Molecular Dynamic Simulation of Heterogeneous Integrating Memristors with COMSO Chips

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Background

The advent of the memristor represents a revolutionary development in the field of electronics. As a fundamental electronic component, the memristor has garnered significant attention due to its unique characteristic - the ability to change its resistance based on the amount of charge that has passed through it, with this change being non-volatile. This property opens up new possibilities in the realms of storage technology and computation, indicating a vast potential for memristors in artificial intelligence, neural networks, and broader data processing technologies.

Direct integration of memristors onto chips, while promising, faces several challenges with current methodologies. One prevalent method involves thin-film deposition, which, despite its precision, struggles with issues of material compatibility and thermal stability, often leading to degraded performance over time. Another approach is the use of nanowire structures, which offers excellent scalability and miniaturization potential, but is hindered by complex fabrication processes that can lead to inconsistent quality and high production costs. A third technique involves the photolithographic patterning of memristor materials, a process well-integrated into current semiconductor manufacturing. However, this method is limited by its resolution and the difficulty in patterning specific memristive materials, restricting the diversity and capability of the

memristors produced. Each of these methods, while innovative, falls short in aspects crucial for the widespread adoption and practical application of memristor technology in chip design.

In response to these challenges, our team has proposed an innovative method for integrating a new type of memristor onto chips. This new approach not only addresses the main drawbacks of existing technologies but also significantly reduces the cost and complexity of the process. To gain a deeper understanding of the working mechanisms of this new type of memristor, molecular dynamics simulations will be employed. This simulation technique allows us to observe and analyze the behavior of memristors at the atomic level, thereby enhancing our understanding of their performance and behavioral patterns on chips.

Objectives

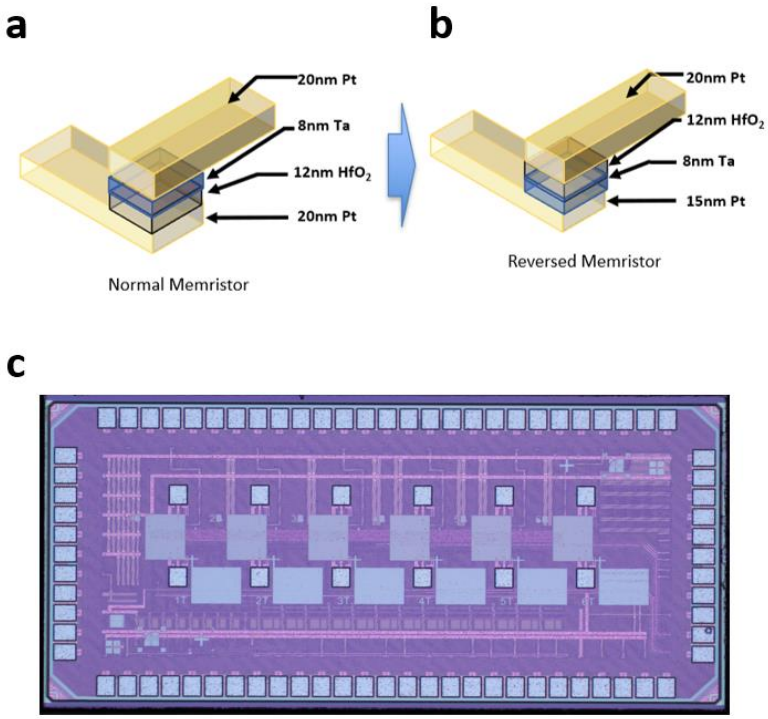

Figure 1. (a) The normal structure of memristors. (b) The structure of reversed memristors. (c) The top view of on-chip memristor under microscope.

The standard structure of memristors, as depicted in Figure 1a, fails to function when integrated with the chip using our proposed method. The new type of memristors used for the integration consist of four parts: bottom electrode (2 nm Ti/ 20 nm Pt/ 8 nm Ta), switching layer (8 nm HfO_2), and top electrode (20 nm Pt). The 3D schematic of the active area are shown in figure 1b. The on-chip memristor can be tuned to multiple conductance states using 10 ns pulses created by a custom-designed tuning circuit. The I-V curves of the memristor demonstrate 1000 conductance states, which is more than 2^8, as shown in figure 2. The greater number of resistance states of the memristor indicates that more information can be processed. Figure 2 shows the linear plot

resistive switching I-V curves of the crossbar, demonstrating that the crossbars have excellent I-V linearity, which is necessary to implement the linear transfer function. Although the structure of the memristor has been reversed, the operating voltage and the performance are the same for both, which means the working mechanism of on-chip memristors is totally different with the normal memristors. Therefore, the dynamic molecular simulation is needed to model the working mechanism of the new type of memristors and analyze why the standard memristor doesn't work on the chip.

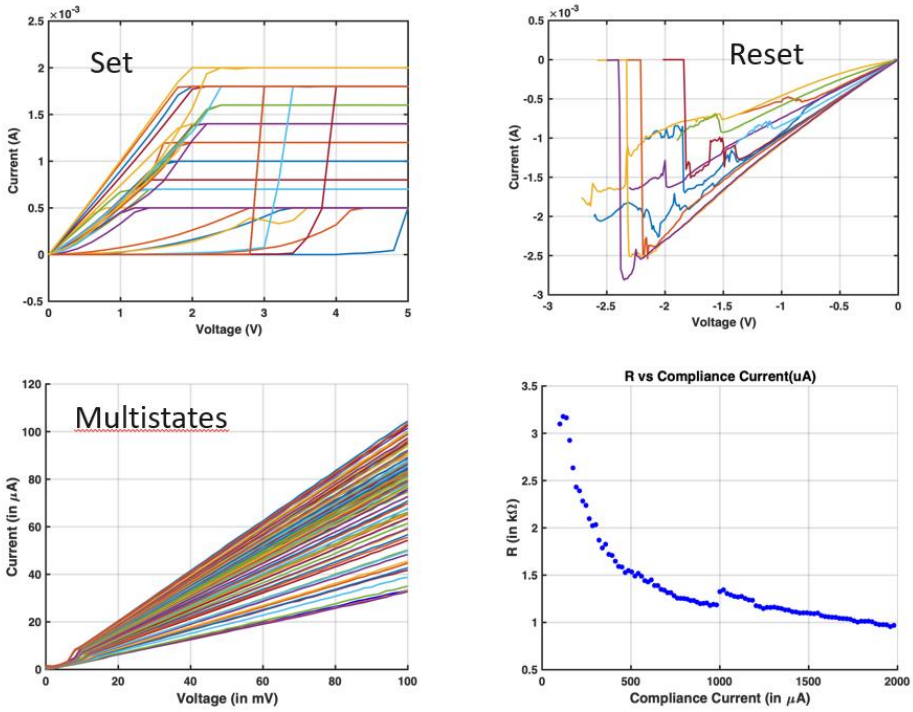

Figure 2. The performance of on-chip memristors during set, reset, and multistates process.

Current Status of Work

Currently, there is no research specifically addressing the working mechanism of on-chip memristors. Through the study of the principles of memristor operation and the analysis of experimental data, we hypothesize that the reason a normal structure cannot function on a chip is due to the high temperature during the Ta deposition process, which leads to Ta diffusing into HfO2, thereby causing the device to temporarily lose its multistate capability.

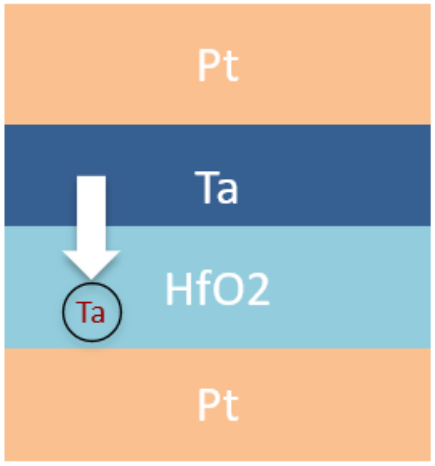

Figure 3. Ta diffuses into HfO2 during deposition.

The primary reason an on-chip memristor can function is due to the generation of oxygen vacancies during the ALD (Atomic Layer Deposition) growth process. The inability of a normal structure to function on a chip is attributed to the high temperature during the Ta deposition process, which results in Ta diffusing into HfO2. Thus, it's essential to conduct separate simulations for these two processes.

