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Avoiding erroneous analysis of MIM diode current-voltage characteristics through exponential fitting



Bradley Pelz, Amina Belkadi, Garret Moddel*

Department of Electrical, Computer and Energy Engineering, University of Colorado, Boulder, CO 80309-0425, United States

ARTICLE INFO	A B S T R A C T
Keywords: MIM diode Optical rectenna Exponential fitting	Accurate fitting of measured current-voltage $[I(V)]$ data is crucial to the correct analysis and understanding of metal-insulator-metal (MIM) diodes, especially for optical rectennas. With the commonly used polynomial fitting of the $I(V)$ data, the order of the fit can drastically affect the diode performance metrics such as resistance, responsivity, and asymmetry. Additionally, the resulting fitting coefficients provide no useful parameters. An exponential-based equation can fit the $I(V)$ data well, can avoid artifacts from the choice of order of the polynomial, and allows for the accurate calculation of diode performance metrics directly from the fitting coefficients. Connecting the performance metrics to fitting coefficients shows a correspondence between zero.

bias responsivity and asymmetry at any given voltage.

1. Introduction

High-speed nonlinear diodes, such as metal-insulator-metal (MIM) diodes, have been increasingly investigated for use in rectennas for optical detection and energy harvesting [1–7]. Optical rectennas are antenna-coupled diode rectifiers that absorb high-frequency electromagnetic radiation and convert it to a DC signal. Measuring the DC I(V) characteristic of fabricated MIM diodes is the first step in experimentally analyzing and testing an optical rectenna. From the DC I(V) characteristics, certain performance metrics, such as differential resistance, responsivity, and asymmetry, given in (1)–(3) respectively, can be extracted. These metrics describe properties that are central in assessing a diode's suitability for use in an optical rectenna.

$$R_d(V) = I'(V)^{-1}$$
(1)

$$\beta(V) = \frac{1}{2} \frac{I''(V)}{I'(V)}$$
(2)

$$A(V) = -\frac{I(V)}{I(-V)}$$
(3)

For an efficient rectenna, a high coupling efficiency between the MIM diode and the antenna is required. The antenna impedance is typically on the order of 100 ohms, and for efficient power transfer the diode resistance should match it [8,9]. For this reason, only diodes that have a relatively low resistance are of interest, despite the higher asymmetry and nonlinearity seen in some high-resistance diodes

[10–13]. A high diode responsivity, which is a measure of rectified DC voltage or current as a function of input power, and a large asymmetry, which is the ratio of forward to reverse current, are required for efficient rectification [9]. Since optical rectennas usually operate at voltages close to zero [14], we use the zero-bias resistance, $R_0 = R_d(0)$, and the zero-bias responsivity, $\beta_0 = \beta(0)$, when analyzing our diodes. Using zero-bias values simplifies the differential resistance and responsivity curves into single quantitative metrics.

While $R_d(V)$ and $\beta(V)$ can be calculated directly from I(V) data using central difference approximation derivatives, a problem often arises when noise in the experimental data gets amplified by the derivatives. To overcome this noise amplification, it is necessary to use some sort of fitting or smoothing. A polynomial fit using least square regression is an attractive option because it is easy to differentiate and integrate, and a polynomial of high enough order can fit any curve to an arbitrarily high degree of accuracy. This arbitrarily high degree of fit accuracy, however, can give misleading results. Runge's function is one well-established example [15,16]. Despite the known problems with polynomial fitting, it has become common practice to fit MIM I(V) data with a polynomial when analyzing MIM diodes [17–26]. In this paper we expose the shortcomings of the polynomial fit for MIM diodes through the analysis of a double insulator MIM diodes. We demonstrate that an alternative fitting procedure can overcome these shortcomings.

The first diode we examine, MIM-1 $(R_d(0) \cong 16 \text{ k}\Omega)$, is a Co-CoO_x-TiO₂-Ti double insulator MIM diode fabricated as described in Herner [26]. While we focus on double insulator MIM diodes, the concepts discussed are appropriate for single insulator MIM diodes as well. We fit

* Corresponding author.

