Atomistic-to-Continuum Simulation of Au-MoS_2-Au Atomristor via Coupled MD-FEM Framework

Mohit Tewari
Department of Electrical Engineering
IIT Gandhinagar
India
tewarimohit@iitgn.ac.in

Ashutosh Krishna Amaram
Department of Materials Engineering
IIT Gandhinagar
India
amaramashutosh@iitgn.ac.in

Tarun Kumar Agarwal
Department of Electrical Engineering
IIT Gandhinagar
India
tagarwal@iitgn.ac.in

***Abstract*— We present a coupled Reactive Molecular Dynamics (MD) and Finite Element Method (FEM) multiscale simulation framework for modeling Au/MoS_2/Au memristor devices. Atomic structures corresponding to different resistance states are obtained by applying voltages within our Reactive MD framework. Subsequently, a python-based workflow is used to voxelise atomic structures for macroscopic electro-thermal FEM simulation. The resulting temperature profiles from FEM simulations are fed back into Reactive MD cycles in an iterative way, enabling dynamic coupling between atomic structure evolution and device-scale thermal effects. We show that the coupled MD-FEM framework can provide realistic atomistic insights into the current-voltage characteristics of reported experiments, which cannot be fully captured by MD or FEM simulations alone. This integrated framework serves as a predictive, atom-to-continuum modeling tool for the designing of the Au/MoS_2/Au memristive devices.**

Keywords—Atomristor, Au-MoS_2-Au, Memristors, Reactive MD, Electro-thermal FEM, Multi-scale modeling.

I. Introduction

Memristors based on two-dimensional (2D) molybdenum disulfide (e.g. Au-MoS_2-Au) can potentially enable energy efficient brain-inspired hardware due to their atomic-scale thickness, low power consumption (<3.02 pJ per operation), and high switching speeds (<5 ns). These devices emulate biological synapses, achieving analog conductance tuning and spike-timing-dependent plasticity (STDP) with recognition accuracies exceeding 96% in neural network applications [1-4]. Despite these advantages these devices exhibit significant cycle-to-cycle instability (C2C) compromising computational accuracy and reliability [1]. This instability originates from stochastic evolution of the filament morphology during SET/RESET cycles, driven by localized electric fields and temperature gradients. In particular, the RESET process relies on thermally activated filament dissolution, where local temperature distributions are reported to directly control the metal ion migration [4].

Atomic-scale Density-Function-Theory (DFT) calculation have been widely employed to get atomic-scale insights into the gold (Au) ion migration into sulfur vacancies in MoS_2. However, due to their incapability to capture ion migration kinetics, these studies propose a simplified picture involving a single Au atom migration into and out of sulphur vacancy in MoS_2 during SET/RESET transitions [5]. However, Reactive molecular dynamics (MD) simulations using reactive force field parameters for Mo/Au/S can reveal filament formation and rupture which involves more complex, multi-gold atom migration driven by electric fields. In another Reactive MD study [6], Au filament in bilayer MoS_2 is ruptured by applying negative voltage along with extremely high temperature of ~2000 K, which could be highly unrealistic and fails to capture dynamic temperature profile within the filament that is experimentally reported for $MoTe_2$ memristors [4].

In this work, we present a coupled modelling framework which captures the effect of both voltage stress and realistic temperature profiles on the filament evolution. To include the filament temperatures originating from the Joule heating, we use electro-thermal calculations within FEM simulations. The temperature profiles obtained from FEM simulations are then fed back to the Reactive MD simulation to capture the temperature driven filament dynamics more accurately. To the best of our knowledge, this is the first reported simulation framework that combines FEM and reactive MD to provide realistic insights into the atomistic filament evolution and has been validated with the current-voltage characteristics of the reported experiments for Au- monolayer MoS_2-Au memristors with bi-sulfur vacancy.

II. Computational Framework

All our Reactive MD simulations are performed using LAMMPS [7] with reactive force field parameters for Mo/Ti/Au/O/S/H [8]. We apply periodic boundary conditions along x and y axis and non-periodic boundary conditions along z-axis in MD simulations. For the initial (0^{th}) iteration, temperature and pressure are set at 300 K using Berendsen thermostat and at ambient conditions using Nose–Hoover barostat, respectively. A timestep of 0.5 fs is used to perform all the simulations. To induce experimentally observed bipolar resistive switching in Au/MoS_2/Au memristor, a triangular voltage profile varying between +38.69 and -38.69 V is applied to Au-MoS_2-Au memristor with bi-sulfur vacancy (Fig. 1a) at a ramp rate of 0.073 V/ps using ECHEMDID package as shown in Fig. 1b. We require these higher voltages than experimentally reported SET/RESET voltages due to the time scale limitations posed by MD simulations [9].

In our coupled approach, we extract the atomistic device structures containing only Au atoms from MD at different voltages (Fig. 1c). These structures are post-processed via a voxelization step (Fig. 1d) to make them suitable for the FEM framework. Voxelisation is performed using python script utilizing pytorch3D library. Fig. 1e shows the complete FEM structure consisting of Si/SiO_2 (500 nm/65 nm) at the bottom and Au/MoS_2/Au memristive device on the top. We scale the applied voltages (Fig. 1f) for FEM simulations to match the realistic experimental RESET voltages, as the higher applied voltages used in MD are necessary only to overcome its limited timescales. Similarly, the current from MD simulations (that are obtained in arbitrary units (a.u.) are scaled to match the RESET current levels.

III. Results and Discussion

Fig. 2a shows the triangular voltage profile applied in the reactive MD simulations. Fig. 2b depicts the initial atomic structure corresponding to the zero voltage at 300K. The atomic structure corresponding to the maximum positive

voltage (i.e. SET transition voltage) and 300K is shown in Fig. 2c, which exhibits a gold atom filament within monolayer MoS_2. Subsequently, Fig. 2d and 2e show atomic structures after the first SET cycle at zero voltage and at maximum negative voltage, respectively. The atomic structure corresponding to the RESET transition voltage (Fig. 2e) clearly demonstrates the absence of an expected gold filament rupture. The absence of filament rupture at 300 K in our MD simulations can be attributed to the absence of the Joule heating. It has been widely studied that the Joule heating plays a significant role to assist the RESET phenomenon for filamentary memristive devices [10].

Therefore, to calculate the corresponding temperature profile for assisting RESET, we employ electro-thermal simulations in FEM which can produce temperatures corresponding to electrical currents at each voltage/time step. The initial device structures obtained from the first Reactive MD simulation for 300K (0^{th} iteration) serve as the input for FEM simulations. To determine the electrical conductivity of the filament at each voltage/time step, we calibrate the FEM-derived current–voltage (I–V) characteristics with the experimental data reported for a 2D MoS_2 memristor with a bi-sulfur vacancy [11] (Fig 3a). As earlier stated, the filament temperature plays a crucial role during the filament rupture, we restrict our FEM simulations to the RESET cycle. Fig. 3b shows the temperature profile (0^{th} iteration) obtained from the FEM simulation based on the 0^{th} iteration MD structures. Using the 0^{th} iteration temperature profile, we perform a subsequent Reactive MD simulation to observe its impact on the filament structure. Fig 4a and 4b show the 1^{st} iteration of the MD atomic structures corresponding to the maximum positive (SET) and the maximum negative (RESET) voltages. Fig. 4b clearly demonstrates the RESET event where the filament constriction is observed corresponding to the negative half of the triangular voltage profile and 0^{th} iteration temperature profile. To further calculate the 1^{st} iteration of temperature profile from FEM simulations, we import the 1^{st} iteration of MD structures which constitutes to a coupled MD-FEM framework. Fig. 3b shows that the 1^{st} iteration temperature profile is reasonably close to the 0^{th} iteration temperature profile, thus indicating a convergence in the coupled framework. This is further depicted in Fig. 4c where the current-voltage characteristics from both MD and FEM simulations show an agreement with the reported experimental characteristics in the RESET region [11]. The validation with experimental results demonstrates the predictive capability of the combined MD–FEM approach.

IV. Conclusion

In this work, we present a coupled multiscale simulation framework that integrates Reactive MD with FEM simulations. This approach bridges the atomistic-level structures and experimental IV characteristics, offering insights into the filament evolution in $Au/MoS_2/Au$ memristors under varying operating conditions. The iterative Reactive MD–FEM coupling allows us to capture realistic and voltage dependent temperature profiles, which in turn affects atomic rearrangements and filament constriction. The presented framework not only gives insights into the structural changes observed during switching but also provides the current-voltage characteristics that can be validated with the experimental results.

