Measurement 120 (2018) 28–33

Contents lists available at ScienceDirect

Measurement

journal homepage: www.elsevier.com/locate/measurement

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

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ARTICLE INFO

Keywords:
MIM diode
Optical rectenna
Exponential fitting

ABSTRACT

Accurate fitting of measured current-voltage [$\boldsymbol{I(V)}$] 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 $\boldsymbol{I(V)}$ 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 $\boldsymbol{I(V)}$ 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.

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

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

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

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-$CoO_x$-$TiO_2$-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

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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
0263-2241/

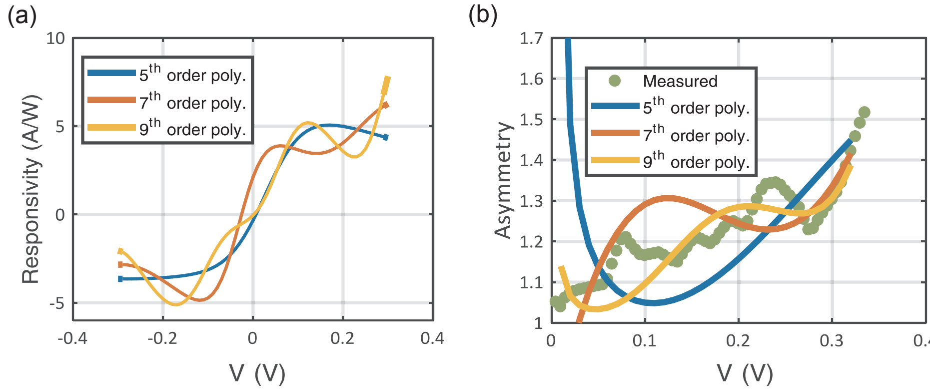

Fig. 1. Effects of polynomial fitting order on a moderate-resistance diode (MIM-1) (a) responsivity as a function of voltage, (b) asymmetry as a function of voltage.

the measured $I(V)$ data for MIM-1 with 5^{th},7^{th}, and 9^{th} 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:

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

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 b strongly 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 $b = \frac{1}{nv_t}$, 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 ($100\,\text{mV} \leqslant V \leqslant 300\,\text{mV}$), 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:

$$R_d(V) = \frac{1}{I_0(b\exp(bV) + d\exp(-dV))} \tag{5}$$

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:

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

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:

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

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: