Dynamic ‘Hour Glass’ Model for SET and RESET in HfO_2 RRAM

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Introduction and purpose: Resistive RAM (RRAM) is considered a promising future memory concept. Its operation relies on the voltage-controlled resistance change of a conductive filament in the dielectric of a MIM stack. In HfO_2, oxygen vacancies (V_o), or, complementary, charged oxygen ions, have been identified as the mobile defect species responsible for forming/breaking the filament [1].

Until now, in all published set/reset models, the filament current-voltage (IV) curves were described by a simple resistive behavior, but experimentally, in the low current range (< 20μA), non-linear IVs with conductance quantization are apparent, indicating a quantum mechanical (QM) model is a necessity.

In this paper, for the first time, the learning from ab-initio and QM conduction are combined to construct a completely new set/reset model. **This model can capture all main features of RRAM device operation and reliability**. It remains fully analytically tractable and **can therefore be implemented in a circuit simulator**.

Sample: X-bar RRAM elements with a TiN/HfO_2/Hf/TiN stack in a 1T-1R configuration are used (fig. 1) for which excellent performance down to 10x10nm has been demonstrated [2]. The process details are also in [2]. In this paper, we use data on 20x20nm or 100x120nm devices.

Model description: By considering formation energies at deposition conditions, we concluded that a sub-stoichiometric HfO_x transient layer exists between Hf and HfO_2, which can act as a source of mobile V_o (Fig. 2a). In the proposed model, the filament, created by subsequent forming, is also described as a volume of sub-stoichiometric HfO_x (Fig. 2b), and ab-initio simulations suggest that in this less-densely structured filament, faster ion diffusion/drift occurs than in the densely packed stoichiometric HfO_2 that surrounds it (Fig 3). Therefore, in a first approximation, we assume that ion diffusion takes place *only inside* the filament, and there is no diffusion from the filament to its surrounding HfO_2. In short, the filament is described as a *container* with boundaries set by the forming process. All ion motion happens exclusively inside this container. Except during forming, no generation or annihilation of V_o is assumed.

The non-linear IV-curves are modeled by a quantum point contact (QPC) approach [3]. The close-range interaction of many V_o’s inside the filament forms a conduction band and in the narrowest point of the filament (=the constriction) current-controlling energy barriers exist (Fig. 4). In HfO_2, experimental data show that the IV-changes during set/reset transients are described by modulations of the constriction width only [4]. Including this knowledge, a more schematic filament representation consists of a top reservoir (TR) and bottom reservoir (BR), connected by a constriction (C) with variable width (Fig. 2c). This resembles an ‘hour glass’ with a variable nozzle size and ‘sand’(=V_o) that moves from TR to BR or vice versa depending on the applied polarity.

The set/reset dynamics are described by the V_o-emission over the interfaces BR/C and TR/C (Fig. 5). For emission *to* the constriction a voltage-modulated energy barrier is assumed, but for emission *from* the constriction, V has no impact, consistent with the QPC voltage distribution (fig. 4b).

The diffusion forces from concentration gradients are accounted for by linearly weighing all emission probabilities by the reservoir occupancy fraction (or its complement).

RESET modeling: Fig. 6 shows a DC reset transient with very slow voltage ramp rate (0.1V/min). V_{trans} is the transition voltage at which the V_o‘s become mobile and the constriction can change size. Many abrupt current jumps are visible. The parts in between the jumps match to IV-curves calculated with the QPC model. A 30-cycle average is also shown. The reset transient is often explained as a filament reduction down to the level where V_o is ‘frozen in’ [5], but the abundant fluctuations in Fig. 6 (*upwards* as well as downwards) suggest that for $V>V_{trans}$, the system is never ‘frozen’, but in a state of *dynamic balance*.

In the hour glass model, this balanced state is calculated by imposing a net zero V_o-flux at both the BR/C and TR/C interfaces. Fitting the model parameters to the measured balance (Fig. 7a) results in a very large TR size, suggesting that the entire HfO_x contact layer acts as a V_o-reservoir, while the BR created by forming is much smaller for a deep reset.