By integrating atomistic insights with continuum-scale temperature information feedback, we establish a robust multiscale simulation framework capable of capturing the filament dynamics and switching characteristics in $Au/MoS_2/Au$ atomristors. This methodology offers a systematic pathway to explore the role of local heating, filament stability, and structural evolution in resistive switching devices, potentially guiding the design of more reliable and efficient neuromorphic and memory technologies.

V. References

[1] M. M. Rehman, H. M. M. U. Rehman, J. Z. Gul, W. Y. Kim, K. S. Karimov, and N. Ahmed, "Decade of 2D-Materials-Based RRAM Devices: Review," Science and Technology of Advanced Materials, vol. 21, no. 1, pp. 147–186, 2020.

[2] R. Xu, H. Jang, M.-H. Lee, D. Amanov, Y. Cho, H. Kim, S. Park, H.-j. Shin, and D. Ham, "Vertical MoS_2 double-layer memristor with electrochemical metallization as an atomic-scale synapse with switching thresholds approaching 100 mV," Nano letters, vol. 19, no. 4, pp. 2411–2417, 2019.

[3] K. A. Nirmal, D. D. Kumbhar, A. V. Kesavan, T. D. Dongale, and T. G. Kim, "Advancements in 2D layered material memristors: unleashing their potential beyond memory," npj 2D Materials and Applications, vol. 8, no. 1, p. 83, 2024.

[4] I. M. Datye, M. M. Rojo, E. Yalon, S. Deshmukh, M. J. Mleczko, and E. Pop, "Localized heating and switching in $MoTe_2$-based resistive memory devices," Nano letters, vol. 20, no. 2, pp. 1461–1467, 2020.

[5] G. Boschetto, S. Carapezzi, and A. Todri-Sanial, "Non-volatile resistive switching mechanism in single-layer MoS_2 memristors: insights from ab initio modelling of Au and MoS_2 interfaces," Nanoscale Advances, vol. 5, no. 16, pp. 4203–4212, 2023

[6] S. Mitra and S. Mahapatra, "Atomistic description of conductive bridge formation in two-dimensional material based memristor," npj 2D Materials and Applications, vol. 8, no. 1, p. 26, 2024.

[7] A. P. Thompson, H. M. Aktulga, R. Berger, D. S. Bolintineanu, W. M. Brown, P. S. Crozier, P. J. In't Veld, A. Kohlmeyer, S. G. Moore, T. D. Nguyen et al., "Lammps-a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales," Computer physics communications, vol. 271, p. 108171, 2022.

[8] Q. Mao, Y. Zhang, M. Kowalik, N. Nayir, M. Chandross, and A. C. van Duin, "Oxidation and hydrogenation of monolayer MoS_2 with compositing agent under environmental exposure: The reaxff mo/ti/au/o/s/h force field development and applications," Frontiers in Nanotechnology, vol. 4, p. 1034795, 2022.

[9] A. K. Amaram, S. Kharwar, and T. K. Agarwal, "Investigation of resistive switching in Au/ MoS_2/Au using reactive molecular dynamics and ab-initio quantum transport calculations," IEEE Electron Device Letters, vol. 46, no. 4, pp. 656–659, 2025.

[10] F. Raffone and G. Cicero, "Unveiling the fundamental role of temperature in rram switching mechanism by multiscale simulations," ACS Applied Materials & Interfaces, vol. 10, no. 8, pp. 7512–7519, 2018.

[11] I.M. Hus, R. Ge, P.-A. Chen, L. Liang, G. E. Donnelly, W. Ko, F. Huang M.-H. Chiang, A.-P. Li, and D. Akinwande, "Observation of single-defect memristor in an MoS_2 atomic sheet," Nature Nanotechnology, vol. 16, no. 1, pp. 58–62, 2021.

