A Versatile Memristor Model With Nonlinear Dopant Kinetics

Themistoklis Prodromakis, Member, IEEE, Boon Pin Peh, Christos Papavassiliou, Senior Member, IEEE, and Christofer Toumazou, Fellow, IEEE

Abstract—The need for reliable models that take into account the nonlinear kinetics of dopants is nowadays of paramount importance, particularly with the physical dimensions of electron devices shrinking to the deep nanoscale range and the development of emerging nanoionic systems such as the memristor. In this paper, we present a novel nonlinear dopant drift model that resolves the boundary issues existing in previously reported models that can be easily adjusted to match the dynamics of distinct memristive elements. With the aid of this model, we examine switching mechanisms, current–voltage characteristics, and the collective ion transport in two terminal memristive devices, providing new insights on memristive behavior.

Index Terms—Memristive devices, memristor model, memristor, nonlinear dopant kinetics.

I. INTRODUCTION

The twentieth century has witnessed an exceptional technological progress that has been mainly driven by the invention of the transistor and integrated circuits. Chemistry and materials science have played a pivotal role in this evolution by enabling the development of active devices with distinct and reliable properties that, over the past 60 years, have been following Moore’s scaling trend [1]. Complementary metal–oxide–semiconductor technology is however approaching the nanoscale floor, with devices attaining comparable dimensions to their constituting atoms. This imposes significant challenges on the performance, reliability, and, eventually, manufacturability of analog and digital circuits. However, in 1959, Feynman [2] proposed that there is plenty of room at the bottom, and he correctly predicted that the operation of emerging devices would rely on the manipulation of just a few atoms; the memristor is nowadays considered as an exemplar device.

Memristive behavior has, in fact, existed for many years [3]–[5], but the phenomenon was not properly deciphered until 2008 when a team from HP Laboratories successfully correlated the characteristics of nanoscale switches in crossbar architectures [6], [7] with the theory originally presented by Chua [8] and later on by Chua and Kang [9]. Since then, the various attributes of memristors, such as their infinitesimal dimensions, their ability to be operated with low power, and their dynamic response have been proclaimed to be fitting in diverse applications, i.e., from nonvolatile memory [10] to programmable logic [11] and beyond [12]. Particular emphasis is however given to the nonlinear nature of the device that resembles the behavior of chemical synapses [13], [14]. While memristors have already been used to demonstrate primitive artificial intelligence [15], this marks a new era for neuromorphic engineering.

To date, memristive dynamics are described through a number of analytical models that approximate the kinetics of intrinsic dopants in linear [16] and nonlinear manners [17]–[19]. On the other hand, memristors come in many flavors, with active cores that are based on oxygen-rich TiO$_2$ films (TiO$_2$/TiO$_{2+x}$) [20], [21], Ag-loaded Si films [14], and TiO$_2$ sol–gel solutions [22], with the switching mechanisms of such nanoionic systems troubling engineers even up to date [23].

In this paper, we present a novel memristor model that takes into account the nonlinear nature of the dopant kinetics and the boundary limiting effects. Section II reviews existing models with distinct attributes being briefly compared. In Section III, we present our modeling approach, which comprises two control parameters for appropriately refining the model to match the distinct dynamics of diverse systems. Finally, a thorough comparison between our model and preexisting models is performed, whereas the paper is concluded by evaluating our model against measured data of in-house fabricated memristors.

II. MEMRISTIVE DYNAMICS WITH LINEAR AND NONLINEAR KINETICS

Memristance was initially postulated [8] as the functional property of memristors that correlates charge and flux, i.e.,

$$ M = \frac{d\phi}{dq}. $$

(1)

Later on, Chua and Kang [9] generalized the concept to memristive systems, i.e.,

$$ v = R(x)i $$

(2)

$$ \frac{dx}{dt} = f(x, i) $$

(3)

where $v$ is the voltage, $i$ is the current, and $R(x)$ is the instantaneous resistance that is dependent on the internal state variable $x$ of the device. This state variable $x$ is bounded within...
the interval [0, 1], and it is simply the normalized width of the doped region \( x = w/D \), with \( D \) being the total thickness of the switching bilayer. At time \( t \), the width of the doped region depends on the amount of charge that has passed through the device; thus, the time derivative of \( w \) is a function of current, which can be described as

\[
\frac{dw}{dt} = U_D = \mu E = \frac{\mu R_{\text{on}}i(t)}{D} \tag{4}
\]

where \( U_D \) is the speed at which the boundary drifts between the doped and undoped regions, \( \mu \) is the average dopant mobility, \( E \) is the electric field across the doped region in the presence of current \( i(t) \), and \( R_{\text{on}} \) is the net resistance of the device when the active region is completely doped.

