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A Novel SPICE compatible behavioral model for molecular electronics having hysteresis effects

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Although molecular electronics is in its infancy, there are many significant advances in understanding and implementing computational functions based on molecular electronic devices. In order to evaluate a molecular electronic circuit, a model is needed. In existing literature, only a few models have been introduced for molecular electronics, all of which do not support the hysteresis phenomenon. To the best of the authors' knowledge, for the first time, this paper introduces a behavioral model in SPICE which is able to imitate hysteresis behavior in a desired molecular circuit. The proposed model is then modified in order to guarantee continuous behavior in its *I/V* curves. Some molecular electronic *I/V* curves from the literature are selected and by utilizing the proposed model, its correct operation are investigated.

Key words: Molecular electronics, behavioral model, hysteresis phenomenon, SPICE.

INTRODUCTION

During the last decades, the feature size of MOS-based circuits has dramatically decreased. The ever decreasing feature size will face serious challenges and alternative technologies should therefore be selected. Due to their performance and density, molecular electronics is a promising candidate for nanoelectronic applications. Molecular electronics has also been proposed as a pathway for high-density nanoelectronic devices (Seminario, 2005). Many efforts have been made by researchers to introduce and describe different structures and technologies based on molecular devices (Strukov and Likharev, 2005; Martin, 2009; Yuqing et al., 2011; Gimenez et al., 2009; Liu et al., 2011). Before manufacturing process of molecular electronic circuits, a model is needed in order to simulate the behavior of the circuit in a reasonable amount of time and with acceptable accuracy. In this paper, a behavioral model for modeling the hysteresis phenomenon in molecular based circuits is proposed. The model is then implemented in SPICE and the correct operation of the model is investigated. Finally for achieving the most accuracy a modification in the proposed behavioral model is made.

MATERIALS AND METHODS

A brief survey of molecular electronics models

In general, there are two major categories for simulating electronic circuits: the physics-based models and the nonphysic-based models or behavioral models. Physics-based molecular device modeling is very difficult due to the unknown underlying physics

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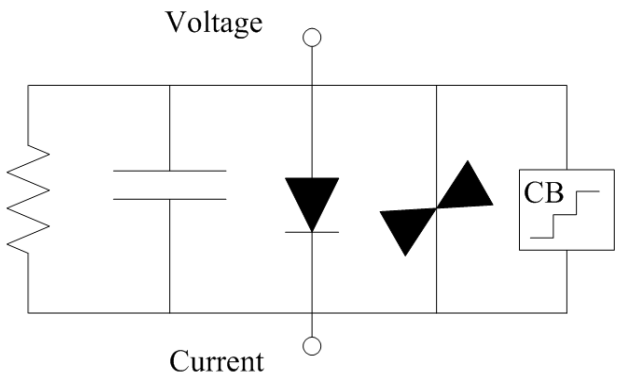

Figure 1. Two-terminal UDM. The main features of this model are capacitance, resistance, thermionic emission, NDR, and coulomb blockade.

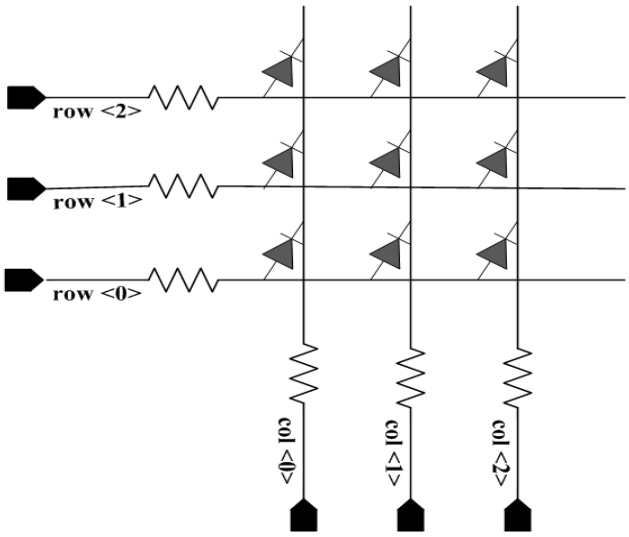

Figure 2. Equivalent circuit schematic of a crossbar technology.

