Physics-Based Compact Model for the Current in Hexagonal Boron Nitride Memristive Devices

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***Abstract*—This paper presents a physics-based compact model for hexagonal boron nitride memristive devices. The use of two-dimensional materials is becoming increasingly popular. In order to evaluate their potential for applications, simulations are necessary or provide helpful support, for example for hardware-based artificial neural networks. For circuit simulations keeping a close link to the device technology, physics-based compact models are required. In this paper, a new approach and implementation of such a model for resistive switching in hexagonal boron nitride memristive devices is presented. Comparison with measurements show good agreement and provide further physical insight to the switching process.**

***Index Terms*—Two-dimensional materials, memristive devices, physics-based, compact model, artificial neural networks, hexagonal boron nitride, resistive switching**

I. Introduction

Memristive devices (MD) are promising candidates for various applications, such as non-volatile memory or hardware-based artificial neural networks [1] [2]. Research in the field of two-dimensional (2D) materials has increased [3]. MDs made of 2D materials offer advantages such as high flexibility, coexistence of volatile and non-volatile switching, good controllability of potentiation and depression processes, and high thermal stability [4]. Multilayer hexagonal boron nitride (h-BN) is particularly suitable as a 2D material [4]. MDs have two states: high-resistive state (HRS) when they are off and low-resistive state (LRS) when they are on [5]. The transition from HRS to LRS is called SET and corresponds to the potentiation of synapses. The transition from LRS to HRS is called RESET and corresponds to the depression of synapses. The h-BN MDs exhibit device-to-device (D2D) variability [6]. Compact models are important for research and evaluation of circuit concepts. To our best knowledge, no physics-based compact model has yet been published that is tailored to the specific physics and properties of MDs with 2D materials. Therefore, an initial physical compact model for h-BN MDs is introduced below.

II. Modeling Approach

The model development consists of three steps which are summarized in this section. First, the current through a single defect in a h-BN layer is estimated. In a second step, the statistical switching process of multiple defects is described. Finally, the total device current is calculated.

A. Defect Current

The physics-based compact model has been developed for the simulation of h-BN MDs (also known as two-terminal metal/insulator/metal (MIM) nanoscale devices). **Figure 1** shows the band diagram (inspired by [1]) of such a device as the basis for the model. First, we focus on monolayer h-BN. It is important to note that we consider boron vacancies within the h-BN layer that act as defects, resulting in a Fermi level close the valence band edge. The distance from the Fermi level of the electrodes to the vacuum level is referred to as ϕ_1 and the distance from the valence band in the h-BN layer as ϕ_2. Between the top and bottom electrodes and the h-BN layer, there is a van der Waals gap of length d. In order for an electron to flow from the top to the bottom electrode, it must tunnel through the two van der Waals gaps. The van der Waals gaps arise because no chemical bond is possible between the electrodes and the h-BN layer, thus creating a vacuum. It is supposed that these are rectangular barriers with tunnel probabilities T_1 and T_2.

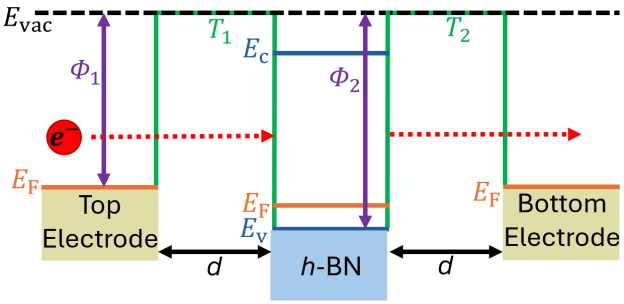

Fig. 1. Representation of the band diagram of a monolayer h-BN MD. There are van der Waals gaps between the electrodes and the h-BN layer. An electron can overcome these with a tunneling probability of T.