When assuming that the generated electric field is small enough, the linear dopant drift model can approximate the dynamics of a memristor. However, this model is invalidated at boundaries \( w < 0 \) or \( w > D \). This is due to the influence of a nonuniform electric field that significantly suppresses the drift of the dopants.

The limitations of this model are revealed when, for example, driving a TiO\(_2\)/TiO\(_2\)-\( \_x \) memristor (\( R_{\text{on}} = 100 \, \Omega \), \( R_{\text{off}} = 16 \, k\Omega \), \( w_0 = 5 \, nm \), \( D = 10 \, nm \), and \( \mu = 10^{-14} \, m^2/V \cdot s \)) into its extreme states, i.e., saturation \( (w = D) \) and depletion \( (w = 0) \). These two extremes can be achieved when the device is biased with a \( \pm 1\)-V sinusoidal stimulus of \( \omega = 1 \, \text{rad/s} \), as demonstrated in Fig. 1. In the case of saturation, \( w \) exceeds the limit value of \( D \) (10 nm), whereas the device’s memristance falls below the 100-\( \Omega \) cutoff value \( (R_{\text{on}}) \). Likewise, in depletion, \( w \) can take negative values with the memristance exceeding the upper limit of \( 16 \, k\Omega \) \( (R_{\text{off}}) \), which is clearly erroneous.

Nonlinear dopant drift can be taken into account by introducing an appropriate window function \( f(x) \) in (4), i.e.,

\[
\frac{dx}{dt} = \frac{\mu R_{\text{on}}i(t)}{D^2} f(x). \tag{5}
\]

This window function models the nonlinear dopant kinetics in the active bilayer and returns a scalar value based on the coordinate of the device’s width \( w \). Any effective window function should therefore fulfill the following conditions:

1) take into account the boundary conditions at the top and bottom electrodes of the device;
2) be capable of imposing nonlinear drift over the entire active core of the device;
3) provide linkage between the linear and nonlinear dopant drift models;
4) be scalable, meaning a range of \( f_{\text{max}}(x) \) can be obtained such that \( 0 \leq f_{\text{max}}(x) \leq 1 \);
5) utilize a built-in control parameter for adjusting the model.

Joglekar and Wolf [18] proposed the following window function:

\[
f(x) = 1 - (2x^2 - 1)^{2p} \tag{6}
\]

with \( p \) as a positive exponent parameter [18]. This window function ensures zero drift at the boundaries, i.e., \( f(0) = f(1) = 0 \). For \( p = 1 \), nonlinear drift is imposed over the entire active region \( D \), whereas for \( p \to \infty \), the model resembles linear dopant drift; thus, aims 1, 2, 3, and 5 are achieved. However, a significant liability of this model lies in the fact that if \( w \) hits any of the boundaries \( (w = 0 \text{ or } w = D) \), the state of the device cannot be further adjusted. This will be, from now on, termed as the “terminal-state problem.”

Bielek et al. [17] addressed this issue by suggesting an alternative window function that included memristive current \( i \) as an additional parameter, i.e.,

\[
f(x) = 1 - (x - \text{sgn}(i)\,i)^{2p} \tag{7}
\]

where \( \text{sgn}(i) = 1 \) for \( i \geq 0 \), and \( \text{sgn}(i) = 0 \) for \( i < 0 \). A positive (negative) current is associated with the increasing (decreasing) width of the doped region. The depleted or saturated device can be brought out of the terminal states when the current reverses direction. This is achieved via the steep throughs at \( x = 0 \) and \( x = 1 \). The features of this particular window function fulfill aims 2, 3, and 5, with limited success, however, in 1 and 4.