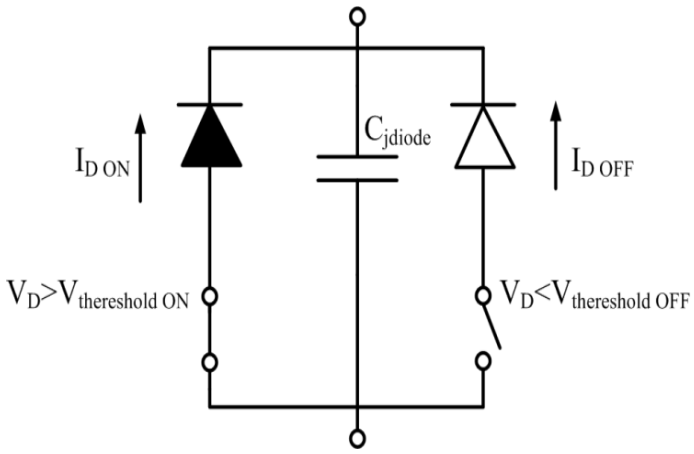

Figure 3. A device model for crossbar technology. Figure source: Ziegler and Stan (2003). Two diodes are used for showing the on-state and off-state of a cross bar junction.

and also the variety of applied materials. However, circuit designers need a model of these devices to evaluate their design performance. The behavioral models introduced for emerging devices have solved this problem and have helped circuit designers to easily design and verify the output of their circuits. In this regard, many efforts have been made (Yan et al., 1995; Yu et al., 1999; Bhattacharya and Mazumder, 2001; Sharifi and Bahrepour, 2009; Sharifi and Banadaki, 2010). For molecular devices three models have been proposed so far.

(i) Ziegler et al. (2002) proposed a circuit model for molecular devices called the universal device model (UDM) (Ziegler et al., 2002). This model is characterized in more detail in Stan et al. (2003), and Rose et al. (2004, 2007). The UDM concept uses empirical equations that describe each fundamental quantum and classical effect that may be relevant to an electronic device (Stan et al., 2003). As shown in Figure 1 the common sub-features used in the UDM are: resistive behavior (linear *I-V* curve), diode-like behavior (exponential *I-V* curve), coulomb-blockade behavior (step *I-V* curve), and tunneling behavior (peak *I-V* curve) for a DC characteristic. The UDM accepts a set of current and voltage data points, which are obtained theoretically or experimentally, and then it produces the appropriate coefficient for the mentioned UDM features. The current equation of a device is achieved by the use of the respective weight of each feature as:

$$I_{UDM}(V) = \alpha_R I_R(V) + \alpha_D I_D(V) + \alpha_T I_T(V) + \alpha_{CB} I_{CB}(V) \quad \text{(i)}$$

(ii) Ziegler et al. (2003) proposed a device model for a crossbar structure which is a main technology in molecular electronics (Ziegler and Stan, 2003). The crossbar technology sandwiches bistable molecules, for example, rotaxanes, between wires at each junction. Figure 2 shows the equivalent circuit of a typical crossbar technology. As shown in Figure 3, the presented model utilizes two diodes for representing the on-state and off-state of a crossbar junction, in parallel with a parasitic junction capacitance. If the applied voltage (V_D) is greater than the on-state threshold ($V_{thresholdON}$), the model switches to the on-state and if the applied voltage (V_D) is lower than the off-state threshold ($V_{thresholdOFF}$), the model switches to the off-state. In this model, the junction capacitance, current-voltage characteristics and switching threshold values should be selected in an appropriate manner in order to obtain a proper mimic of crossbar structure based devices (Ziegler and Stan, 2003).

(iii) Ci Lei et al. (2007) introduced a device model (Lei et al., 2007, 2008) in which the electron transport properties of a molecular system were studied by viewing it as a one electron elastic scattering problem. The Breit-Wigner resonance formula was used to model a general crossbar structure. In this model, the transmitted current (I) through the metal-molecule-metal junction is proportional to the transmission probability ($T(E)$) for a range of energy levels around the Fermi energy of the source lead and it is computed using Landauer's formula as Equation (2).

$$I(V) = \frac{2e}{h}\int_{-\infty}^{\infty} dE\,T(E)\left(\frac{1}{\exp[(E-\mu_s)/kT]+1} - \frac{1}{\exp[(E-\mu_d)/kT]+1}\right) \quad \text{(ii)}$$

where μ_s and μ_d are the electro-chemical potentials of the source and drain respectively. In addition the transmission probability $T(E)$ used in the Landauer formula is approximated by the Breit-Wigner formula as follows.

$$T(E) = \frac{4\Gamma_1\Gamma_2}{(E-\varepsilon_0)^2 + (\Gamma_1+\Gamma_2)^2} \quad \text{(iii)}$$