When the h-BN MDs are in HRS, an electron must tunnel through the barriers with probability T_1 and T_2 (**figure 2 (a)**). When a positive voltage between top and bottom electrode is applied, metal atoms detach from the top electrode and form a bridge to the h-BN layer (**figure 2 (b)**) [2]. If the voltage was too low, it disappears after the voltage is switched off (volatile switching). If the voltage was high enough, a

permanent bridge consisting of several metal atoms forms (non-volatile switching). Once the bridge is formed, the h-BN MD is in the LRS and an electron only has to tunnel through T_2 (**figure 2 (c)**).The h-BN layer has boron vacancies given by a certain defect density (**figure 2 (d)**). The metal atoms preferentially form a bridge to these defects.

The modeling approach is based on the fact that over time, when a voltage V is applied, more and more bridges form to the defects, where n_{LRS} indicates the number of defects in the LRS per area (**figure 2 (e)**). Defects without bridges are in the HRS and supply the current dI_{HRS}, while defects with bridges are in the LRS and supply the current dI_{LRS}. The total current over time can be determined from the evolving number of defects with and without bridges (**figure 2 (f)**).

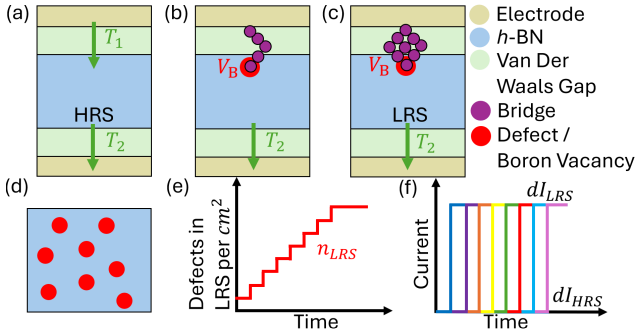

Fig. 2. (a) Structure of the h-BN MD in the HRS. (b) Formation of a metal atom bridge from the top electrode to a defect in the h-BN layer. (c) Structure of the h-BN MD in the LRS. (d) Representation of the defects (boron vacancies) in the h-BN layer. (d) Representation of how the metal bridges develop over time. (f) Switching currents of single defects at different time steps.

Based on this, physical formulas were determined to calculate the current through the h-BN MD. In the model, we divide the device into spatial cells that can either switch into LRS or remain in HRS, with a density of N_0 cells per area. The current dI_{LRS} through a single cell in the LRS (metal bridge formed to a defect in this cell) is calculated using

$$dI_{LRS} = I_0 \cdot T_2 \cdot \sinh\left(-\frac{V}{V_0}\right), \tag{1}$$

where the prefactor I_0 is an empirical fitting parameter, $sinh(-V/V_0)$ describes the exponential dependence of the tunnel current, T_2 is the tunnel probability, and V_0 is a voltage coefficient. To calculate the current dI_{HRS} through a cell without a bridge (i.e. a cell without a defect, or a cell with a defect in HRS), the tunneling probability T_1 and T_2 must be taken into account, as two barriers must be tunneled through here.

$$dI_{HRS} = I_0 \cdot T_1 \cdot T_2 \cdot \sinh\left(-\frac{V}{V_0}\right). \tag{2}$$

The tunnel probability can be calculated using

$$T_{1/2} = \exp\left(-\frac{2d}{\hbar} \cdot \sqrt{2m_0\Phi_{1/2}}\right), \tag{3}$$

which is valid for a rectangular barrier [7]. To calculate the current densities, we denote the defect density in the device by D^0, i.e. the number of cells with defects per area.