The reset transient reaches a saturation level (corresponding to a minimal achievable constriction size, Fig. 7c) depending on the forming power (fig. 8). Higher forming power leads to a high reset saturation level, which can also be fitted with the hour glass model by increasing the BR capacity and the amount of participating V_o while keeping α and R_{th} constant (Fig. 7b). We conclude that the forming determines the filament geometry and size, and this information is kept throughout all subsequent cycles, validating the absence of V_o-generation/recombination. Note that in the hour glass model the filament never breaks, but only narrows until a current-blocking potential barrier is raised due to QM confinement in the constriction.

The existence of the dynamic balance is further exemplified by disturb measurements at reset polarity directly after reset (fig. 9). Intuitively, one would expect a stable low current or even further current lowering. The hour glass model, however, predicts correctly that the system evolves eventually to the balance line at *high* current.

Note that the first DC reset directly after forming systematically shows a current overshoot before the dynamic balance is reached (Fig. 10). Indeed, directly after forming most V_o are in the BR, resulting always first in a constriction growth before equilibrium is approached.

SET modeling: Set transients were measured with a high resistive load and low voltage resolution. After subtracting the V-drop over the load resistance, the actual set transient is revealed (fig.11a). Starting from low current, the set voltage first needs to reach V_{trig} to start the transient. Then, a fast ‘snap back’ is seen to a lower voltage. The current further increases at nearly fixed voltage until compliance is reached.

This behavior is easily explained by calculating the line of equal probability for the BR to C defect emission as a function of V and I (fig. 11a). This line defines (with a fixed probability) the transition from immobile to mobile V_o. The set transient is detailed out in Fig. 11b on an experimental example. The constriction growth is triggered when the transition line is reached at V_{trig}. The constriction widens fast in discrete steps (jumps to curves with integer defect numbers n_C) along a line determined by the resistive load until the transition line is again reached. The current oscillates further upwards along the transition line at nearly constant V_{trans}.

The transition voltage curve in Fig. 11 is polarity independent due to the voltage-symmetry of the QPC conduction, and therefore the $|V_{trans@set}| = |V_{trans@reset}|$, which is experimentally confirmed. The hour glass model also predicts an increase of V_{trans} as a function of the voltage ramp rate, in agreement with the experimental data (Fig. 12).

Conclusions: An analytic dynamic hour glass model for HfO_2 RRAM is demonstrated, describing the reset as a dynamic equilibrium process and the set as a constriction growth limited by ion mobility and current compliance. The dependence on time, voltage and forming conditions is in good agreement with experiments. Since the model is fully analytical, it can be implemented in a circuit simulator.

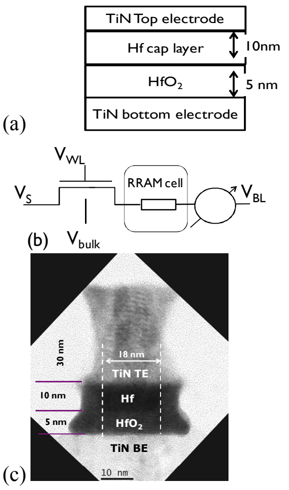


Fig. 1: (a) Schematic drawing of the stack used in this study and **(b)** the 1T1R (1 Transistor- 1 Resistor) configuration. **(c)** A cross section SEM image of the 20x20 nm RRAM stack.

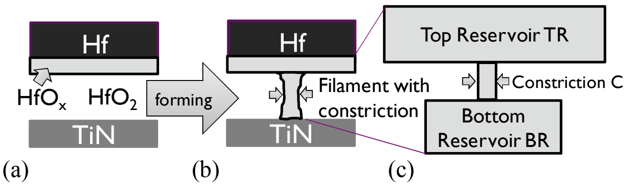


Fig. 2:(a) Stoichiometric HfO_x is present between Hf electrode and HfO_2 dielectric. **(b)** Forming 'extends' the HfO_x region to the filament. **(c)** Filament is modeled as a container with a top and a bottom V_o reservoir (TR and BR), connected by a constriction C with variable width.

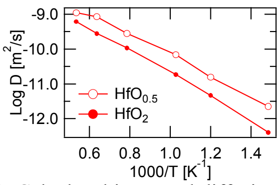


Fig. 3: Calculated increased diffusion constant in sub-stoichiometric HfO_x

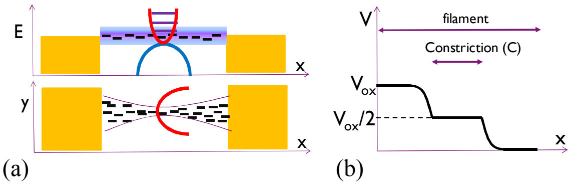


Fig. 4: (a) Energy diagram (top) and spatial schematic drawing (bottom) of a filament. Many interacting defects form a conduction band. The current-controlling energy levels originate from the spatial confinement in a constriction, modeled as parabolic potential well [3]. **(b)** Schematic voltage drop in the filament. V drops symmetrically at the interfaces of the constriction C. For wider cross section, the field penetrates in the constriction yielding the classical limit.

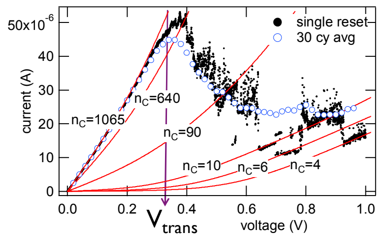
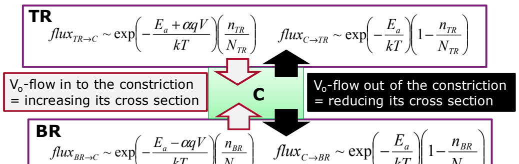


Fig. 6: Example of a slow DC reset (0.1V/min). The current jumps abruptly to different levels. The smooth curves are QPC calculations for integer number of defects n_C in the constriction. Extensive calibration to data (not shown here) was done to determine the IV curve corresponding to a single defect.



$$flux_{TR\to C} \sim \exp\left(-\frac{E_a+\alpha qV}{kT}\right)\left(\frac{n_{TR}}{N_{TR}}\right) \qquad flux_{C\to TR} \sim \exp\left(-\frac{E_a}{kT}\right)\left(1-\frac{n_{TR}}{N_{TR}}\right)$$

$$flux_{BR\to C} \sim \exp\left(-\frac{E_a-\alpha qV}{kT}\right)\left(\frac{n_{BR}}{N_{BR}}\right) \qquad flux_{C\to BR} \sim \exp\left(-\frac{E_a}{kT}\right)\left(1-\frac{n_{BR}}{N_{BR}}\right)$$

$$T = T_{ambient} + \frac{IV}{n_C}R_{th} \quad \textbf{(Eq. 1)} \qquad n_{total} = n_C + n_{BR} + n_{TR} \quad \textbf{(Eq. 2)}$$

Fig. 5: Flow equations at the TR/C and BR/C interfaces (reset polarity). N_{BR} and N_{TR} are the maximum V_o-capacity of the BR and TR resp. The amount of V_o's is given by n_{BR} and n_{TR}. The number of defects making up the constriction is n_C. Temperature is calculated using a power density per defect IV/n_C (Eq. 1) . The total amount of V_o's is given by n_{total} in Eq. 2 (no generation/annihilation). Current I is calculated with the QPC model (see [3]).

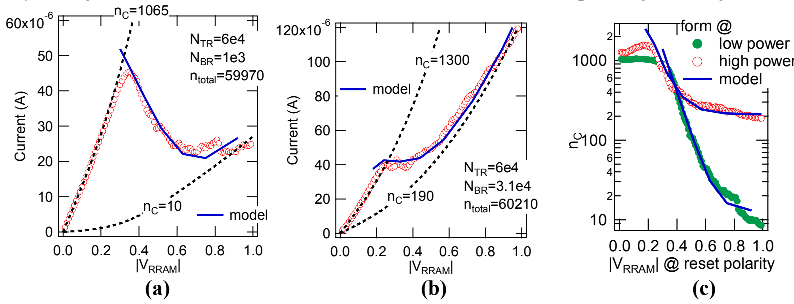


Fig. 7: (a) The reset transients for a low reset saturation ($n_{C,min}$=~10 defects) or **(b)** high reset saturation ($n_{C,min}$=~190 defects). From a transition voltage of ~0.3 V on, the system stays in dynamic balance, fitted with the hour glass model. **(c)** shows the evolution of n_C. Increasing n_{total} and N_{BR} results in high reset saturation $n_{C,min}$, occurring for high forming power.In all three figures we used α=0.32 and $R_{th}=10^8$K/W