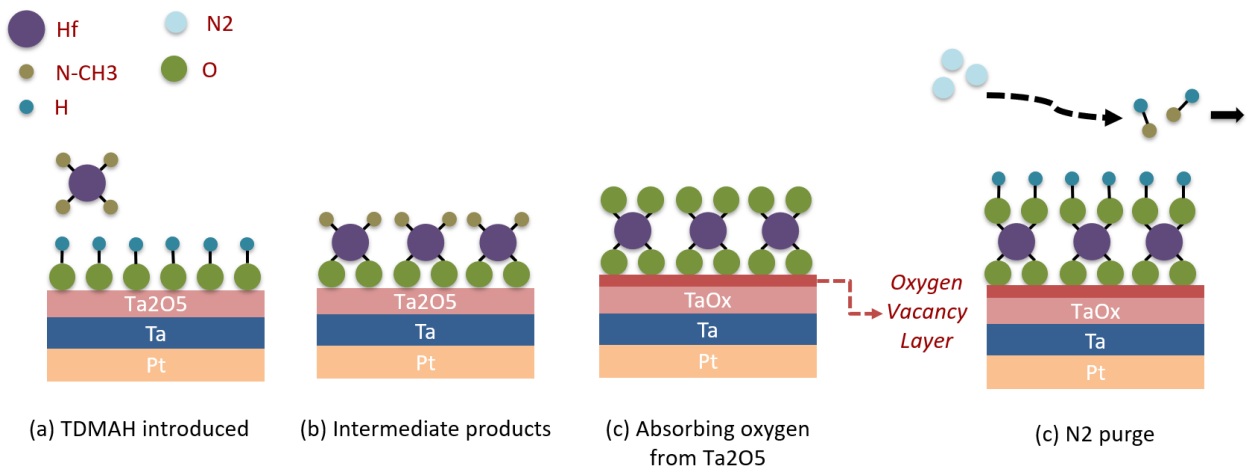

Figure 4. Oxygen drift during ALD process.

Techniques to be used

The diffusion of tantalum Ta into HfO2

Classical Molecular Dynamics Methods: This approach involves parameterized potential functions to describe interactions between atoms. For Ta and HfO2 systems, multi-body potential functions like the Embedded Atom Model (EAM) or Buckingham potential may be required to accurately represent interactions between metals and oxides.

Temperature-Accelerated Dynamics (TAD): Since diffusion is a high-temperature process, TAD can be used to accelerate the simulation, allowing diffusion events to be observed in shorter simulation times.

Dynamic Monte Carlo (KMC) Simulations: This method is suitable for simulating the diffusion of Ta atoms in HfO2, especially when the diffusion process is slow.

Oxygen drift during ALD process

Reaction Dynamics Simulations: This simulation focuses on the chemical reaction process and can be achieved by combining molecular dynamics with reaction path analysis. This involves

constructing the potential energy surface for the reaction between TDMAH and Ta2O5 and simulating the reaction dynamics at high temperatures.

Ab Initio Molecular Dynamics (AIMD): AIMD can accurately describe complex chemical reactions at the atomic scale, particularly useful in handling the complex reaction mechanisms between TDMAH and Ta2O5. This method computes electronic structures and atomic movements directly from quantum mechanical principles.

Density Functional Theory (DFT)-Based Molecular Dynamics: This approach combines the accuracy of DFT calculations with the dynamic simulation capabilities of molecular dynamics, suitable for simulating complex electronic and atomic interactions during the reaction process between TDMAH and Ta2O5.

Expected Results

Through the aforementioned simulations, we are able to validate the diffusion of tantalum (Ta) into hafnium dioxide (HfO2). These simulations not only confirm the diffusion process but also provide critical insights into the dynamics of this interaction at an atomic level. Simultaneously, we observe the drift of oxygen from tantalum pentoxide (Ta2O5). This is a crucial aspect of the process, as it leads to the formation of oxygen vacancies, particularly at the interface between Ta and HfO2. The creation of these oxygen vacancies is pivotal, as they play a significant role in the electronic properties of the memristor, impacting its conductivity and overall performance. By closely examining these phenomena, we can gain a deeper understanding of the material's behavior, which is essential for optimizing the performance of memristors and developing more efficient and reliable electronic devices.