), \quad \text{and} \quad \hat{y} = y + \epsilon \eta(x,y) + \mathcal{O}(\epsilon^2).
\]

(7)

When \( \epsilon \to 0 \), \( \xi = \delta / \delta \epsilon \) and \( \eta = \delta \hat{y} / \delta \epsilon \). In other words, they are the instantaneous rates of change of the applied bias and the current w.r.t. \( \epsilon \). We intend to transform the \((x,y)\) coordinate system with its ODE to a canonical system in which the ODE is possibly easier to solve through some inherent symmetry that may exist. There are several ways to define a canonical coordinate system \([14]\). For instance, we can define a constrained new system \((f(x,y), g(x,y))\) such that the above-mentioned conditions of the existence of a symmetry group. For instance, we can choose \( y' = \eta / \xi = 1/r \), for \( r \neq 0 \) such that the general solution is \( y = (x/r + m) \). If we assign \( m \) as the invariant axis then

\[
m = f = y - \frac{x}{r},
\]

(8)

Hence the possible canonical coordinate and transformed derivative are:

\[
(f, g) = \left( y - \frac{x}{r}, \frac{x}{\delta r} \right), \quad \frac{dg}{df} = \frac{(1/r^2)}{(-1/r + \hat{y})}.
\]

(9)

This then leads to Eq. 4. To illustrate simply, if we assume that bias does not depend on bias, then \( \alpha'(x) = 0 \), so that the transformed derivative becomes

\[
\frac{dg}{df} = \frac{1}{\delta} + \left( -\frac{r}{p\delta} \right) \left( (b - c)e^{brf} + c \right)e^{-crf}.
\]

(10)
Figure 2. Plots of the $H(I)$-I and $dV/d\ln(I)$ Cheung-Cheung functions for 40 mW/cm$^2$ in two identified linear regions i.e. Region A = 0.6-1.2V, Region B = 2.3-4.8V.

Integrating this result w.r.t $f$ gives the canonical space equivalent of Eq. 1:

$$g(f) = -\frac{f}{\delta} + \frac{1}{p\delta}\left[1 - e^{brf}\right]e^{-crf}. \quad (11)$$

The invertibility can be checked by applying $g\delta=(y - f)$ in Eq. 10 to get

$$y = \frac{1}{p}\left[1 - e^{brf}\right]e^{-crf}, \quad \text{where } f = y - \frac{x}{r}. \quad (12)$$

3. Results and discussions

3.1. Comparison with the Cheung-Cheung method

We can examine experimental I–V characteristics in the vicinity of $\varepsilon$. That is, if $\delta\varepsilon\to\Delta\varepsilon$ in Eq. 5, then $\hat{x} = x + r\Delta\varepsilon$, and $\hat{y} = y + \Delta\varepsilon$. Then finding $r$ for an experimental data set is straightforward i.e. $r=(\hat{x} - x)/(\hat{y} - y)$. One can also compensate the I–V data set for $r$ by immediately changing to the above derived canonical system i.e.

$$(x - yr)\Big|_x \equiv (V - IR)\Big|_V,$$
Figure 3. Plots obtained using the new method, in (a) both Curve 1 $\neq$ Curve 2 (40-60 mW/cm$^2$), and Curve 1 = Curve 2 (40-40 mW/cm$^2$) are plotted. Plot (b) shows the $R_s$ vs. applied bias.

since $R_s$ is then calculable at each $(V, I)$ point. The Cheung-Cheung method (CCM) [3], defined in terms of the same variables above, employs the following functions:

$$\frac{dV}{d\ln I} = R_s I + \frac{n kT}{q}, \quad \text{and} \quad H(I) = R_s I + n \Phi_b,$$

where

$$H(I) = V - \frac{n kT}{q} \ln \left( \frac{I}{A^* T^2} \right).$$

CCM therefore gives two estimates of $R_s$ which, unfortunately, can differ significantly. Additionally, the intercepts of the first and second plots respectively estimate $n$ and $\Phi_b$. Table 1 shows the results of the method on the Al/p-Si/Bi$_2$Se$_3$/Al diode under the two test cases. For the experimental diode used, $A^*=32$ A/K$^2$cm$^2$, $A=1$mm, and $T=300K$. This allows $\Phi_b$ to be calculated graphically.

Fig. 3 presents the results of the calculations using the new method. In Fig. 3(a), the calculations based on Curve 1 = Curve 2 when $P=40$ mW/cm$^2$ are practically identical to Curve 1 $\neq$ Curve 2 in all the given bias region. This means that the method can be applied with good accuracy to measurements that have only one characteristic curve. In Fig. 3(b) the series resistance varies with with applied bias $V_a$ in the forward bias region approximately according to:

$$R_s = R_0 e^{-\alpha V_a},$$

where $\alpha$ is a constant. We determined $R_0=13.2$ k$\Omega$ and $\alpha$ as shown in Table 1. Some existing literature have experimental data that support these calculations [20, 6, 21]. The compared literature results have relied on electrical and capacitance-voltage impedance measurements. Fig. 3(b) shows that diode forward current starts around 0.48V, which we suggest to indicate the built-in potential, $V_{bi}$. The barrier height can be calculated by writing Eq. 2 linearly as $\ln y=(cz+\ln w)$, where $z$ is the resistance compensated bias, and $w=(1/p)$. The ideality factor is then found from $c$, and the barrier height from the intercept given by $A^* T^2 e^{-\Phi_b}$. Table 2 summarises the results of the Cheung-Cheung method on the Al/p-Si/Bi$_2$Se$_3$/Al Schottky photo diode. The results in Table 2 suggest that resistance decreases with illumination. From a physical perspective the conductance is expected to increase with illumination i.e. the resistance decreases. This is supported by the calculated $\alpha$ results in Table 1.
Table 1. Calculated $n$ and $\Phi_b$ using new method in the two bias regions.

| $P$ (mW/cm$^2$) | Bias (0.1V-1.0V) | Bias (1.0V-4.8V) |
|----------------|------------------|------------------|
|                | $n$              | $\alpha$/V       | $\Phi_b$/eV     |
| 40 - 60$^a$    | 10.3             | -1.832           | 0.557           |
| 40 - 40$^b,c$  | 10.8             | -1.914           | 0.557           |

$^a$ Curve 1 $\neq$ Curve 2.
$^b$ Curve 1 = Curve 2.
$^c$ $\alpha = -2.22 \times 10^{-3} P - 0.41$
$^d$ $\alpha = 3.51 \times 10^{-3} P - 2.03$

Table 2. Calculated $R_s$, $n$ and $\Phi_b$ using the Cheung-Cheung method in the two identified regions.

The maximum variance 9%. Region A = 0.6-1.2V, Region B = 2.3-4.8V,

\[
dV/d\ln(I) \text{ vs } I 
\]

| $H(I)$ vs $I$ |
|---------------|
| A | B | Average |
| $n$ | $R_s$/k$\Omega$ | $R_s$/k$\Omega$ | $\Phi_b$/eV | $R_s$/k$\Omega$ | $\Phi_b$/eV | $R_s$/k$\Omega$ | $\Phi_b$/eV |
| 40 | 4.1 | 6.84 | 34.6 | 0.56 | 6.79 | 0.723 | 0.62 | 0.534 | 6.82 | 0.59 |

$^e$ using $dV/d\ln(I)$
$^f$ using $H(I)$

3.2. Other possible symmetry actions

The foregoing discussion outlines how the actions of other factors that impact the symmetry of the characteristics of a given device may be investigated. For instance, since semiconductor devices are impacted by temperature, one can investigate the influence of temperature on the symmetry by introducing an additional variable into the ordinary differential equation such that it takes the form $z' = \omega(x, y, z)$, where $x$ is the applied bias, $y$ is the temperature, and $z$ is the diode current. Any symmetry present may either be deduced intuitively by inspection of the serialized curves, or analytically through a suitable ansatz. For instance, one can intuitively follow the plots and assign a function $\ln(\ldots)$ along a given coordinate ($x$, or $y$) while the other coordinate remains invariant. Once the linearized tangent vectors are found then the vector fields can be described mathematically. Often, the empirical data may be available that hints at some inherent symmetry. For instance, the experiment of varying the temperature of a p-n junction diode whose forward current is kept constant produces a set of curves, hence the title term “serialized” when the experiment is repeated at different forward currents [22, 23]. Thus a visual inspection may facilitate the investigation of the potential symmetries.

4. Conclusions

We have presented a new method based on mathematical symmetry to determine parameters in serialized empirical measurements. An more illustrative than group theoretic approach has been followed deliberately to practically illustrate extraction of series resistance, to compensate the I-V characteristics of an device. Although the illustration is done using Schottky diodes, the method should be applicable in principle to other devices that have well-known analytical solutions for which serialized curves can be drawn. Our method argues that if a symmetry can be proved, then important parameters can be extracted from the reduced or canonical equations of the system. The method presented is applicable over the entire region of bias. As is evident above, this is in sharp contrast to many well-used I–V methods in the literature, such as the CCM itself. The method presents a clear route to the extraction of the device parameters over the entire region of bias. Also, unlike the CCM method against which it is compared, it provides a route to consistently calculate the a given parameter, such as $R_s$, and to provide a way to quantify its functional dependence. For Schottky diodes we show that such a symmetry exists and depends on the series resistance, is translational, and unique. The resulting method is simple, and is directly applicable to single traces as well as to multiple curves without unnecessary approximations.
The illustrations are based on data that is available for a specific diode that has the structure Al/p-Si/\(\text{Bi}_2\text{Se}_3\)/Al. The results are compared with the Cheung-Cheung method. The presented method gives results that agree with literature reports as far as the series resistance, ideality factor and barrier height are concerned. This work spawns a wide scope for future research in the symmetry approach that has not been attempted prior to our investigations. For instance, the actions of actions temperature, device doping, and many other factors on the symmetries can similarly be quantified.

