Comprehensive Numerical Modeling of Filamentary RRAM Device

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INTRODUCTION: Resistive Random-Access Memory (RRAM) is a promising nano-scale memory device which operates via bipolar resistive switching between the insulating (OFF) and conducting (ON) states. The switching is due to formation or destruction of a conducting filament in its insulator layer, yet the underlying physics remains poorly understood. Thus, based on our thermodynamic description [1], we built a numerical RRAM model in COMSOL Multiphysics® which is manipulated with MATLAB® to simulate RRAM device operation and its I-V characteristics.

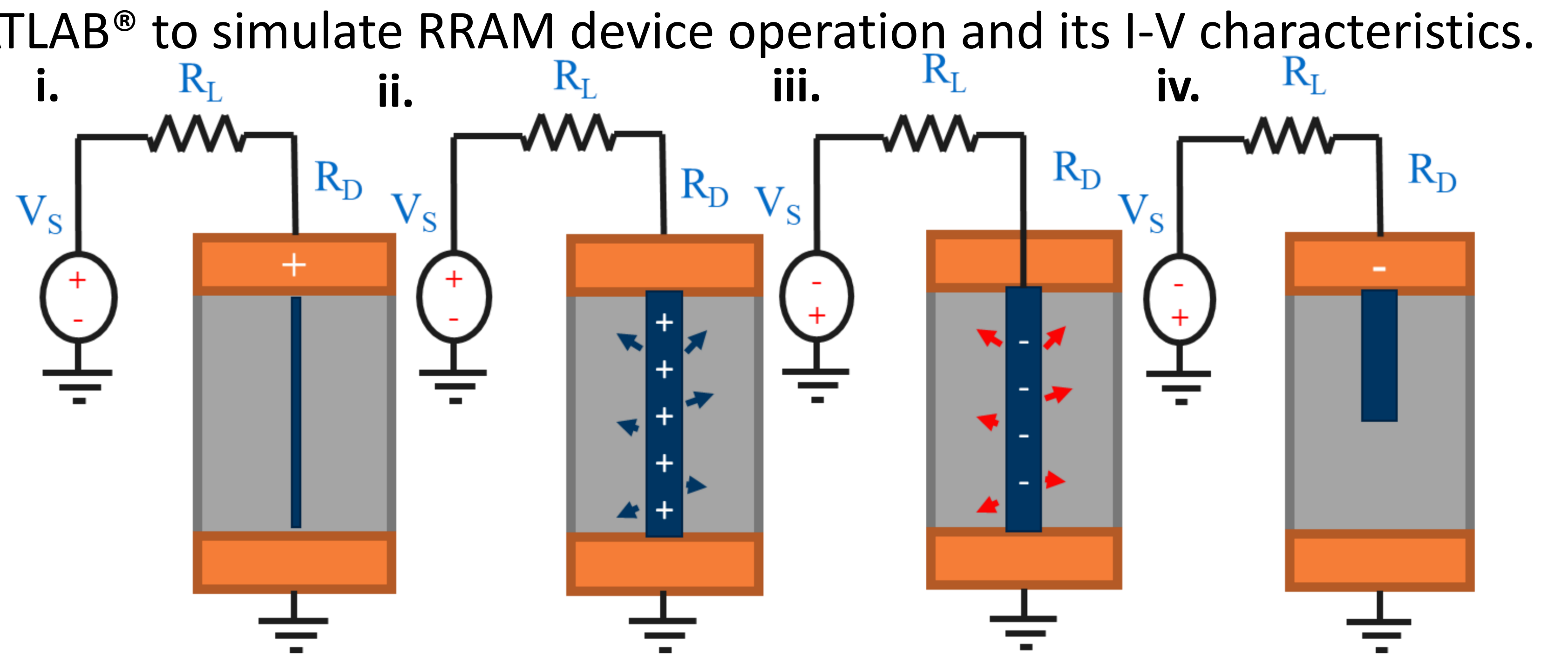
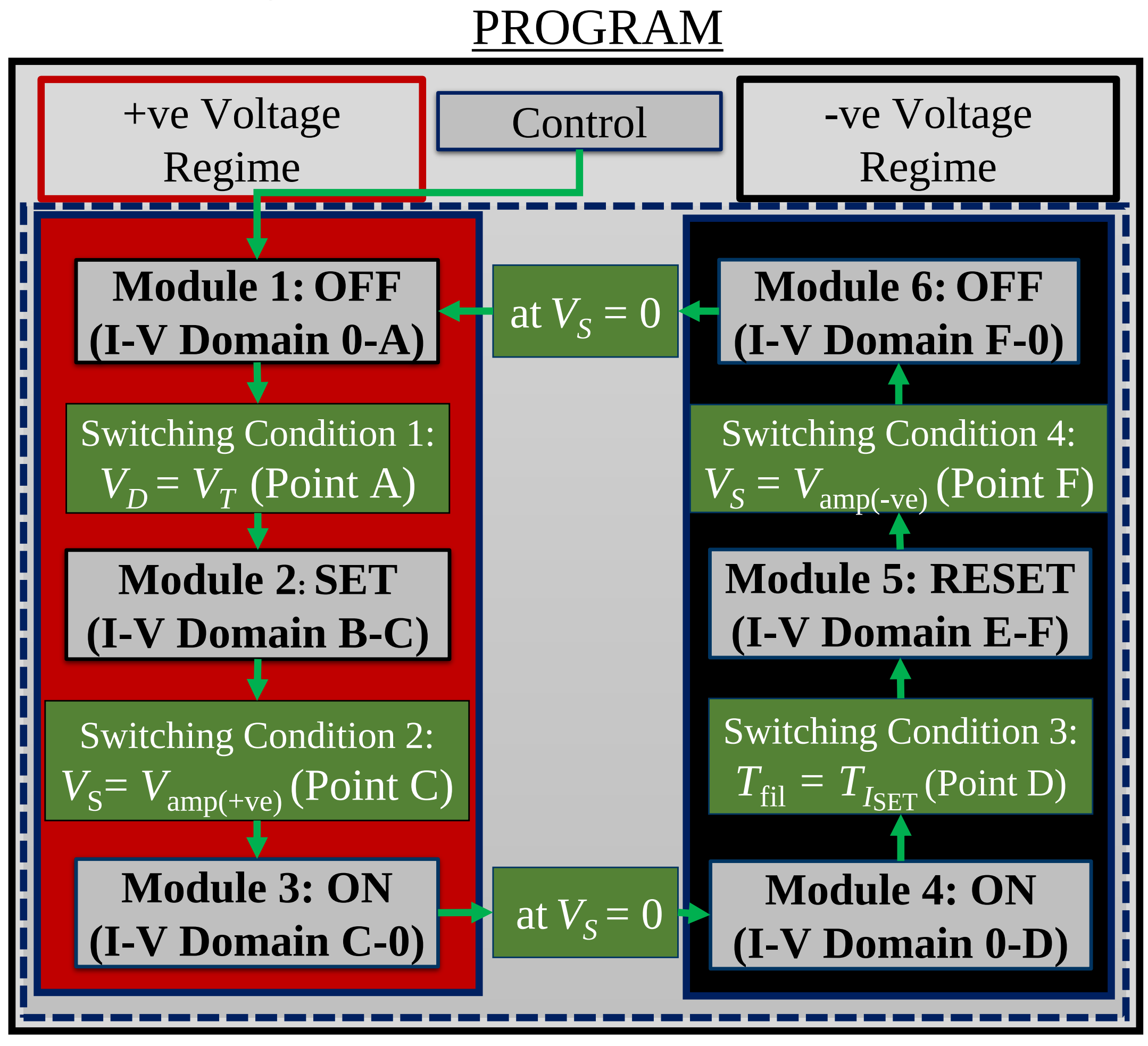