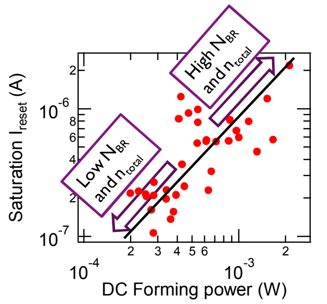


Fig. 8: The relation between the DC forming power and the saturation reset level. The forming history is stored through the parameters N_{BR} and n_{total}

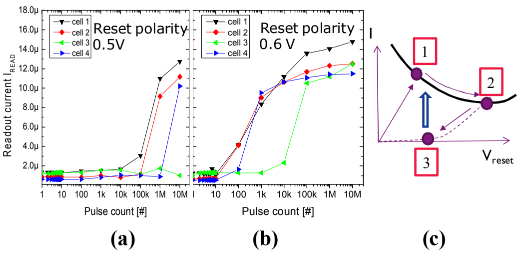


Fig. 9: Disturb measurements (100ns pulses) at **(a)** 0.5 and **(b)** 0.6V in reset polarity. **(c)** Schematic explanation: (1) transition voltage is reached, 1→2) reset along dynamic balance line. 2→3) fast down ramp to the OFF state. (3) system tends to return to the ON state (upwards), but because of the low voltage, a time delay is seen (Figs. a en b).

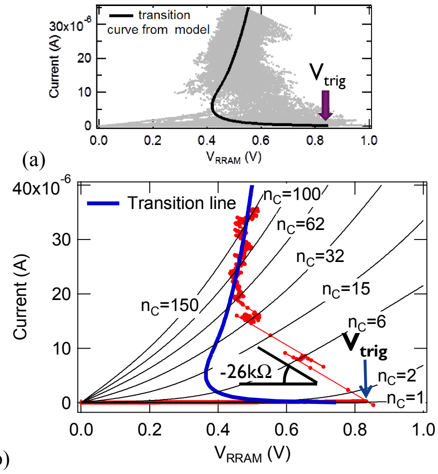


Fig. 11: SET behavior with high resistive load and small voltage step. Fig. **(a)** shows 100 set curves on a single RRAM cell. Systematically, a trigger voltage needs to be overcome, followed by a rapid 'snap back' to a lower voltage. The voltage transition line calculated with the model is shown. Fig. **(b)** shows an example of a single set curve. QPC IV-curves for corresponding integer number of constriction defects n_C are added. The resistive load was 26kOhm. V_o start to move at V_{trig}. The constriction grows rapidly until the transition line is again reached.

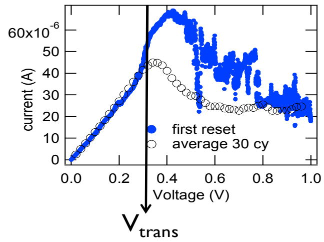


Fig. 10: The first reset transient after forming (in DC conditions) systematically shows a current overshoot before moving to the balance line.

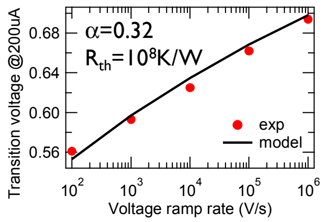


Fig. 12: The transition voltage as a function of the ramp rate can be fitted by the hour glass model.

REFERENCES: [1] C.H. Wang et al., IEDM 2010. / Xu et al, VLSI Symp, 2008. / Bersuker et al, IEDM 2010. [2] B. Govoreanu et al., IEDM 2011. [3] R. Degraeve et al, IEDM 2010 / E. Miranda, APL 92 (2008). [4] R. Degraeve et al, to be presented at VLSI-TSA 2012. [5] D. Ielmini et al., IEDM 2011.