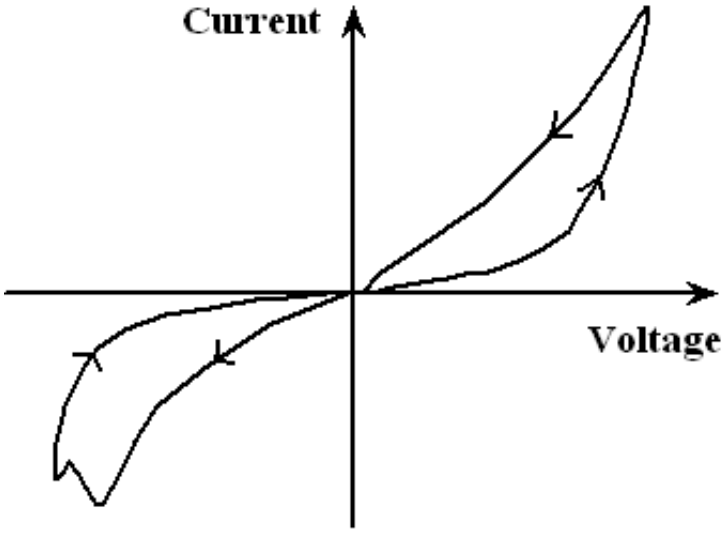

Figure 4. A generic *I-V* curve for a typical molecular hysteresis switch. Figure source: Rose and Stan (2007).

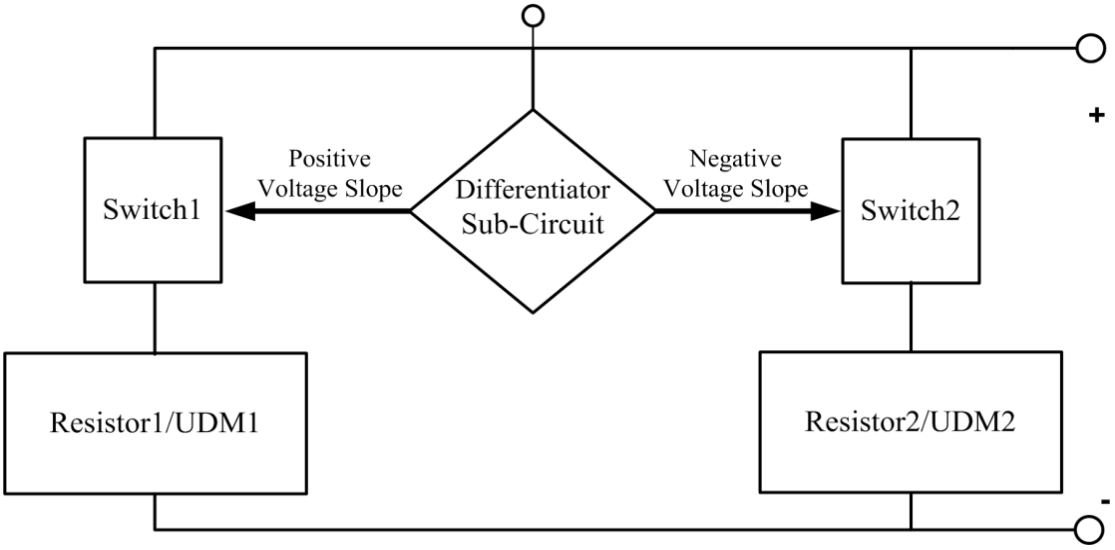

Figure 5. Block diagram for the proposed behavioral model. The differentiator sub-circuit selects one of the resistors/UDM modules. And the selected resistors/UDM modules generate appropriate current.

The hysteresis phenomenon

Hysteresis is a non classical behavior and refers to a device's ability to switch between stable behaviors. Hysteresis not only depends on the current environment but also depends on its past environment. To predict the future behavior of a hysteresis progress, either its internal state or its history must be known (Mielke and Roubicek, 2003). If a given input alternately increases and decreases, then the output tends to form a loop.

Although hysteresis curves have different shapes, many molecular switching devices have an *I-V* characteristic such as that presented in Figure 4 (Rose and Stan, 2007). This curve illustrates that, in general, molecular electronic *I/V* curves have hysteresis in the first and third quadrant. Also in each quadrant there are two different paths called reverse and forward paths which signifies positive or negative voltage slope, respectively.

Introducing a behavioral model for hysteresis

Circuit designers need a complete and easy to use model for describing the behavior of a molecular electronic device used in a computational or memory circuit. Although the models mentioned before are applicable, they do not support hysteresis phenomenon. This paper bridges the existing gap by introducing a behavioral model for hysteresis phenomenon usually appeared in molecular electronic circuits. Figure 5 shows the proposed behavioral model which comprised of a differentiator sub-circuit for identifying the positive/negative slopes of a molecular device voltage and two resistor/UDM modules. As seen from Figure 5, the sign of the

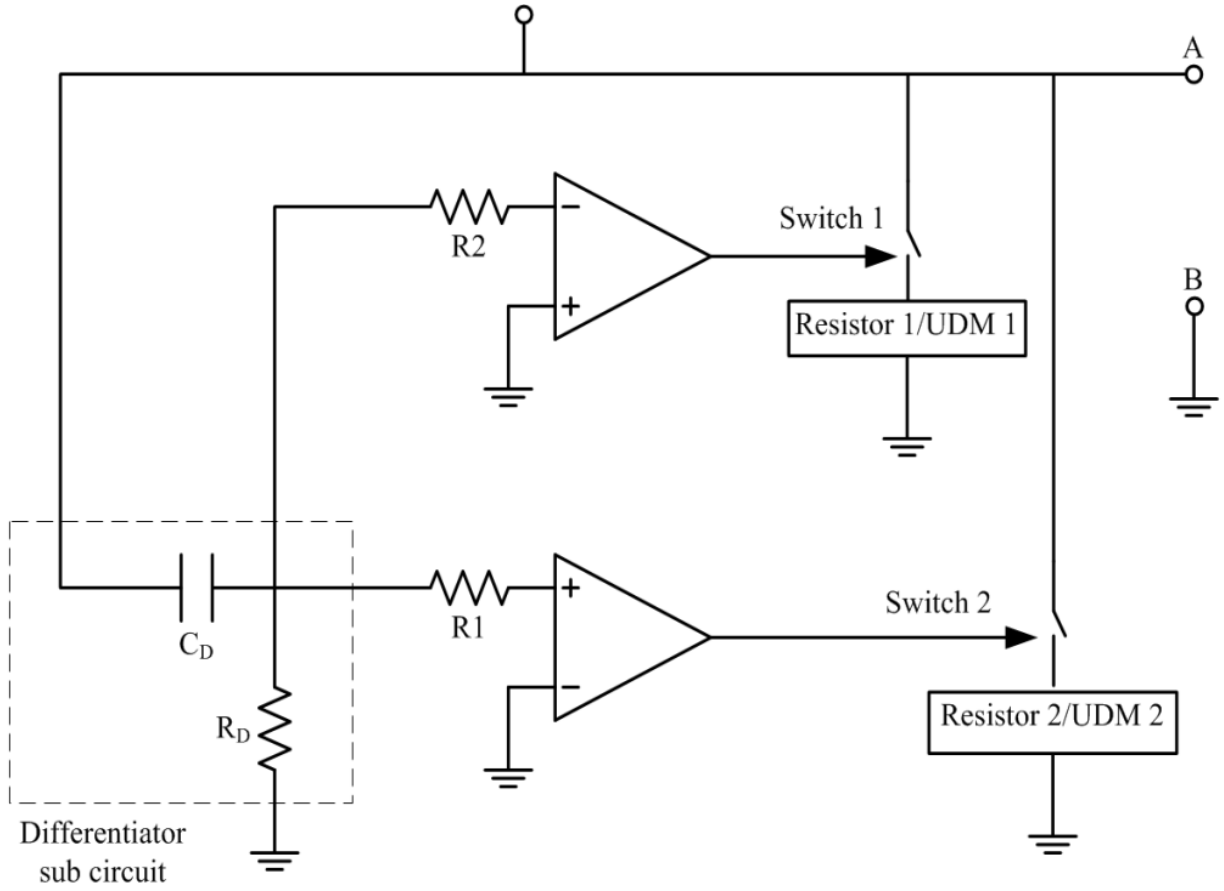

Figure 6. The proposed circuit model for imitating hysteresis behavior. This model consists of a differentiator sub-circuit, two switches and two resistor/UDM modules.

voltage slope is achieved using a differentiator sub-circuit which selects one of the resistor/UDM modules for producing the appropriate device current. The positive slope signifies increasing voltage that in the hysteresis curve means forward path and the negative slope indicates decreasing voltage that in the hysteresis curve means reverse path. The proposed circuit for the LHM and GHM is presented in Figure 6. As shown, this model utilizes simple circuit elements in order to generate hysteresis behavior in molecular electronics circuit.

RESULTS

By considering the proposed behavioral model for hysteresis phenomenon in previous section, there are two different approaches for implementing the model: i) the linear hysteresis model (LHM) and ii) the general hysteresis model (GHM). The LHM uses two different resistors for generating appropriate current values and hence, it has minimum possible complexity. In Figure 6 the Resistor 1 and Resistor 2 values may be approximated by the average of the forward and reverse slope values appeared in the first and third quadrants of given *I/V* curves. In fact this model imitates the *I/V* characteristics of a device in linear format. Figure 7(a) shows *I/V* curves for the ZnO/aluminum stack (Lüssem, 2006) and a dashed line in Figure 7(b) depicts the simulation outputs using the LHM. This approach has two main drawbacks: i) it eliminates the details of the reverse or forward paths and changes them to two simple lines with different slopes and ii) since the amount of slopes in the first and third quadrant of a specific curve may be different in the forward or reverse paths, this model replaces these amounts by their average values which means less accuracy. In the GHM, the resistors are replaced with proper UDMs; hence, the simulation output is more accurate. This approach helps to save the details of *I/V* curves with more precision. The solid line in Figure 7(b) shows the simulation output of the *I/V* curve for the ZnO/aluminum stack using the GHM. As another example, the *I-V* curve for the ITO/aluminum stack (Lüssem, 2006) is selected (Figure 8(a)). In Figure 8(b) the dashed line and solid line depict the simulation outputs using the proposed LHM and GHM respectively. As depicted in Figures 7(b) and 8(b) there is a very good agreement between the GHM and the original *I/V* curves. For modeling the ZnO/aluminum and ITO/aluminum stack curves the applied characteristics in the proposed circuit are: C_D=1 nF, R_D=100 KΩ and *R2*=*R3*=1 KΩ.