Strukov et al. [16] proposed the following window function:

\[
f(w) = w(D - w)/D^2 \tag{8}
\]

which can be rewritten in terms of the state variable giving \( f(x) = x^2 - x^2 \). This window function was also exercised by Benderli and Wey [19] to form a SPICE macromodel of TiO\(_2\) memristors. The boundary condition at the OFF-state when \( w = 0 \) is resolved since \( f(x) = 0 \), whereas it also imposes nonlinear drift over the bulk of the device. However, this particular window function lacks in flexibility, whereas the terminal-state problem remains prevalent. It is interesting to note that this

\[1\] We should note here that, in practice, an impeding drift term also exists, as described by Strukov et al. [24], which is however omitted here for simplicity and for enhancing the versatility of our model.
window function is, in fact, a scaled version of Joglekar’s model (by a factor of 4) when \( p \) is set to 1. Table I summarizes the attributes of the aforementioned window functions. At this point, we also like to acknowledge the possibility of the dopants drift exceeding the values that are calculated through the preexisting linear and nonlinear models, particularly in the bulk of the memristor giving \( f(x) > 1 \). An example where such a case is valid is shown in [25], where programmable nanowires exhibit a hysteric behavior along with gain.

III. NOVEL MEMRISTOR MODEL

The nonlinear nature of the dopants is typically dominating at the two extremes \((w \to 0 \text{ and } w \to D)\). This can be modeled through a parabola that is symmetric at \( x = 0.5 \) and is of the form

\[
f(x) = -Ax^2 + Bx + C \tag{9}
\]

where the three constants \( A, B, \text{ and } C \) are determined through

\[
\left| \frac{df}{dx} \right|_{x=0.5} = 0 \tag{10}
\]

\[
f(0.5) = 1 \tag{11}
\]

\[
f(0) = f(1) = 0. \tag{12}
\]

A simple calculation shows that \( f(x) = -4x^2 + 4x \), which coincides with Joglekar and Wolf’s window function when \( p = 1 \), but is still considerably different from \( f(x) = 1 - (2x - 1)^2 \). Expanding the terms in the brackets gives \( f(x) = 1 - (4x^2 - 4x + 1) \). It is immediately obvious that all terms containing state variable \( x \) can be grouped under the influence of an exponent control parameter, yielding a family of curves. In addition, introducing \(+1\) outside the brackets ensures \( f_{\max}(x) = 1 \).

The purpose of having a control parameter as an exponent is to incorporate scalability and flexibility in window function \( f(x) \) that describes the dopant kinetics. Although Joglekar and Wolf’s \( p \) parameter is successful in creating a family of distinct curves, it lacks the necessary scalability, i.e., scaling \( f(x) \) either upward or downward. Motivated by this observation, we proceed to modify Strukov’s window function since it is based on a smooth parabolic function. Completing the square and ensuring \( f_{\max}(x) = 1 \) yields

\[
f(x) = x - x^2 = -[(x - 0.5)^2 - 0.25] \tag{13}
\]

\[
= 1 - [(x - 0.5)^2 + 0.75]. \tag{14}
\]

Finally, control parameter \( p \) is introduced, i.e.,

\[
f(x) = 1 - [(x - 0.5)^2 + 0.75]^p \tag{15}
\]

where \( p \in \mathbb{R}^+ \). This new window function is demonstrated in Fig. 2 for various values of \( p \), where it can be observed that, for \( p = 1 \), it becomes identical to Strukov’s model.

The introduced control parameter \( p \) acts in three distinct roles. It allows the window function to scale upward, which implies that \( f_{\max}(x) \) can take any value within \( 0 \leq f_{\max}(x) \leq 1 \). In addition, \( p \) can take any positive real number, unlike the constraint of the control parameter being an integer in the models proposed by Joglekar and Wolf [18] and Biolek et al. [17], allowing a greater extent of flexibility. Values of \( p = 1, 2, 4, 8, \text{ and } 10 \) can be chosen to impose distinct nonlinear drift over the entire bilayer (see Fig. 2), whereas a very large value of \( p \) can provide linkage with the linear dopant drift model.

The boundary issues are now resolved with the window function returning a zero value at the active bilayer edges, whereas the drift of the dopants is strongly suppressed near the metal contact interfaces. On the other hand, the terminal-state problem is eradicated by adopting a feedback implementation. Therefore, the proposed window function, as represented by (15), satisfies all the prerequisites and improves on the shortcomings of existing models.

