

# Conduction properties of nanoscale switching filaments in HfO<sub>2</sub>-based resistive memories

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## Abstract

Resistive switching (RS) in MIM devices offers new opportunities for ultra-scaled nonvolatile memories. In resistive memories (ReRAM), the resistance values used to store the information are achieved by ion motion and chemical reaction. In this way, ReRAM is expected to overcome the scaling limits of the conventional devices, which are based on the trapping/detrapping of electrons by confining potential barriers. RS is most often based on the creation and partial destruction of a conductive filament (CF) of nanoscale dimensions. Understanding the conduction properties of the CF in the Low-Resistance State (LRS) and the High-Resistance State (HRS) and linking these properties to the shape and nature of the CF is of great importance to improve the understanding of RS and to boost ReRAM applications.

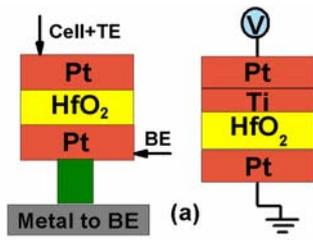
Many different conduction models have been proposed for the HRS including trap-assisted tunneling (TAT), Poole–Frenkel, thermally activated hopping, space-charge limited current, and Quantum Point Contact model (QPC), among others. Although the results might somehow depend on the considered oxide material, in the case of HfO<sub>2</sub> there is strong experimental evidence supporting the importance of tunneling in the HRS. On the other hand, experimental evidence of conductance quantization has been recently reported in a variety of ReRAM devices, including HfO<sub>2</sub>-based structures [1].

The QPC model is based on the idea that the CF can be modeled as a quantum wire, and it is based on the Landauer approach to conduction along narrow mesoscopic constrictions. The constriction of the CF determines the energy of the subbands available for quasi-one-dimensional transport along the CF. If the CF is wide, the position of this first subband is below the cathode Fermi level, the conduction is linear and the conductance is a multiple of  $G_0=2e^2/h$ . If the CF is narrow, the energy of the first subband might be above the Fermi level and conduction is limited by a tunneling barrier which, depending on its height and thickness, results in a CF conductance several orders of magnitude below  $G_0$  and strongly non-linear  $I(V)$ . This is shown in the experimental characterization of two types of HfO<sub>2</sub>-based ReRAM structures (Fig.1) repetitively cycled in the unipolar switching mode (Fig.2). The distribution of resistance is much wider in the HRS than in the LRS (Fig.3 & 4). In the LRS, it only depends on the area of the CF while in the HRS, it is determined by the thickness of a spatial gap (tunneling barrier) in the CF. A small change of the gap thickness causes an exponential reduction of the transmission coefficient in the HRS. In this work, we depart from first-principle calculations (Fig. 5) of electron transport along paths of oxygen vacancies in HfO<sub>2</sub> to reformulate the QPC model in terms of a bundle of such vacancy paths. In this way we reduce the number of QPC free parameters and provide a direct link between the microscopic structure of the CF and its electrical properties. This multi-scale QPC model has been applied to the two different HfO<sub>2</sub> devices (Fig. 1) operated in the unipolar and bipolar RS modes. The fitting of the  $I(V)$  characteristics is excellent in the complete resistance range (Fig.4). Extraction of the model parameters from a statistically significant number of CFs (cycle to cycle variations) allows revealing significant structural differences in the CF of these two types of devices and RS modes. An example of the results obtained in Pt/HfO<sub>2</sub>/Pt structures operated in the unipolar mode (Fig.6). In this case, only one channel contributes to conduction in the HRS while several channels are active in the LRS (proportional to CF conductance). While the thickness of the barrier is zero in the LRS, it increases logarithmically with CF conductance in the HRS. In this case, the CF is found to be symmetric (likely with hourglass shape). The results obtained in the bipolar switching of Pt/Ti/HfO<sub>2</sub>/Pt structures (not shown in this abstract) are significantly different and point out to conical CF shape with a significant gap even in the LRS, which shows a non-linear  $I(V)$  contrary to what happens in the unipolar switching case.

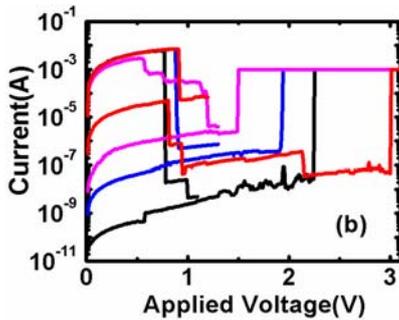
## References

[1] S. Long, X. Lian, C. Cagli, X. Cartoixà, R. Rurali, E. Miranda, D. Jiménez, L. Perniola, M. Liu and J. Suñé, *Applied Physics Letters*, 102 (2013) 183505.