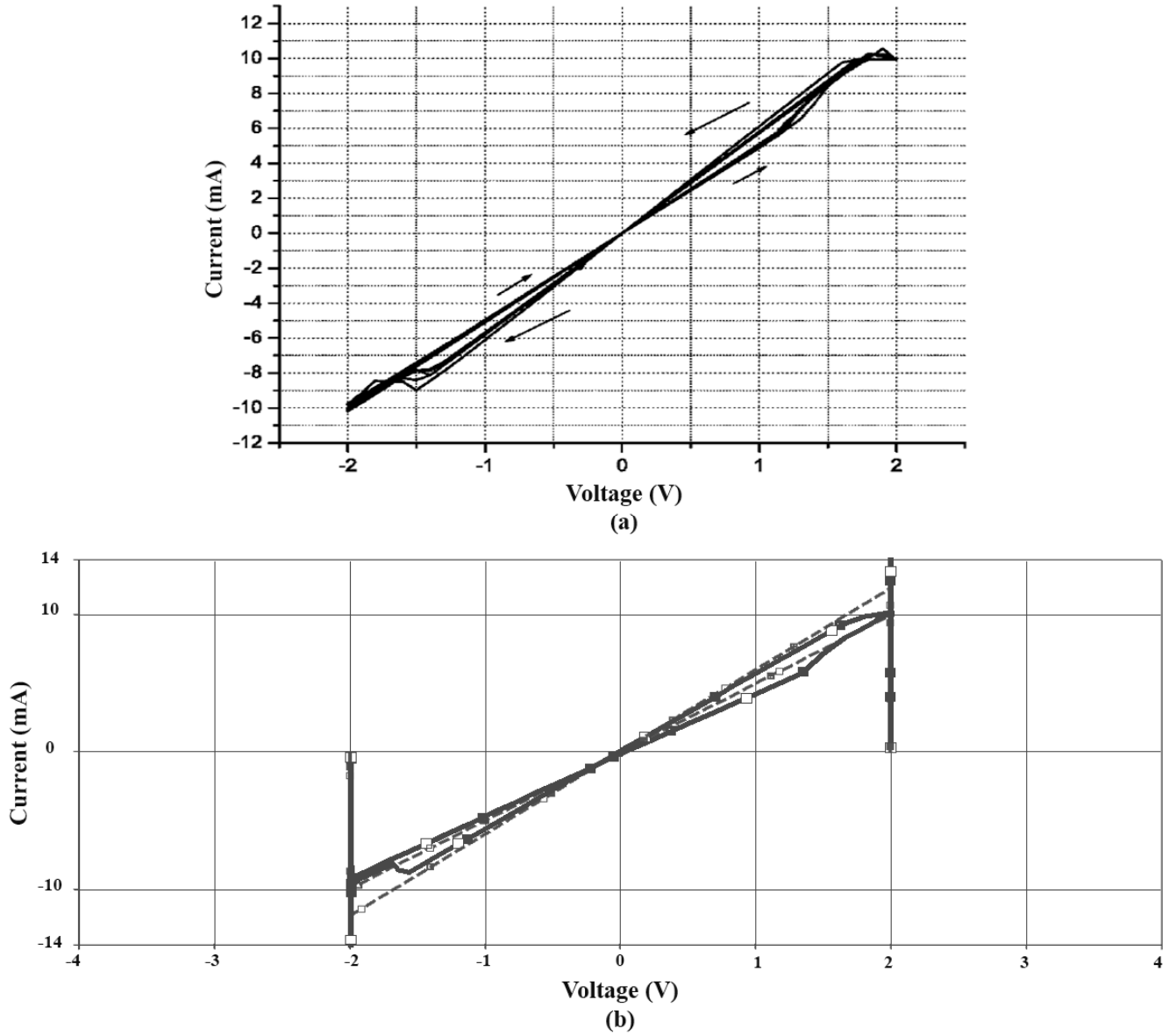

Figure 7. (a) *I-V* characteristic of the ZnO/aluminum stack which shows hysteresis behavior. Figure source:Lüssem (2006). (b) The simulation result curves by the use of the LHM (dashed line) and GHM (solid line). For achieving the LHM output the forward and reverse slope values are specified by utilizing two different resistors (166 Ω and 200 Ω respectively).

DISCUSSION

The proposed behavioral model is easy to use and operates in a short period of time and with very good accuracy. However, the model has a main disadvantage in that it cannot produce a smooth and continuous output when the input signal changes its direction (rising and or falling points). However, for overcoming this disadvantage this model is modified by adding a simple integrator circuit (Figure 9) to points A and B of the proposed circuit model. The effect of this modification is found in Figure 10. Figure 10(a) provides the applied voltage to the device which its *I/V* curve was previously shown in Figure 7(a); Figure 10(c) and (b) demonstrate the response of the device to the applied voltage with and without utilizing the proposed integrator circuit, respectively. As mentioned before, utilizing two resistors in the LHM instead of the GHM leads to more simplicity. However, in the forward and reverse paths the discontinuous behavior is appeared (Figure 10(b)). As seen in Figure10(c), exploiting a simple integrator circuit makes these points disappear. As an instance, in the appendix, the SPICE NETLIST of the proposed hysteresis circuit model for Figure 7 is presented.