When the device is in the HRS, it is supposed that no bridges have formed for any defect. Similarly we assume that in LRS a bridge has been formed at all defects. Based on these considerations, we obtain for the relation between the current densites in LRS and HRS the following expression:

$$\frac{J_{LRS}}{J_{HRS}} = \frac{D^0 \cdot dI_{LRS} + \left(N_0 - D^0\right) \cdot dI_{HRS}}{N_0 \cdot dI_{HRS}}. \tag{4}$$

Considering $dI_{HRS} = dI_{LRS} \cdot T_1$, **equation (4)** can be solved for the defect density D^0 as follows:

$$D^0 = N_0 \cdot \frac{\frac{J_{LRS}}{J_{HRS}} - 1}{\frac{1}{T_1} - 1}. \tag{5}$$

B. Statistical Switching Process

In the following, we derive the model equations for switching from HRS to LRS. However, the approach can be transferred for modeling the process from LRS to HRS.

For the statistical process of forming atomic metal bridges we assume an exponential distribution with rate parameter λ:

$$f_\lambda(t) = \lambda \cdot \exp\left(-\lambda \cdot t\right). \tag{6}$$

This exponential relationship in the development of defects was already identified in earlier work on a statistical model for calculating expected variations in devices whose function is based on defects [8]. The calculation of λ is motivated by an Arrhenius equation:

$$\lambda = \lambda_0 \cdot \exp\left(\alpha \cdot \frac{q \cdot V - E_A}{kT}\right). \tag{7}$$

The formation of bridges to the defects (SET cycle), as well as their breakage (RESET cycle), and therefore the rate parameter of the exponential distribution depends on the applied voltage V. Parameter E_A is the activation energy for movement of metal atoms into a defect or for releasing from a defect. Parameter α is a field enhancement factor, i.e., how the voltage actually affects the barrier on an atomic scale, and λ_0 is an empirical fitting parameter. We denote n_{LRS} as the number of defects (or rather cells with defects) per area which at time t have already switched to the LRS. Therefore, the number of remaining defects per area as candidates for switching is given by D^0 - n_{LRS}. By applying the exponential distribution function, the number of defects per area, which are forming a bridge within time interval dt can be calculated by:

$$d_{nLRS} = \left(1 - \exp\left(-\lambda \cdot dt\right)\right) \cdot \left(D^0 - n_{LRS}\left(t\right)\right). \tag{8}$$

For a numercial implementation, we calculate the defect density in LRS at time t_1 = t_0 + dt by:

$$n_{LRS}(t_1) = n_{LRS}(t_0) + d_{nLRS}(t_0). \quad (9)$$

The procedure for switching from LRS to HRS is analogous to switching from HRS to LRS. However, **equation (8)** must be modified for this purpose:

$$d_{nLRS} = -(1 - \exp(-\lambda \cdot dt)) \cdot (n_{LRS}(t)). \quad (10)$$

In addition, the difference is that different parameter values E_A and α are used for SET and RESET.

C. Total Device Current

Equation (1) and **(2)** can be used to calculate the current through a single cell in the LRS and HRS, respectively. **Equation (8)** - **(10)** can be used to determine the number of cells in LRS per area (n_{LRS}). Finally, from these parameters the total current I through a MD having an area A can be calculated:

$$I = \left(n_{LRS} \cdot dI_{LRS} + \left(D^0 - n_{LRS}\right) \cdot dI_{HRS}\right) \cdot A. \quad (11)$$

Please note, that the model has been derived for monolayer h-BN. However, under the assumption that a high defect density supports interlayer transport of electrons, the model can be applied to multilayer h-BN too.

III. Verification with Measurements

The h-BN MD from [6] is used for the verification of the model. The electrodes are made of gold (Au) and h-BN is used as the 2D material. The h-BN layer consists of several layers and is approximately 6 nm thick. Since the h-BN layer has a high defect density, it can be assumed to allow interlayer transport, which means that the equations of the model are applicable. The defect density D^0 from the device is approximately $7.5 \cdot 10^9 \mathrm{cm}^{-2}$ [6]. The cross-sectional area A is $5\,\mu\mathrm{m}$ x $5\,\mu\mathrm{m}$ [6].