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E-mail address: moddel@colorado.edu (G. Moddel).

https://doi.org/10.1016/j.measurement.2018.01.054

Received 4 August 2017; Received in revised form 15 November 2017; Accepted 29 January 2018 Available online 07 February 2018

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Fig. 1. Effects of polynomial fitting order on a moderate-resistance diode (MIM-1) (a) responsivity as a function of voltage, (b) asymmetry as a function of voltage.

the measured I(V) data for MIM-1 with 5th,7th, and 9th order polynomials. These fits generate smooth responsivity curves shown in Fig. 1(a). However, these responsivity curves vary greatly between the different fit orders, which is evidence that these results are misleading. The asymmetry curves in Fig. 1(b) also show substantial variation, not only from each other, but from the data. Unlike $R_d(V)$ or $\beta(V)$, the asymmetry does not rely on I(V) derivatives, and so it can be calculated directly from the interpolated I(V) data. The interpolation is necessary to ensure that the currents at both the positive and negative voltage are taken at a uniform voltage distance from V = 0. Even though the asymmetry can be calculated from the data directly, the noise of the measurement is still clearly evident, which again demonstrates the need for quality fitting. These curves show that the polynomial fits do a particularly poor job of estimating the asymmetry at low voltages due to the polynomials ability to not pass through the origin. Because of these erroneous results, we developed an alternative, more robust fitting model.

2. Calculating performance metrics from the exponential model

The electron tunneling responsible for the rectification in MIM diodes is fundamentally an exponential process [27]. To overcome limitations of the polynomial fit, we propose an alternative approach using least square regression to fit an equation based on exponentials. This fit facilitates an understanding of how well the diode will operate in a circuit (e.g., in a rectenna,) and provides a useful basis for diode improvement. The proposed exponential-based fit is:

$$I(V) = ae^{bV} + ce^{dV} = I_0(e^{bV} - e^{-dV})$$
(4)

17.7.

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In practice, we use the first version of the equation to perform the fit as it is a convenient MATLAB built-in fitting function, 'exp2'. After the fit is complete, we check that the variation between *a* and *c* is less than 1% and set I_0 to the average of *a* and *c* and force the sign conventions in the second version of the equation. In this equation, parameter bstrongly influences the I(V) at positive voltages while parameter d affects the curve at negative voltages. The parameter I_0 scales the curve, thus modifying the diode resistance. The first indication that (4) is an appropriate form for a diode fit is that when d = 0 and $b = \frac{1}{nv}$, where n is an ideality factor and v_t is the thermal voltage, the equation simplifies to the Shockley diode equation, which describes an ideal semiconductor diode [28]. Simmons proposed a similar exponential form for a trapezoidal high-barrier diode [27]. We note that Simmon's equation does not describe our MIM diodes accurately because for low-barrier height MIM diodes at intermediate voltages (100 mV $\leq V \leq 300$ mV), the equation simplifies to a symmetric I(V) formula and overestimates the tunnel current [29]. In contrast to the polynomial fits, when the exponential fit is used the resistance, responsivity, and asymmetry are directly determined by the fitting coefficients in a physically meaningful way. In this paper, we calculate resistance, responsivity and

asymmetry for two MIM diodes of different material sets that were fabricated by different techniques. These different diodes show slightly different I(V) curvature and fitting techniques. We demonstrate that the exponential fitting is a superior alternative to the polynomial fit.