[12] R. J. Dolleman, D. Lloyd, M. Lee, J. S. Bunch, H. S. Van Der Zant, and P. G. Steeneken, "Transient thermal characterization of suspended monolayer MoS_2," Physical Review Materials, vol. 2, no. 11, p. 114008, 2018

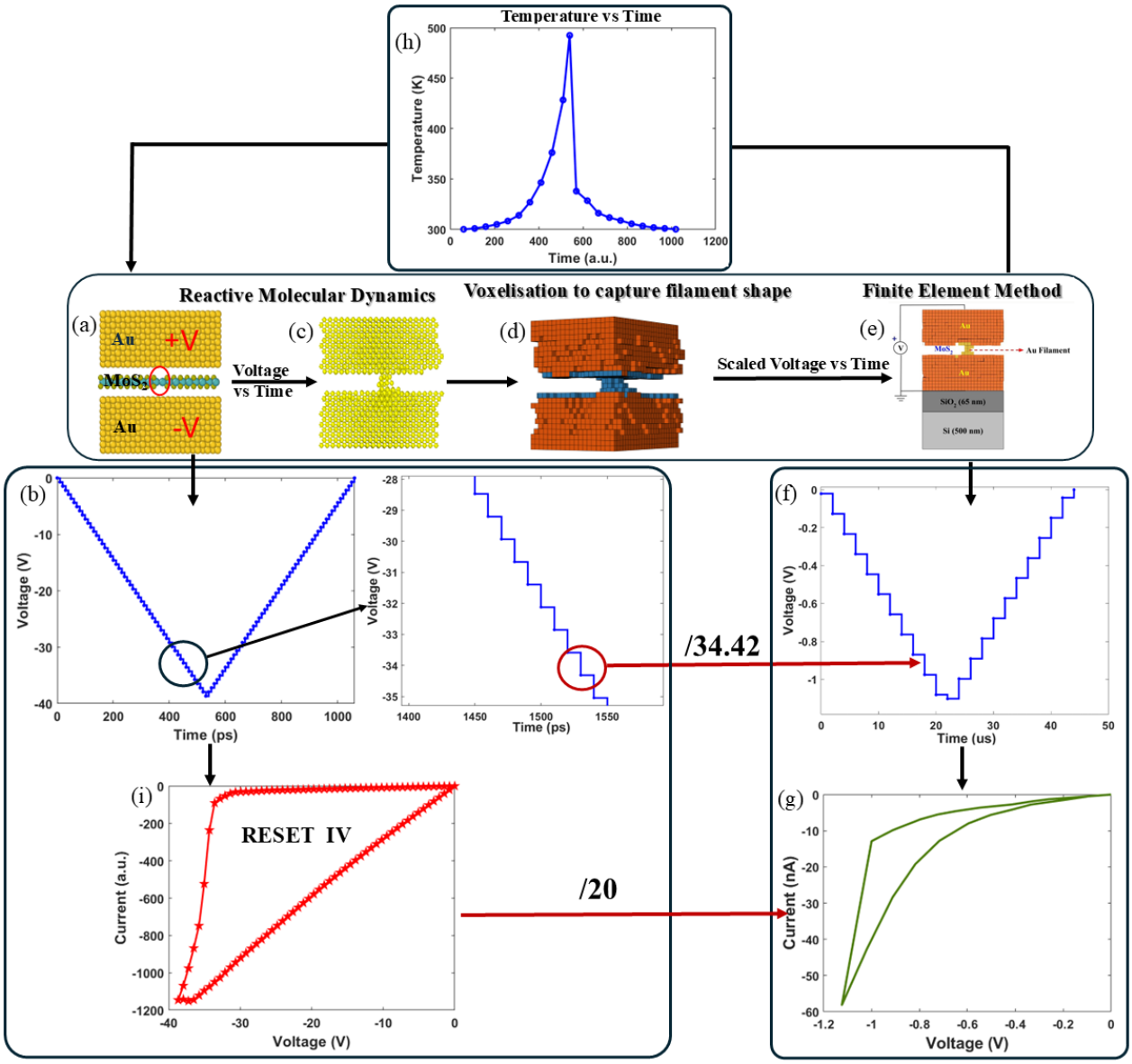

Figure 1. Multiscale Coupled Framework with FEM and Reactive MD Simulations, (a) Initial Structure with bi-sulfur vacancy, (b) Voltage vs Time for RESET cycle, (c) The atomic structure exported from MD simulations with only Au, (d) Voxelisation of the atomic structure, (e) Structure imported for FEM simulation with SiO_2/Si substrate, (f) Scaled voltage profile in FEM simulations, (g) IV characteristics in FEM after fitting conductivity corresponding the experimental result [11], (i) Reactive MD IV characteristics after applying the RESET cycle voltage (Fig. 1b) along with the temperature profile obtained from electro-thermal calculations in FEM simulation framework.