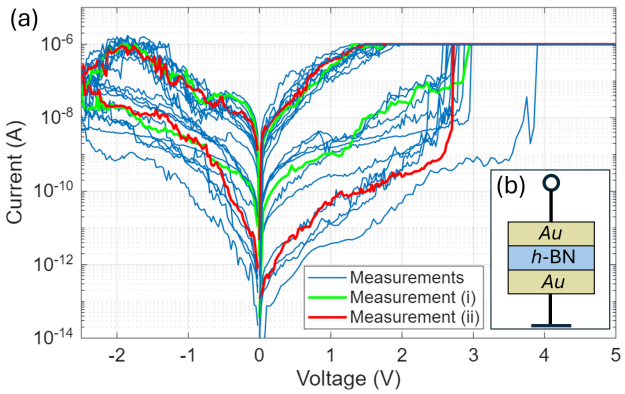

Fig. 3. (a) Measurements of 12 h-BN MDs showing D2D variability, with measurement (i) marked in green and measurement (ii) marked in red. (b) Representation of the $Au/h\text{-BN}/Au$ structure of the MD.

Figure 3 shows the measurements of 12 h-BN MDs. These show a D2D variability. A voltage of up to $5\,\mathrm{V}$ was applied for the SET cycle and a voltage of up to $-2.5\,\mathrm{V}$ for the RESET cycle. Two measurement data sets with different characteristics are marked, to which the model is to be fitted.

According to the measurement, the voltage V shown in **figure 4** is applied to the compact model.

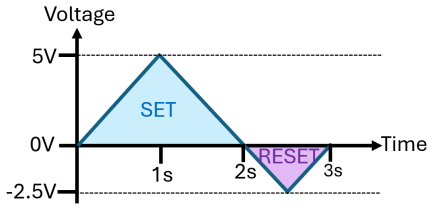

Fig. 4. Programming pulse according to the measurement procedure for fitting the model. Programming takes a total of $3\,\mathrm{s}$ and ranges between voltages of $-2.5\,\mathrm{V}$ and $5\,\mathrm{V}$.

The physics-based compact model was fitted to measurements (i) and (ii), the results of which can be seen in **figure 5 (a)** and **(b)**. The physical parameters D^0 and A are known [6], for ϕ_1 the work function of Au was taken as $5.1\,\mathrm{eV}$, the barrier height ϕ_2 is used as fitting parameter because electron affinity and band gap of h-BN varies with processing [3]. Furthermore, d, I_0, E_A, α, V_0, and λ_0 were adapted during fitting. The parameters α and E_A are different for the SET and RESET cycles because different amounts of energy are required for the formation and decomposition of the metal bridges to the defects [2].

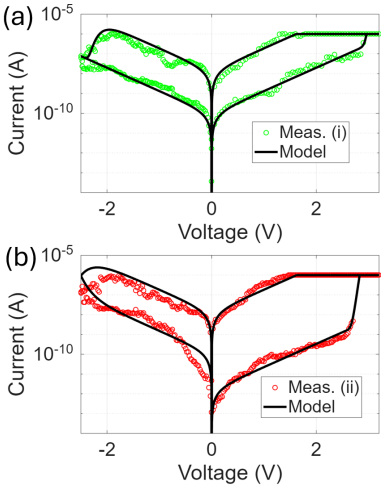

Fig. 5. (a) Fitting result model to measurement (i). (b) Fitting result model to measurement (ii).

The comparison between measurement data and model shows good agreement, confirming the modeling approach. The parameter values for the fitting are shown in **table I**. The difference in ϕ_2 between the two fittings is particularly striking. ϕ_2 lies between approximately $5\,\mathrm{eV}$ and $8\,\mathrm{eV}$ depending

on h-BN processing [1] [3]. Therefore, the $7.6\,\mathrm{eV}$ in fitting (ii) is reasonable. A smaller value had to be selected for fitting (i). However, a boron vacancy can also lie in a certain distance from the valence band edge, so smaller barrier heights are physically possible.

TABLE I
TABLE OF MODEL PARAMETERS AND THEIR VALUES FOR FITTING TO MEASUREMENTS (I) AND (II).

