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Master / Semester Thesis

Atomistic Modelling of Resistive Memory Arrays

Non-volatile Valence-Change Memory (VCM) memory devices are being explored for several applications in computing, including as on-chip memory and analog computing primitives. These devices are metal-oxide-metal stacks, across which an applied voltage results in the formation/dissolution of conductive nano-filaments of point defects. As their operating area can be localized to the nanoscale, they can be integrated into incredibly high-density planar- (**Fig. 1a**) and vertical arrays. The ultimate scaling limit of these devices is however fundamentally limited by finite-size effects and non-idealities. Evaluating their potential involves understanding the scales at which the operating physics can still be reliably achieved, and the nature of the failure mechanisms encountered beyond them.

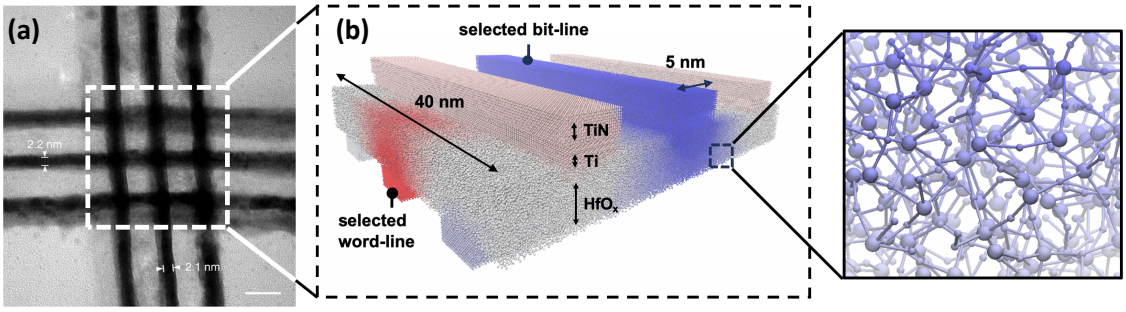

Fig. 1: (a) A fabricated 3x3 array of HfO_x resistive memory [1]. Each device is roughly 2.2 nm. **(b)** Atomic structure of an TiN-HfOx/Ti-TiN crossbar array with similar physical dimensions to the fabricated 3x3 array, consisting of roughly 1 million Hafnium, Oxygen, Titanium, and Nitrogen atoms in the switching layer and contacts. [2]

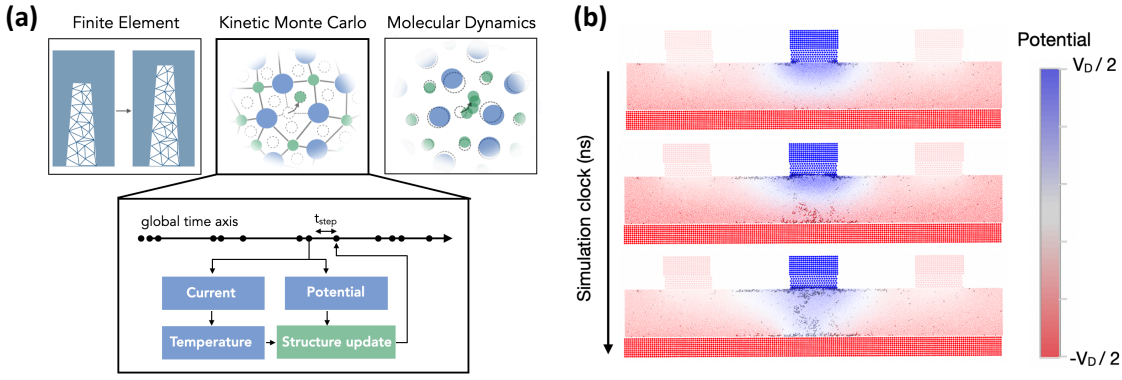

Fig. 2: (a) Overview of the modelling framework developed to simulate the kinetics of resistive switching. **(b)** Example kinetic `electroforming' process to build a conductive filament across the center device in the 3x3 array (as in Fig. 1) under an applied bias, transitioning it into an ON state. [2-3]

We have developed a specialized atomistic Kinetic Monte Carlo solver which can handle simulations of domain sizes with over a million atoms **(Fig. 2)** [2-3]. We are now interested in leveraging the capabilities of this application to (1) simulate the effects of coupling between neighbouring devices in planar- and 3D-stacked array architectures and (2) study the effects of non-idealities such as wire resistance and sneak current pathways, connecting trends from simulations to experimental results when available.

Interested candidates please contact: Manasa Kaniselvan → mkaniselvan@iis.ee.ethz.ch
Dr. Marko Mladenović → mladenovic@iis.ee.ethz.ch
ETH Professor : Prof. Mathieu Luisier → mluisier@iis.ee.ethz.ch

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Prerequisites

- An interest in using theory and simulations to understand the operation of nanoscale semiconductor devices
- Good programming skills in C++/Python and a background in numerical methods
- (*Optional*) A familiarity with atomistic simulation methods such as Molecular Dynamics (MD) and lattice Kinetic Monte Carlo (KMC)

References

[1] Pi, Shuang, et al. "Memristor crossbar arrays with 6-nm half-pitch and 2-nm critical dimension." Nature Nanotechnology 2019.
[2] Kaniselvan, M*; Maeder, A*; Mladenović, M; Luisier, M; Ziogas, A.N; “Accelerated Kinetic Monte Carlo Simulations of Atomistically-Resolved Resistive Memory Arrays”. (Accepted paper) *International Conference on High Performance Computing, Networking, Storage and Analysis (SC24)* 2024
[3] Kaniselvan, M.; Luisier, M.; Mladenović, M; “An Atomistic Model of Field-Induced Resistive Switching in Valence Change Memory” *ACS Nano* 2023