Material Parameter	Au	MoS_2 and Filament
σ (S/m)	$\frac{1.4\times10^7}{1+0.0025\times(T-T_0)}$ [4]	0.312 (MoS_2 fitting) and fitting parameter for Filament
κ (W/ (m.K))	$\sigma \times L_0 \times T$ [4]	34.5 [12]
Cp (J/kg K)	129 [4]	373 [12]
ε	-1×10^7	4.3

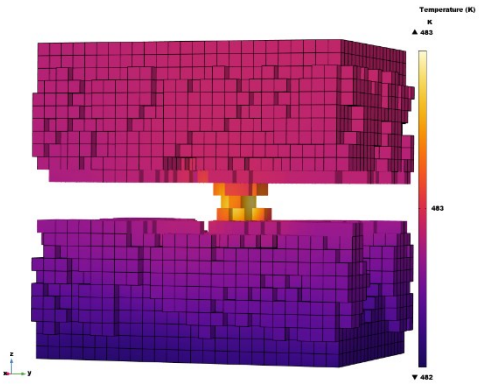

Table 1. Material Parameters used for FEM Simulations where $L_0 = 2.44\text{x}10^{-8}$ is the Lorentz number and T_0 is the temperature of the previous step which initially starts from 300 K. (The figure highlights the electro-thermal simulation within COMSOL Multiphysics corresponding to the material parameters given in Table. 1)

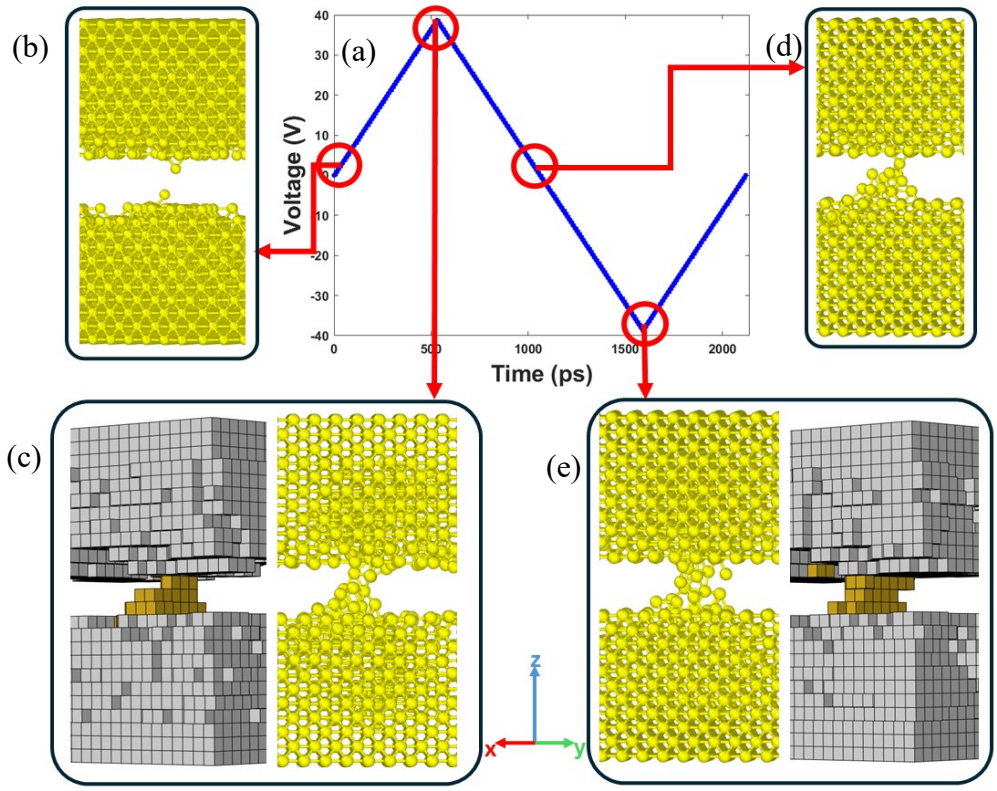

Figure 2. (a) Triangular Voltage profile applied to the Au/MoS_2/Au Memristor at 300K; Atomic structures corresponding to b) zero voltage, (c) the maximum positive applied (SET) voltage and its voxelised structure, d) zero voltage after the first SET cycle, e) maximum negative (RESET) voltage and its voxelised structure.