2.1. Resistance

To effectively match the diode resistance, R_d , to the antenna, it is necessary to understand the relationship between the diode I(V) and $R_d(V)$. Substituting the exponential equation for the diode I(V), (4), into the diode differential resistance equation, (1), results in:

$$R_d(V) = \frac{1}{I_0(bexp(bV) + dexp(-dV))}$$
(5)

From (5), we can calculate the zero-bias differential resistance R_0 . At V = 0, the exponential terms vanish and R_0 can be expressed simply as:

$$R_0 = \frac{1}{I_0(b+d)}$$
(6)

2.2. Responsivity

Since responsivity provides the connection between optical input power and DC output, it is useful to understand the relationship between the I(V) and $\beta(V)$. Substituting the exponential I(V) equation, (4), into (2), we obtain the voltage-dependent responsivity:

$$\beta(V) = \frac{1}{2} \left(\frac{b^2 \exp(bV) - d^2 \exp(-dV)}{b \exp(bV) + d \exp(-dV)} \right)$$
(7)

Just as with resistance, the first parameter of interest is the zero-bias responsivity, since we are often interested in rectenna operation at or near zero bias. The responsivity at zero bias is:

$$\beta_0 = \frac{1}{2}(b-d) \tag{8}$$

Zero-bias responsivity is dependent only on the two coefficients in the arguments of the exponentials in (4). From (4) we can see that at large voltage magnitudes, one exponential dominates the I(V) equation. Similarly, from (7), we see that at large positive voltages $\beta(V)$ asymptotically approaches $\frac{1}{2}b$ and at large negative voltages $\beta(V)$ approaches $-\frac{1}{2}d$.

2.3. Asymmetry

The asymmetry gives insight into a diode's ability to efficiently rectify. Again, substituting (4) into (3) and simplifying gives the voltage dependent asymmetry:



Fig. 2. Comparison of 5^{th} , 7^{th} , and 9^{th} order polynomial fits (dashed grey, labeled in Fig. 1) and exponential fit (solid orange, $I_0 = 3.3 \times 10^{-6}$ A, b = 10.0 V⁻¹ and d = 8.9 V⁻¹) for MIM-1 ($R_d(0) \cong 16$ kΩ). (a) Measured diode DC I(V) characteristics (green circles) and I(V) fits versus voltage, V. (b) Calculated fit residue. (c) Calculated fit responsivity. (d) Calculated fit asymmetry and interpolated data asymmetry (green circles). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

$$A(V) = e^{(b-d)V} = e^{2\beta_0 V}$$
(9)

This asymmetry equation is rewritten in terms of β_0 using (8), thus showing a direct correspondence between the diode asymmetry and zero-bias responsivity.

3. Exponential fit of I(V) data

Our interest in relatively low resistance diodes [29] dictates that the MIM insulators be thin (<5 nm). Thus, the maximum measured voltage range for our diodes, to avoid dielectric breakdown, is the on the order of several hundred millivolts. For MIM-1, the exponential fit coefficients are as follows: $I_0 = 3.3 \times 10^{-6}$ A, b = 10.0 V⁻¹ and d = 8.9 V⁻¹. Using (6) and (8), these coefficient values correspond to a $\beta_0 = 0.55$ A/W and a $R_0 = 16$ k Ω . The quality of the fit is assessed in two ways: First, the fit residue, which is calculated from the I(V) data minus the I(V) fit, indicates how well the model fits the data. Second, comparing the fit asymmetry to the interpolated data asymmetry shows how closely the model estimates performance metrics.

For MIM-1, the exponential fit is of similar quality to the polynomial fit. In Fig. 2(a), the three polynomials $(5^{th},7^{th})$, and 9^{th} order fits) and exponential I(V) curves are all nearly indistinguishable from the data and each other. A closer look at the fit quality in Fig. 2(b) reveals that all fits have comparably low residues. However, as shown earlier, changing the order of the polynomial fit results in a wide range of responsivity curves. Fig. 2(c) shows the exponential fit responsivity curve overlaid on Fig. 1(a), the polynomial fits responsivity curves. Fig. 2(d) shows the exponential fit asymmetry overlaid on the polynomial and interpolated data asymmetry from Fig. 1(b). Clearly, the exponential fit does a superior job of representing the diode asymmetry.

The second diode examined is a Ni-NiO-TiO₂-Cr double insulator diode, MIM-2. MIM-2 ($R_d(0) \cong 4 \text{ k}\Omega$) has a lower resistance than MIM-1 and was fabricated with a shadow-mask technique [30]. Diodes with

lower resistances often suffer less variation between different polynomial fit orders, but even when the polynomial fits are well behaved, the resulting polynomial equation fails to provide the same connection among diode properties that the exponential fit provides.