In the peculiar case where the dopant’s drift is such that \( f_{\max} \geq 1 \), the proposed window function can be adjusted, i.e.,

\[
f(x) = j \left(1 - [(x - 0.5)^2 + 0.75]^p\right) \tag{16}
\]

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![Fig. 2. Plot of our proposed window function](image-url)
Fig. 3. Proposed window function \( f(x) = j(1 - [(x - 0.5)^2 + 0.75]^p) \) versus normalized width of the doped region \( x \) with \( p = 10 \) and \( j \) varying.

where \( p \) and \( x \) are as previously defined, and \( j \) is a scalar acting as a second control parameter. For any particular \( p \), \( f(x) \) can be scaled upward or downward with a suitable value of \( j \). The alternative window function with \( p \) fixed at 10 is illustrated in Fig. 3. As \( j \) varies, a family of curves is formed, allowing easy modification of the model.

**IV. RESULTS AND DISCUSSION**

A. Solving the “Terminal-State” Problem

The presented model has been evaluated by simulating the response of a single memristor with identical parameters to the one presented in Section II. Particular emphasis is given when the device is driven into depletion and saturation since these extremes have been identified to be problematic in existing models. Our window function was first implemented with \( p = 10 \) to impose nonlinear drift across the whole bilayer. The resulting \( I-V \) curve is depicted in Fig. 4. When compared with previously reported data [16]–[19], this pinched hysteresis loop is shown to be asymmetrical, whereas the OFF-state of the device is highly nonlinear. The first observation arises due to the different switching rates of the ON- and OFF-states, whereas the second can be explained as a nonohmic characteristic of the OFF-state. These results are in good agreement with measured data provided in [7] and [24].

When the device is driven into its OFF-state, the corresponding memristance remains high, which is illustrated in Fig. 5 for \( 6 \leq t \leq 7 \) s. It is also evident that the width \( w \) of the doped region does not exceed \( D \), whereas the memristance is correctly limited by \( R_{on} = 100 \). When the bias polarity is reversed, the depletion extreme is modeled, and it is demonstrated in the same figure that the device does not take any erroneous states, i.e., \( w \leq 0 \) or \( M > R_{off} \). This demonstrates that our model is essentially free of the terminal-state problem.

B. Accounting for Nonlinear and Linear Dopant Kinetics

In the case of the linear dopant drift model, it takes 650 ms to drive the memristor into saturation, as denoted in Fig. 1. However, for the same applied bias, the proposed nonlinear dopant drift model requires a significantly larger time frame of 3.15 s to reach saturation at \( w = 9.892 \) nm, with a corresponding memristance of 271.6 \( \Omega \). Likewise, this divergence is investigated for a nonsaturation condition for 1 \( \mu C \) of charge. If a linear dopant drift model is assumed, the change in \( w \) is calculated to be \( \Delta w = 1.2 \) Å, where a nonlinear dopant drift model results into \( \Delta w = 0.14 \) Å. Moreover, it is observed that, for the same stimulus, the net displacements of \( w \) are 4.892 and 4.673 nm for the positive and negative bias polarities, respectively. This is in agreement with the notion that the ON and OFF switching rates are not identical, due to the asymmetric nature of the device.

Next, we set \( p = 40 \) to approximate the linear dopant drift model and test the robustness of our window function by applying a large voltage bias, as shown in Fig. 6. Under a 10-V sinusoidal biasing scheme, the device is driven harder, but caution is exercised to ensure the current flow does not exceed the maximum allowable current given by \( V_{\text{max}}/R_{on} = 100 \) mA. It is illustrated that the device remains in saturation most of the time. In addition, the memristor is capable of memorizing the exact amount of charge that has passed through it, even when the device is saturated, which was also validated by Biolek et al.
Fig. 6. Modeling of memristance $M$ and doped region width $w$ modulation at saturation ($w \rightarrow D$) and depletion ($w \rightarrow 0$) for a sine wave of $\pm 10$ V at 1 rad/s. Our proposed model was implemented for $p = 40$ and $j = 1$, demonstrating an effective solution to the “terminal-state problem.”

[17], in contradiction to the original HP memristor model [16]. The same argument also holds when the bias polarity is reversed and the device is driven to its OFF-state.