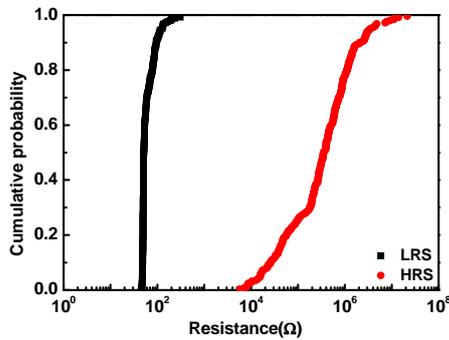
## Figures



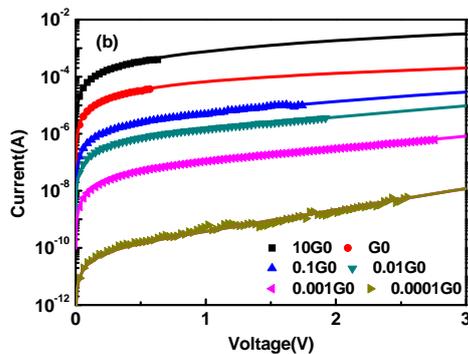
**Fig. 1.** Schematic representation of the characterized ReRAM samples.



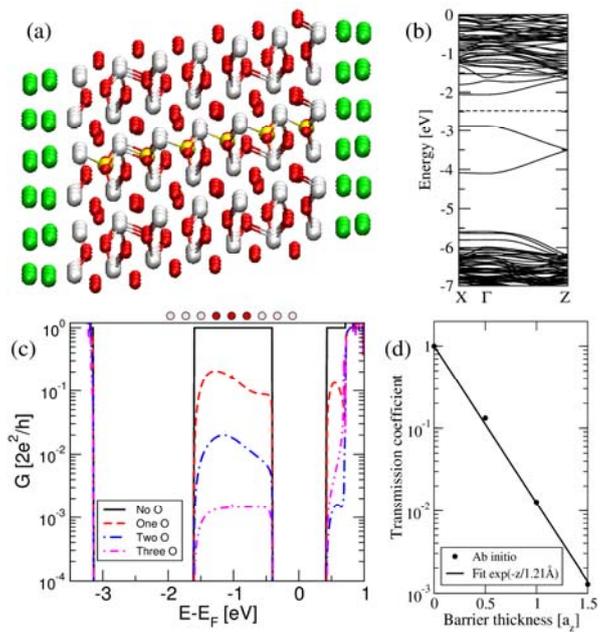
**Fig. 2.** Examples of set/reset cycles of a Pt/HfO<sub>2</sub>/Pt sample operated in the unipolar switching mode.



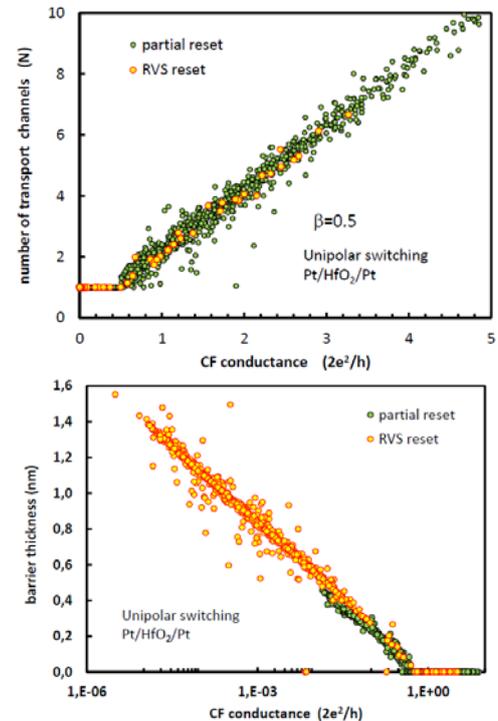
**Fig.3.** Distribution of resistances in the LRS and HRS during Pt/HfO<sub>2</sub>/Pt unipolar cycling.



**Fig. 4.** Fitting of the  $I(V)$  characteristics to the multi-scale QPC model in the whole (LRS & HRS) range of CF resistances.



**Fig.5.** First-principles calculations (using SIESTA) of oxygen vacancy paths in metal/HfO<sub>2</sub>/metal structures. (a) Representation of a vacancy path in monoclinic hafnia; (b) Calculated bandstructure showing the dispersive band in the HfO<sub>2</sub> gap due to the single-vacancy path; (c) Calculated conductance for the full vacancy gap and with 1,2, and 3 reoxidized vacancies; (d) transmission coefficient as a function of energy barrier thickness (each reoxidized vacancy introduces barrier of one half of the lattice parameter).



**Fig. 6.** Scatterplots of extracted QPC parameters as a function of CF conductance in Pt/HfO<sub>2</sub>/Pt operated in the unipolar switching mode. (a) Only one channel is obtained in the HRS while it increases linearly with  $G$  in the LRS (being of the order of the quantum of conductance). (b) While no barrier is present in the LRS, its thickness increases logarithmically with the CF conductance in the HRS.