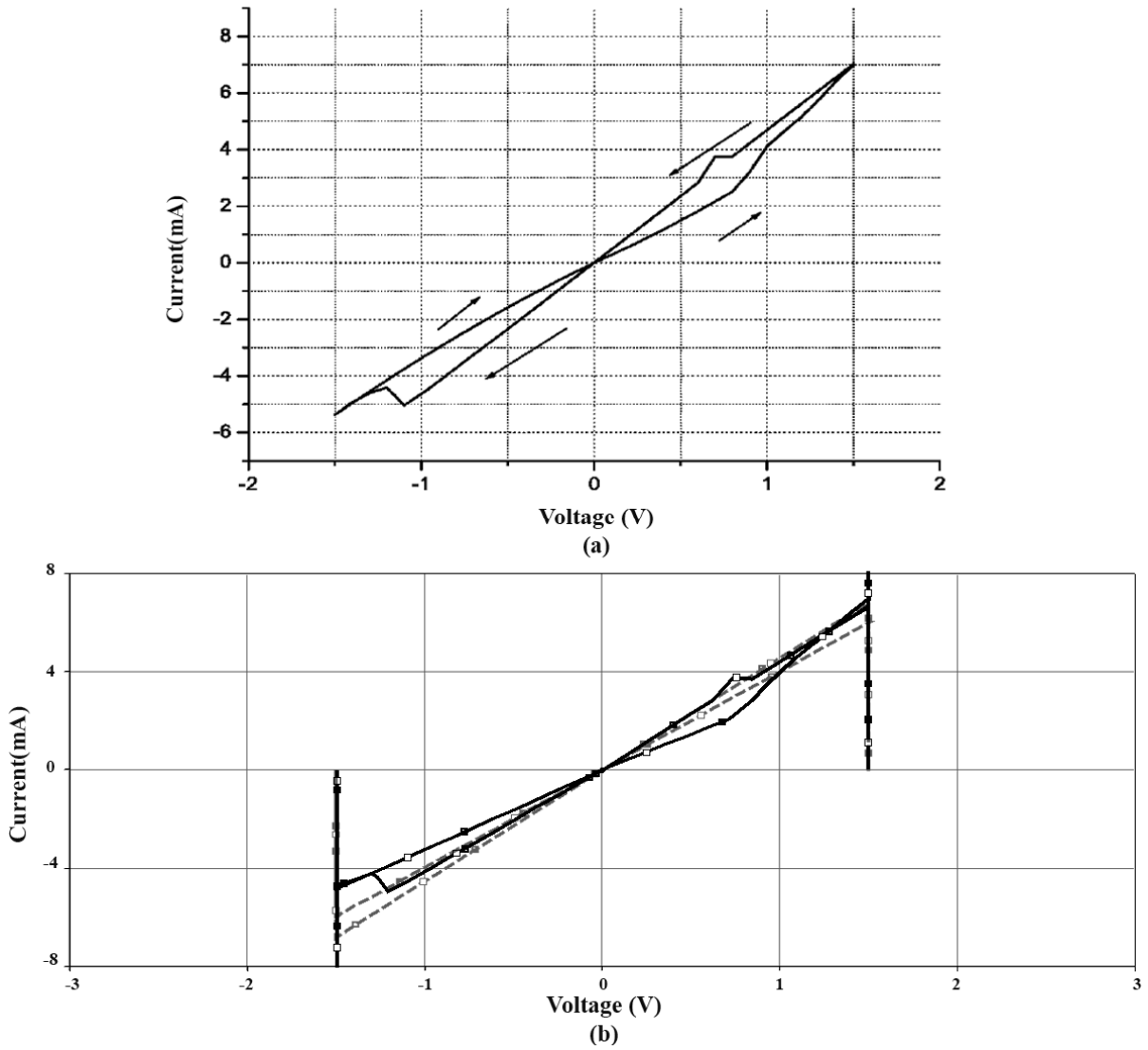

Figure 8. (a) *I-V* characteristic of the ITO/aluminum stack which shows hysteresis behavior. Figure source: Lüssem, (2006). (b) The simulation result curves by the use of the LHM (dashed line) and GHM (solid line). For achieving the LHM output the forward and reverse slope values are specified by utilizing two different resistors (250 Ω and 219 Ω respectively).

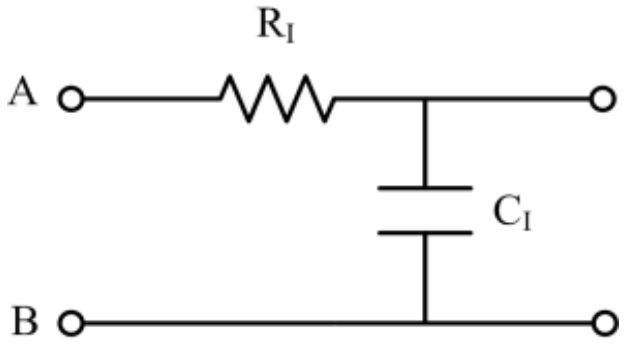

Figure 9. Applying simple integrator circuit helps to achieve continuous curves in the output.

Conclusions

Since molecular electronics attracts much attention in literature; some effort has been made to model molecular electronic behavior. However, all of the proposed models do not support the hysteresis phenomenon. To the best of the authors' knowledge, for the first time, this paper proposes a behavioral model for the hysteresis phenomenon in simulating molecular electronic devices. The proposed behavioral model is implemented in SPICE with two different approaches (the LHM and GHM) and the correct operation of each approach is investigated. The proposed model is then modified by adding a simple integrator circuit for solving the discrete points' problem.

