Molecular dynamics simulation of the full operation cycle of a HfO_2-based RRAM cell

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Resistive random access memories (RRAMs) are considered the most promising candidates for next generation, high-scaling, ultrafast, and low power consumption memories. RRAM cells, that typically consist of a metal-insulator-metal (MIM) stack, store bits by reversibly changing the resistivity of the insulator between a high resistance state (HRS) and a low resistance state (LRS). In order to enable this reversible change, the devices normally require an initial and irreversible process called electro-forming, which is basically a current-controlled breakdown of the pristine highly resistive oxide layer [1].

In most RRAM devices, the switching between LRS/HRS originates from the formation/rupture of a nanoscale conductive filament (CF) in the dielectric layer. In the valence change mechanism (VCM) of operation, a variation in local stoichiometry arising from the presence of oxygen vacancies changes the valence of the metallic ions rendering them conductive [1].

In this contribution we present molecular dynamics (MD) simulations of a HfO_2-based RRAM cell evolving in time under the influence of a changing external bias, in order to obtain atomistic information of the filament formation and rupture dynamics during all the stages of operation of the RRAM cell [2]. Our simulations explicitly capture all the relevant processes involved in the switching of the device, including redox reactions, oxygen migration, growth of vacancy-rich regions and the effect of temperature. We studied cells with metallic Hf as AE and our simulations reproduce the substoichiometric layer generated at the oxide/AE interface during the fabrication of the devices. A detailed, 3D, analysis of the motion of O ions during forming, reset, and set reveal unexpected phenomena. During forming, net oxygen migration towards the active electrode dominates the formation of the CF. Our results support the viewpoint that the filament rupture during reset is governed by lateral oxygen migration, induced by the complex 3D electric fields from the neighboring ions and irregular electrode shape during reverse in the bipolar case, or by effect of temperature under unipolar operating conditions. Finally, simulations of the set process demonstrate negligible vertical oxygen migration, in contrast to the forming process, and the filament forms by the rearrangement of oxygen atoms in the lateral directions.

Acknowledgment

M.L.U and X.C. acknowledge financial support by the Spanish Ministerio de Ciencia e Innovación under Grants No. RTI2018-097876-B-C21 (MCIU/AEI/FEDER, UE) and No. PID2021-127840NB-I00 (MICINN/AEI/FEDER, UE). Computational support from nanoHUB and Purdue University is gratefully acknowledged.

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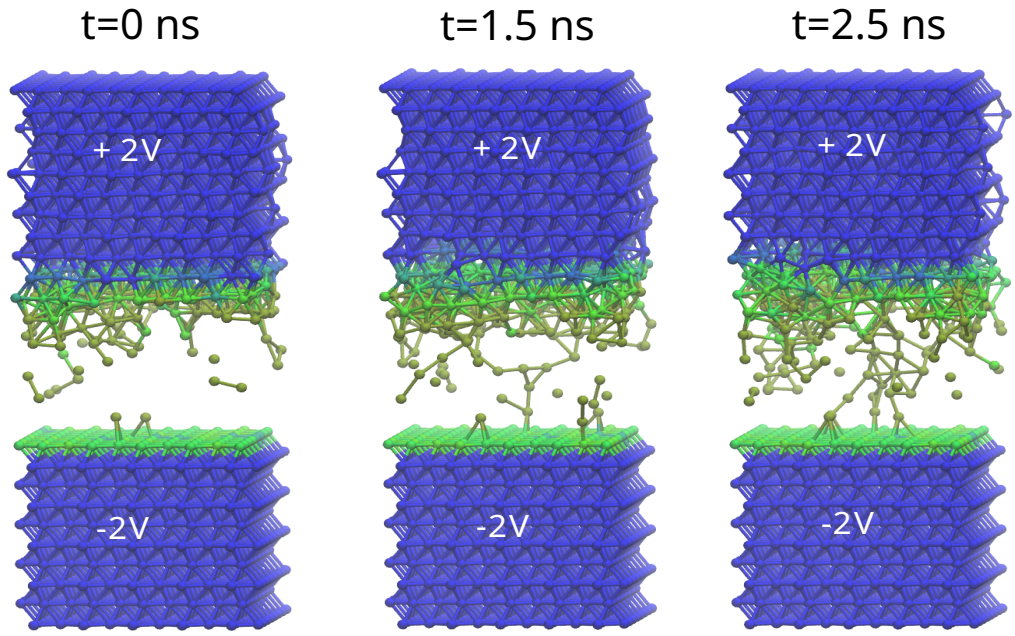

Fig. 1. Snapshots of filament formation during *forming*. Adapted with permission from M. .L. Urquiza et al., ACS Nano vol. 15, 12945 (2021).

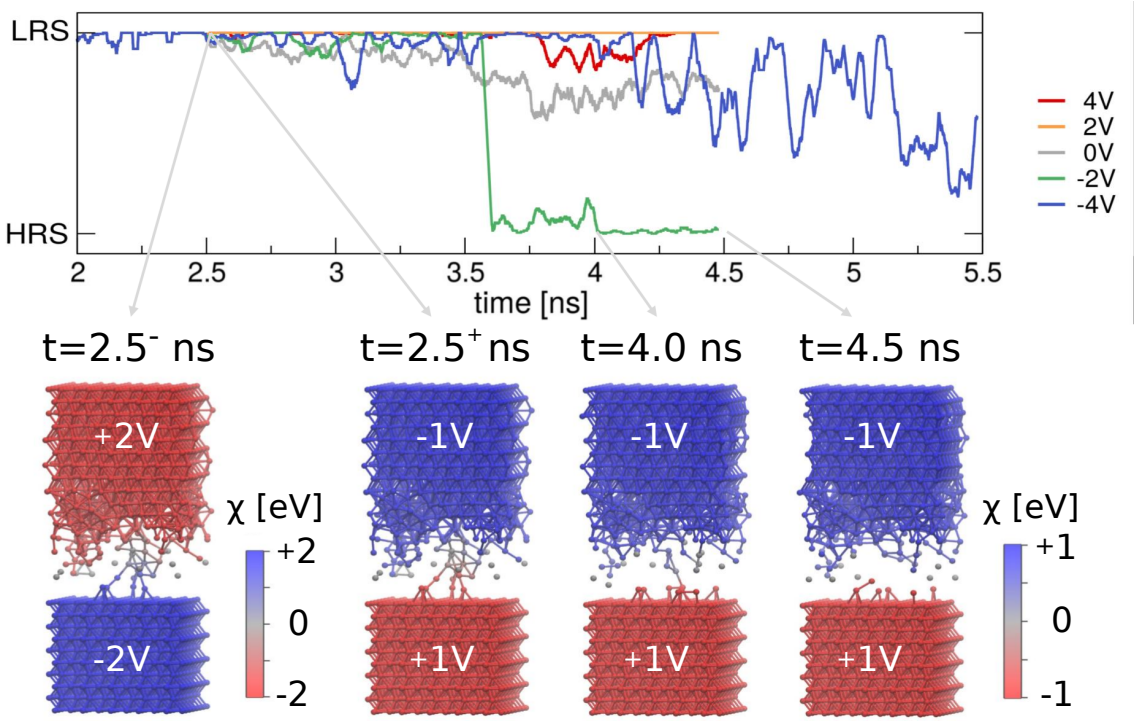

Fig. 2. Snapshots of filament rupture during *reset*. Reproduced with permission from M. .L. Urquiza et al., ACS Nano vol. 15, 12945 (2021).