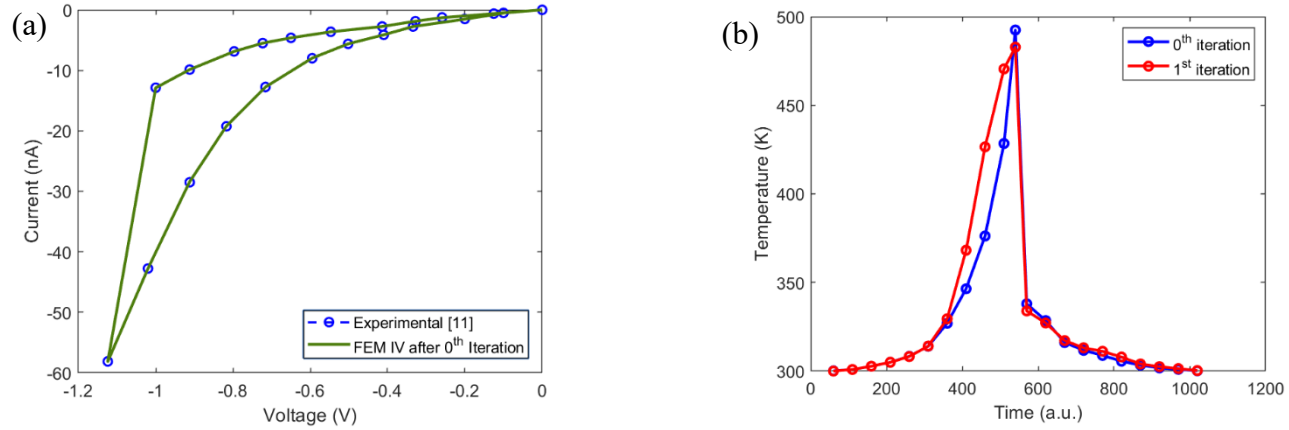

Figure 3. (a) FEM IV characteristics fitted to the experimental IV characteristics to calibrate the filament conductivity. (b) Temperature profiles obtained for 0^{th} and 1^{st} iteration from FEM simulations.

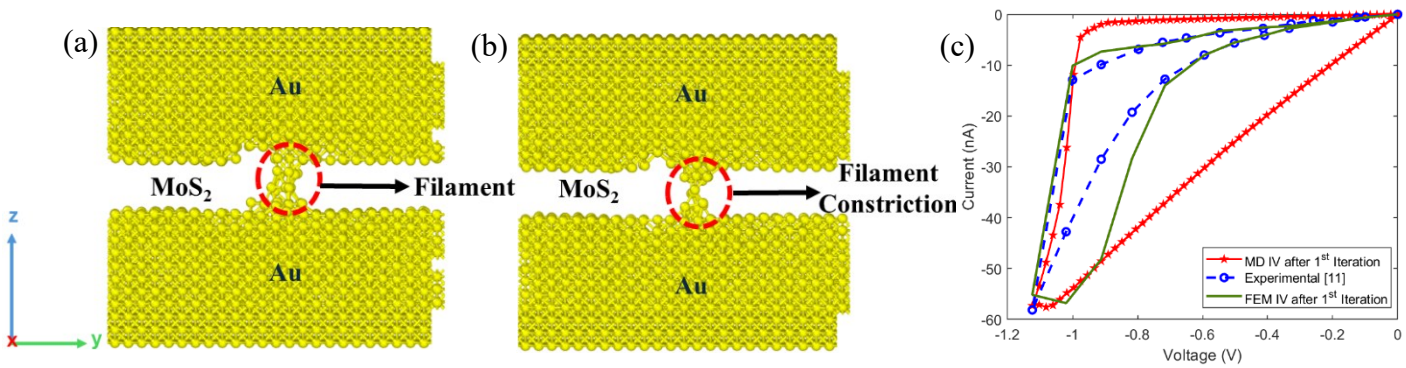

Figure 4. Atomic structures corresponding to (a) the SET voltage and (b) the RESET voltage, obtained from Reactive MD simulations after the 1^{st} iteration. (c) Validation of FEM IV characteristics and MD IV characteristics after the 1^{st} iteration with the reported experimental IV for RESET cycle.