References

[1] H. Norde, A modified forward I-V plot for Schottky diodes with high series resistance, Journal of Applied Physics 50 (7) (1979) 5052–5053.
[2] E. H. Nicollian, J. R. Brews, E. H. Nicollian, MOS (metal oxide semiconductor) physics and technology, Vol. 1987, Wiley New York, 1982.
[3] S. Cheung, N. Cheung, Extraction of Schottky diode parameters from forward current-voltage characteristics, Applied Physics Letters 49 (2) (1986) 85–87.
[4] Y. Zhang, Z. Zhang, B. Lin, Z. Fu, J. Xu, Effects of Ag doping on the photoluminescence of ZnO films grown on Si substrates, The Journal of Physical Chemistry B 109 (41) (2005) 19200–19203.
[5] G. Güler, Ö. Güllü, Ş. Karataş, O. F. Bakkaloglu, Analysis of the series resistance and interface state densities in metal semiconductor structures, Journal of Physics: IOP Conference Series 153 (2009) 012054. doi:10.1088/1742-6596/153/1/012054.
[6] H. E. Lapu, A. Köke, D. A. Aldemir, A. F. Özdemir, Ş. Altindal, Effect of illumination on electrical parameters of Au/(P3DMTFT)/n-GaAs Schottky barrier diodes, Indian Journal of Physics (2019) 1–8doi:10.1007/s12648-019-01644-y.
[7] J. H. Werner, Schottky barrier and pn-junction I/V plots—small signal evaluation, Applied Physics A 47 (3) (1988) 291–300.
[8] E. H. Rhoderick, R. H. Williams, Metal-semiconductor contacts, Clarendon Press, 1988.
[9] S. Chand, J. Kumar, Electron transport and barrier inhomogeneities in palladium silicide Schottky diodes, Applied Physics A 65 (4) (1997) 497–503.
[10] D. E. Yıldız, Ş. Altindal, H. Kanbur, Gaussian distribution of inhomogeneous barrier height in Al/SiO_2/p-Si Schottky diodes, Journal of Applied Physics 103 (12) (2008) 124502. doi:10.1063/1.2936963.
[11] A. M. Chowdhury, R. Pant, B. Roul, D. K. Singh, K. K. Nanda, S. Krupanidhi, Double Gaussian distribution of barrier heights and self-powered infrared photoresponse of InN/AIn/Si (111) heterostructure, Journal of Applied Physics 126 (2) (2019) 025301. doi:10.1063/1.5100066.
[12] S. Khanna, S. Neeleshwar, A. Noor, Current-voltage-temperature (IVT) characteristics of Cr/4H-SiC Schottky diodes, Journal of Electronic Devices 9 (2011) 382–389.
[13] N. K. Ibragimov, Group analysis of ordinary differential equations and the invariance principle in mathematical physics (for the 150th anniversary of Sophus Lie), Russian Mathematical Surveys 47 (4) (1992) 89–156.
[14] R. Ocaya, F. Yakuphanoglu, Ocaya–Yakuphanoglu method for series resistance extraction and compensation of Schottky diode I–V characteristics, Measurement 186 (2021) 110105. doi:10.1016/j.measurement.2021.110105.
[15] H. Durmuş, Ü. Atav, Extraction of voltage-dependent series resistance from IV characteristics of Schottky diodes, Applied Physics Letters 99 (9) (2011) 093505.
[16] M. Sağlam, A. Ayyildiz, A. Gönuş, A. Türüt, H. Efeoğlu, S. Tüzemen, Series resistance calculation for the Metal-Insulator-Semiconductor Schottky barrier diodes, Applied Physics A 62 (3) (1996) 269–273.
[17] V. Mikhailashvili, G. Eisenstein, R. Uzdin, Extraction of Schottky diode parameters with a bias dependent barrier height, Solid-State Electronics 45 (1) (2001) 143–148.
[18] P. E. Hydon, Symmetry methods for differential equations: a beginner’s guide, Cambridge University Press, 2000.
[19] R. O. Ocaya, Introduction to Control Systems Analysis Using Point Symmetries: An Application of Lie Symmetries, AuthorHouse UK, 2016.
[20] A. Mekki, R. Ocaya, A. Dere, A. A. Al-Ghamdi, K. Harrabi, F. Yakuphanoglu, New photodiodes based graphene-organic semiconductor hybrid materials, Synthetic Metals 213 (2016) 47–56.
[21] A. B. Ulusan, A. Tataroglu, Ş. Altindal, Y. Aziziyan-Kalandaragh, Photoreponse characteristics of Au/(CoFe_2O_4-PVP)/n-Si/Au (MPS) diode, Journal of Materials Science: Materials in Electronics (2021) 1–8doi:10.1007/s10854-021-06124-w.
[22] A. Hussain, Temperature dependent current–voltage and photovoltaic properties of chemically prepared (p) Si/In) Bi_2S_3 heterojunction, Egyptian Journal of Basic and Applied Sciences 3 (3) (2016) 314–321.
[23] R. Ocaya, An experiment to profile the voltage, current and temperature behaviour of a P–N diode, European Journal of Physics 27 (3) (2006) 625.