C. Adjusting the Window Function

The versatility of our model is illustrated in Fig. 7(a), where the $I$–$V$ characteristic curves of our memristor model are plotted for nine representative cases. These cases combine three distinct $j$ values ($j = 0.5, 1,$ and 1.5), whereas $p$ is set to 100 to resemble a linear drift model and to $p = 1$ and $p = 10$ to establish a nonlinear drift window function. The benefits of having two calibration parameters are further revealed in Fig. 7(b), where the corresponding time evolution of our device’s memristance is calculated for all nine cases. The inset in the same figure depicts the total calculated charge when our model device is simulated with the same $p$ and $j$ values, as previously utilized. Parameter $j$ is responsible for vertically scaling the window function, whereas $p$ rather supports lateral scaling, and both essentially modulate the effective mobility of the device. This model indeed demonstrates higher flexibility from the preexisting ones that can be beneficial in describing devices of distinct dynamics.

D. Evaluation Against Preexisting Models

As a figure of merit, Fig. 8 depicts the $I$–$V$ characteristics of our standard memristor as calculated by the proposed model and the models presented in Section II. Wherever applies, $p$ was set to 1 to obtain a fairer comparison. For a 2-V peak-to-peak sine wave of $\omega = 1$ rad/s, our proposed model coincides with Strukov’s model, which cannot be however scaled in its original description. Joglekar’s and Biolek’s models, however, significantly diverge, and particularly, the latter demonstrates some discontinuities, which are evident in the negative voltage domain. To further illustrate the versatility of our model, we have matched the corresponding $I$–$V$ responses of Joglekar’s and Biolek’s models by setting $j = 4/p = 1$ and $j = 0.5/p = 200$, respectively.

E. Reproducing the Response of a $\text{TiO}_2/\text{TiO}_2^{2+}$ Memristor

As a final test, the proposed model was employed to emulate the response of an in-house fabricated memristor. The device was developed based on the process flowchart described in [20], with a 20-nm-thick $\text{TiO}_2/\text{TiO}_2^{2+}$ bilayer. A microphotograph
of the device and the interfacing pads is presented in inset A in Fig. 9. The device was characterized with a symmetric triangular wave of ±4 V at ω=0.82 rad/s, and it was simulated with the following parameters: $D = 20 \text{ nm}$, $w_0 = 10 \text{ nm}$, $R_{\text{off}} = 250 \text{ Ω}$, and $R_{\text{on}} = 25 \text{ Ω}$. At the same time, the control parameters of the proposed model were set to $j = 1.3$ and $p = 3$.

Fig. 9 illustrates the measured, along with the simulated, $I–V$ characteristic responses of the device, with the arrows indicating the biasing sequence. Clearly, the experimental and simulated results are in very good agreement. Some discrepancies appear above 2 V and below −3.5 V, which are however associated with the bipolar switching of the device between its high- and low-resistive states and are only signified when observing the device’s current in a logarithmic scale. A better matching is observed in inset B in the same figure, where the $I–V$ relation is linearly plotted. A small disagreement between the measured and simulated data is shown to exist on the peaks of both hysteric loops, which are due to the 100-mA compliance current of our instrumentation and is thus insignificant.

V. Conclusion

A versatile memristor model has been presented that renders the nonlinear kinetics of the mobile dopants within the active bilayer of the device. The drift of the dopants is described through a novel parabolic window function that resolves issues that typically appear when the device is driven at its extremes, i.e., depletion and saturation. In addition, two control parameters $j$ and $p$ are introduced that enable diverse scaling of the window function, which is shown to support both linear and nonlinear dopant kinetics. This flexibility is particularly important as it allows our model to be utilized in memristive systems of dissimilar mechanics. Finally, the proposed model was validated with measured results from key publications and an in-house fabricated TiO$_2$/TiO$_2$+x memristor, with the measured and simulated data matching rigorously.

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REFERENCES

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Boon Pin Peh, photograph and biography not available at the time of publication.

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Prof. Toumazou is a Fellow of The Royal Society and the Royal Academy of Engineering. He is a member of many professional committees and has made outstanding contributions in the fields of low-power analog circuit design and current mode circuits and systems for biomedical and wireless applications. He was invited to deliver the 2003 Royal Society Clifford Patterson Prize Lecture, entitled “The Bionic Man,” for which he was awarded The Royal Society Clifford Patterson Bronze Medal. He was the recipient of the IEEE Circuits and Systems Society Education Award for pioneering contributions to telecommunications and biomedical circuits and systems, as well as the Silver Medal from the Royal Academy of Engineering for his outstanding personal contributions to British engineering.