Model Parameter	**Fitting Measurement (i)** SET | RESET	**Fitting Measurement (ii)** SET | RESET
A / cm^2	$2.5 \cdot 10^{-7}$	$2.5 \cdot 10^{-7}$
d / m	$0.27 \cdot 10^{-9}$	$0.27 \cdot 10^{-9}$
ϕ_1 / eV	5.1	5.1
ϕ_2 / eV	4.1	7.6
D^0 / cm^{-2}	$7.5 \cdot 10^{9}$	$7.5 \cdot 10^{9}$
I_0 / A	$7 \cdot 10^{-9}$	$7 \cdot 10^{-9}$
V_0 / volts	0.37	0.37
α / -	1 | 0.17	1 | 0.113
E_A / eV	2.75 | 0.5	2.6 | $1 \cdot 10^{-4}$
λ_0 / $\frac{1}{s}$	0.001	0.001
m_0 / kg	$9.11 \cdot 10^{-31}$	$9.11 \cdot 10^{-31}$
T / K	300	300

Figures 6 (a) and **(b)** show how the number of defects in the LRS per area change over time, clearly illustrating the difference between the two measurements. In **(a)**, all defects are in the HRS at the beginning. After approximately $0.63\,\mathrm{s}$, a bridge has formed across all of these defects and they have switched to the LRS. For RESET operation, after $3\,\mathrm{s}$, these bridges are all broken down again and all defects switch back to the HRS, i.e., the initial state. In **(b)**, all defects are already in the LRS at the SET after approximately $0.59\,\mathrm{s}$. However, the voltage (or time) is insufficient to switch all defects back to the HRS. Therefore, bridges remain after the RESET and the initial state has not yet been reached.

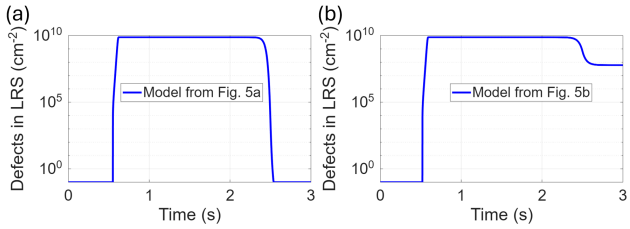

Fig. 6. Development of defects in LRS per cm^2 in the model. (a) Model from Fig. 5a, fitted to measurements (i), (b) model from Fig. 5b, fitted to measurements (ii).

IV. CONCLUSION

The first physics-based compact model for h-BN memristive devices presented here exploits the development of atomic bridges to the defects in the h-BN layer. This results in two states: defects with bridges in the LRS, and defects without bridges in the HRS. The statistical formation and reduction of these bridges could be described physically. In addition to the number of defects per area with and without bridges, it is necessary to calculate how much current flows through a single defect with and without a bridge. Here, the tunneling of electrons through the van der Waals gaps between the electrodes and the h-BN layer was used as the physical basis. In defects in the HRS, an electron must tunnel through two barriers, and in defects in the LRS, because of the bridge an electron must tunnel only through one barrier. Assuming rectangular barriers, a physical description of the currents in the LRS and HRS could be established. Combining both considerations, a physical equation for calculating the total current through the h-BN memristive device could be determined. This model was verified with two different measurement data sets and shows good agreement. It was possible to plot the development of defects in the LRS per area over time.

The definition of the compact model allows for an easy integration into circuit design tools. It can assist research and analysis of 2D-material-based memristive devices and help to explore design concepts on circuit level. The measurements show D2D variability, which due to the physical foundation of the model could be related to variations of the band structure of h-BN and uncomplete breaking of atomic bridges during the RESET process. Combining these findings with the results presented in [8] could bring these variations to a statistical analysis on circuit level. The model was verified here using h-BN memristive devices. However, the model is fundamentally applicable to memristive devices with layers of other 2D materials.

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