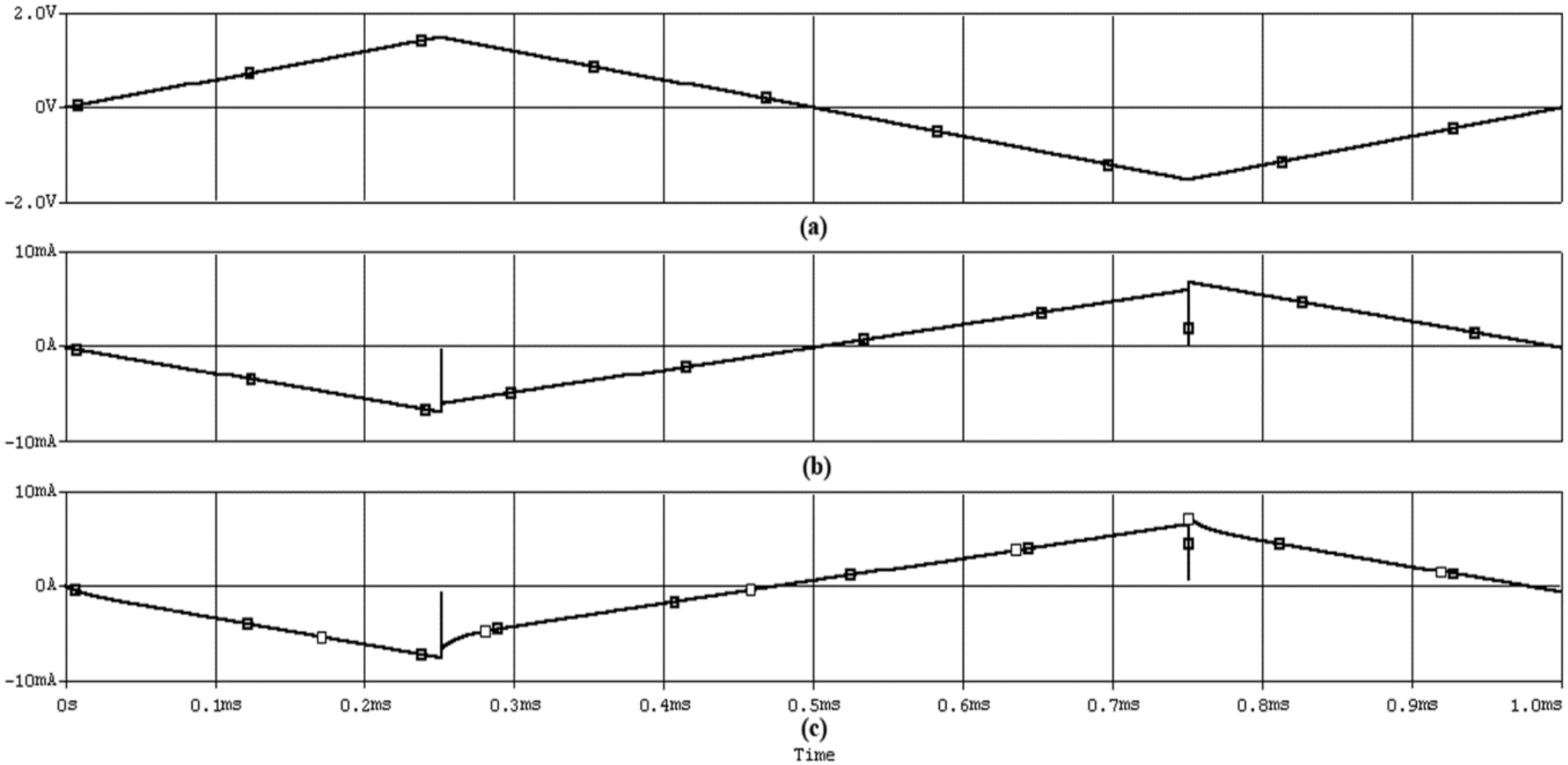

Figure 10. The effect of using integrator circuit in the proposed circuit for modeling the Figure 7 *I/V* curve. (a) Applied voltage. (b) Current curve without exploiting the integrator circuit. (c) Current curve after modification and with exploitation of the integrator circuit. The applied characteristics are: C_I=100 nF and R_I=0.1 KΩ.

This model helps the circuit designer to evaluate a design with more simplicity and accuracy.

APPENDIX

In this appendix, a SPICE NETLIST for the simulation result of Figure 7 curve is demonstrated. This simulation uses the modified GHM approach.

```
C_C21      N34624 N34628 1n
R_R2       0 N34754 20
C_C1       N09392 N11976 1n
R_R1       0 N11976 1k
R_R3       0 N09392 100k
X_S2       N59306 0 N09392 N24506 SCHEMATIC1_S2
V_V1       N09392 0
+PWL 0 0 250us 2 750us -2 1000us 0
G_G220     N34754 N24506 TABLE {V(N34754,
```

```
N24506)}
+ [(0,0) (1.25,6 m) (1.4,8 m) (1.5,8.5 m) (1.75,10 m)]
R_R5        N627581 N09392 1k
C_C11       N24506 N34754 1n
C_C2        0 N627581 10n
R_R4        N34628 0 10
C_C12       N24506 N34754 1n
G_G230          N34754  N24506  TABLE  {V(N34754,
N24506)}
+ [(-2, -10 m) (0, 0)]
E_U2        N23820 0 VALUE {LIMIT(V(N11976, 0)*1E6, -
1V, +1V)}
E_U1        N59306 0 VALUE {LIMIT(V(N11976, 0)*1E6, -
1V, +1V)}
G_G130    N34628 N34624 TABLE {V(N34628, N34624)}
+ [(-2,-10m) (-1.6, -8.2 m) (-1.5, -9 m) (0, 0)]
G_G120    N34628 N34624 TABLE {V(N34628, N34624)
}
+ [(0, 0) (1.5, 9 m) (1.75, 10 m)]
X_S1    0 N23820 N34624 N09392 SCHEMATIC1_S1
C_C22       N34624 N34628 1n
.subckt SCHEMATIC1_S2 1 2 3 4
S_S2        3 4 1 2 Sbreak
RS_S2       1 2 1G
.ends SCHEMATIC1_S2
.subckt SCHEMATIC1_S1 1 2 3 4
S_S1        3 4 1 2 Sbreak
RS_S1       1 2 1G
.ends SCHEMATIC1_S1
```

Conflict of Interests

The author(s) have not declared any conflict of interests.

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