We now repeat the fitting procedure for MIM-2, comparing the exponential model to the 7th order polynomial fit. Just as with MIM-1, both the 7th order polynomial and exponential fits are nearly indistinguishable from the raw I(V) data, and therefore are not shown. Unlike MIM-1, however, once we examine the residue plot, Fig. 3(a), we can see that the exponential fit is substantially less accurate than the polynomial, especially at higher voltage magnitudes. The exponential fit tends to overstate the magnitude of the current at higher voltages. This systematic error corresponds to a curvature of the I(V) data that does not increase with voltage as quickly as the fit does. The fundamental nature of the exponential model does not allow for this reduction in curvature because away from V = 0, only one of the exponential terms in (4) dominates. One physical explanation of this reduced curvature of the I(V) is an unaccounted for series resistance. This series resistance also accounts for the flattening of the asymmetry curve in Fig. 1(b), rather than the unbounded exponential growth predicted by (9).

A small portion of the resistance is due to the inability, in practice, to remove 100% of the parasitic lead resistance even with 4-point probe measurements, while the remainder is associated with the MIM diode junction itself. In Fowler-Nordhiem tunneling, electrons are transported through the dielectric barrier partially by tunneling, and partially by conduction in the conduction band of the insulator [31]. This transport through the conduction band adds to the series resistance. The distance an electron travels in the conduction band depends on the insulator thickness and the energy band structure, which changes for different voltages. Therefore, the series resistance depends on the voltage, *V*. To fit this adequately while avoiding unnecessary complexity, we choose the simplest form that meets the physical requirements for this voltage.



Fig. 3. Comparison of 7th order polynomial fit (dashed blue) and exponential fit (solid orange, $I_0 = 2.65 \times 10^{-5}$ A, b = 5.53 V⁻¹ and d = 4.82 V⁻¹) for MIM-2. (a) Calculated fit residue. (b) Calculated fit asymmetry and interpolated data asymmetry (green circles) (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

dependent series resistance: (1) resistance is always positive, and (2) it has a continuous first derivative. Thus, the voltage-dependent series resistance, R_{ν} , is approximated as follows:

$$R_{\nu}(V) = R_s + \alpha V^2 \tag{10}$$

where R_s is the constant portion of the series resistance, and α is the coefficient for the voltage-dependent portion. The relatively low zerobias resistance of MIM-2 makes the inclusion of this additional voltagedependent series resistance necessary for an accurate fit, unlike for MIM-1 where the diode resistance was large enough that the series resistance was negligible.

4. Modified exponential fit

Previously, when (4) described the diode I(V), it was unnecessary to distinguish between the voltage on the diode, V_D and the measured voltage, V, as $V_D = V$. With the addition of a series resistance, R_v , there is a third voltage to consider, the resistor voltage, V_R . The voltage, which is measured over the diode and resistor series combination, can be separated into two components:

$$V = V_D + V_R \tag{11}$$

The diode voltage, V_D , from (11) can be expressed in another form:

$$V_D = V - R_v(V)I \tag{12}$$

where V_D is the diode voltage, and $R_v(V)I$ gives the voltage across the voltage-dependent series resistor. Even though we are now including a series resistance in our analysis, the diode I(V) data is still represented by (4), which can be rewritten to clarify which voltage the I(V) relationship applies to:

$$I(V_D) = I_0 (e^{bV_D} - e^{-dV_D})$$
(13)

The relationship between the measured current, I(V) and the measured voltage, V, can be found by substituting (12) into (13) for V_D and is described by:

$$I(V) = I_0(e^{b(V-I(V)R_v(V))} - e^{-d(V-I(V)R_v(V))})$$
(14)

Since the current in (14) is recursive, the fit coefficients cannot be obtained through least squares regression as done for (4) in Section 3. However, with the addition of a few preliminary data manipulation steps, and a comparison of a series of least squares regression fits, we can solve for the five coefficients (R_s,α,b,d , and I_0). Appendix A explains this procedure in detail.

To compare the results of the modified exponential fit with the unmodified version, we plot I(V)'s, residues, responsivities and asymmetries. Fig. 4(a) shows that for the data, the unmodified exponential fit, and the series resistance exponential fit are all indistinguishable in the I(V) plot. Fig. 4(b) present the fit residue for the exponential and

the modified exponential fits. This shows that the addition of the series resistance improves the fit, compared to a simple exponential without an additional resistance. Fig. 4(c) shows the responsivity of both exponential fits, and that, as expected, the addition of the series resistance reduces the curvature of the I(V) at higher voltages. Finally, Fig. 4(d) shows the asymmetry for both exponentials with the interpolated asymmetry data. Clearly, the exponential with the series resistance does a much more accurate job of representing the asymmetry than the unmodified exponential.

Just as we did for the fit without the series resistance, we want to determine the relationship between our model and the diode performance metrics. Because of the complex relationship between *I* and *V* in (14), there are not useful analytic expressions for voltage-dependent diode resistance, responsivity or asymmetry. However, we can find expressions for zero-bias resistance and responsivity, because those complex voltage dependent expressions simplify at V = 0 V.

4.1. Zero-bias resistance

The diode resistance is simply the series combination of a resistor and the exponential resistance in (5). At V = 0, the voltage-dependent resistance part of R_v vanishes and leaves only R_s . Thus the zero-bias resistance can be expressed as follows:

$$R_0 = \frac{1}{I_0(b+d)} + R_s = R_0^{exp} + R_s$$
(15)

If we refer to the resistance in (6) as R_0^{exp} , we get the second form, where we see the zero-bias resistance is the sum of the constant portion of the series resistance and the zero-bias resistance from the unmodified exponential. Using (15) for MIM-2 fitting results gives $R_0 = 4.1 \text{ k}\Omega$.

4.2. Zero-bias responsivity

While the complexity of (14) leads to a voltage-dependent responsivity that provides little insight into the diode characteristics, the responsivity at zero-bias can be calculated as:

$$\beta_0 = \frac{1}{2}(b-d) \left(\frac{1}{1+R_s I_0(b+d)}\right)^2$$
(16)

Using (16) for MIM-2, we find $\beta_0 = 0.65$ A/W. If we refer to the responsivity in (8) as β_0^{exp} , (16) simplifies to the following:

$$\beta_0 = \beta_0^{exp} \left(\frac{1}{1 + R_s / R_0^{exp}} \right)^2 \tag{17}$$

As R_s gets large relative to R_0^{exp} , the zero-bias responsivity is reduced relative to β_0^{exp} . Of course, if $R_s = 0 \Omega$, then $\beta_0 = \beta_0^{exp}$.



Fig. 4. Comparison of exponential (orange dots, with Eq. (4) parameters $I_0 = 2.65 \times 10^{-5}$ A, b = 5.53 V⁻¹ and d = 4.82 V⁻¹) and modified exponential (solid purple, $I_0 = 1.83 \times 10^{-5}$ A, b = 8.64 V⁻¹, d = 7.07 V⁻¹, $R_s = 334$ Ω and $\alpha = 1125 \Omega/V^2$) fits for MIM-2 ($R_d(0) \cong 4 \text{ k}\Omega$). (a) Measured diode DC I(V) characteristics (green circles) and I(V) fits versus voltage, V. (b) Calculated fit responsivity. (d) Calculated fit asymmetry and interpolated data asymmetry (green circles). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

5. Conclusion

Inaccurate fitting of fabricated MIM didoes can lead to erroneous analyses of a diode's I(V) characteristics and its performance metrics. We found that polynomial fitting can misstate responsivity and asymmetry values, two of the main metrics used to assess the performance of diodes in optical rectennas. Using the wrong order polynomial fit for a high resistance diode can drastically affect the resulting responsivity curve. Different order polynomial fits can even imply different diode polarity. Here, we have presented an exponential fitting method as an alternative to the commonly used polynomial fitting procedure. The exponential fit provides several advantages in analyzing MIM diodes such as fewer fitting parameters and a simple relationship between the fitting parameters and the diode performance metrics. One example of the relationships provided is that the diode asymmetry is directly linked to the zero-bias responsivity. Another is a simple function relationship showing how series resistance degrades responsivity. This exponential model can be used to develop a broader understanding of MIM diode I(V) characteristics, and the connections between performance metrics.

We have analyzed the exponential fit for two diodes, one with high

Appendix A. Modified exponential fitting procedure

resistance and one with low resistance. For the low resistance diode, an additional voltage-dependent series resistance was necessary to get an accurate fit. The high resistance diode can be fit by either the modified or unmodified exponential fit and achieve the same results. The addition of these exponential fitting procedures to existing analysis techniques will help avoid potentially misleading results, and give added confidence to derived performance metrics.

Acknowledgment

The authors would like to thank David Doroski and Brad Herner for their assistance in fabricating the MIM devices and Miena Armanious, Ayendra Weerakkody and John Stearns for their helpful discussions. This work was carried out in part under contract from RedWave Energy Inc. and funded in part by the Advanced Research Projects Agency -Energy (ARPA-E), U.S. Department of Energy, under Award Number DE-AR0000676. Also, research reported in this publication was supported by competitive research funding from King Abdullah University of Science and Technology (KAUST). G. Moddel holds stock in RedWave Energy, Inc.

To fit the data to (14), we find the pair of R_s and α values that allow the best fit for (13) to the modified I(V) data. Given a pair of R_s and α values, the *V* in the (*V*,*I*) data set can be converted to V_D using (12). When the data is converted to (V_D ,*I*) ordered pairs, (13) is now an appropriate model to fit the data. Coefficients I_0 , *b*, and *d* can be determined using least squares regression, as done in Section 3.

To determine the optimum R_s and α , we pick the pair of R_s and α values that give the highest coefficient of determination, R^2 , for the fit of (13) to modified (V_D ,I) data sets. To make this comparison of different values for R_s and α , we first establish a range of interest. The additional series resistance must be smaller than the smallest measured absolute diode resistance, which can be approximated as $V_{max}/I(V_{max})$, where V_{max} is the maximum measured voltage. Thus for R_s , we are interested in the following range:

$$0 \leq R_s \leq V_{max}/I(V_{max})$$

For α , we examine this range:

(A.1)

(A.2)

$0 \leq \alpha \leq 1/V_{max}I(V_{max})$

A new (V_D,I) pair is generated for every α and R_s combination. The exponential model in (13) is used to fit the resulting V_D vs *I*. The combination of R_s and α values that have the highest coefficient of determination, R^2 , for the fit to (13) is chosen for the final model. For MIM-2, we have a maximum R^2 when $R_s = 334 \ \Omega$ and $\alpha = 1125 \ \Omega/V^2$. These R_s and α values lead to $b = 8.64 \ V^{-1}, d = 7.07 \ V^{-1}$, and $I_0 = 1.83 \times 10^{-5} \ A$. This fit procedure is also suitable for MIM-1, and shows that the series resistance is, in fact, negligible in that case. The highest R^2 is found when both $R_s = 0 \ \Omega/V^2$, resulting in identical *b*,*d*, and I_0 values established in Section 3.

Now that we have the fit coefficients for MIM-2, we can generate the fit I(V) needed to plot the responsivity, resistance and residue. Because the current in (14) is recursive, several steps are required to plot the resulting fit. First, we plug (13) in for the current in (12) to get an equation that relates *V* and V_D . Since this results in a transcendental equation, we must numerically solve for V_D values for a set of voltages, *V*, over any range of interest, generally (±400 mV). Once we have V_D , we can calculate *I* using (13). Now that we have *V* and *I* we can easily plot *I*(*V*), the residue, the asymmetry, or generate resistance and responsivity curves using central difference approximation derivatives.

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