Figure 1. Resistive switching in a generic metal-insulator-metal multilayered RRAM device.
i. Narrow filament forms and shunts RRAM (SET), ii. filament charges and polarizes its surrounding (blue arrows), iii. reversing source polarity, oppositely charges filament which is energetically unfavorable w.r.t surrounding polarization (red arrow) iv. dissolution of filament (RESET).

COMPUTATIONAL METHODS: A Program is devised in MATLAB® consisting of control, modules, and switching conditions that mimic switching operation in a COMSOL® modeled RRAM device.


PROGRAM

+ve Voltage Regime

Control

-ve Voltage Regime

Module 1: OFF (I-V Domain 0-A)

Switching Condition 1: $V_D = V_T$ (Point A)

Module 2: SET (I-V Domain B-C)

Switching Condition 2: $V_S = V_{amp(+ve)}$ (Point C)

Module 3: ON (I-V Domain C-0)

at $V_S = 0$

Module 4: ON (I-V Domain 0-D)

Switching Condition 3: $T_{fil} = T_{I_{SET}}$ (Point D)

Module 5: RESET (I-V Domain E-F)

Switching Condition 4: $V_S = V_{amp(-ve)}$ (Point F)

Module 6: OFF (I-V Domain F-0)

at $V_S = 0$

Figure 2. Flowchart of the program that simulates RRAM switching operation

OFF/ON	**SET/RESET**
Electric Currents module	
$\nabla . \boldsymbol{J} = 0$, $\boldsymbol{J} = \sigma_c \boldsymbol{E} + \epsilon \frac{\partial \boldsymbol{E}}{\partial t}$, $\boldsymbol{E} = -\nabla V$	$\nabla . \boldsymbol{J} = 0$, $\boldsymbol{J} = \sigma_c \boldsymbol{E}$, $\boldsymbol{E} = -\nabla V$
Heat Transfer in Solids module	
$\rho C_P \frac{\partial T}{\partial t} - \nabla . (\kappa \nabla T) = Q_s$	$-\nabla . (\kappa \nabla T) = Q_s$
Multiphysics module	
$Q_S = \boldsymbol{J} . \boldsymbol{E}$	$Q_S = \boldsymbol{J} . \boldsymbol{E}$
Additionally, *Electric Circuit* module is used to connect a power source and load resistor to RRAM in series	

Table 1: Utilized COMSOL Modules and Differential Equations

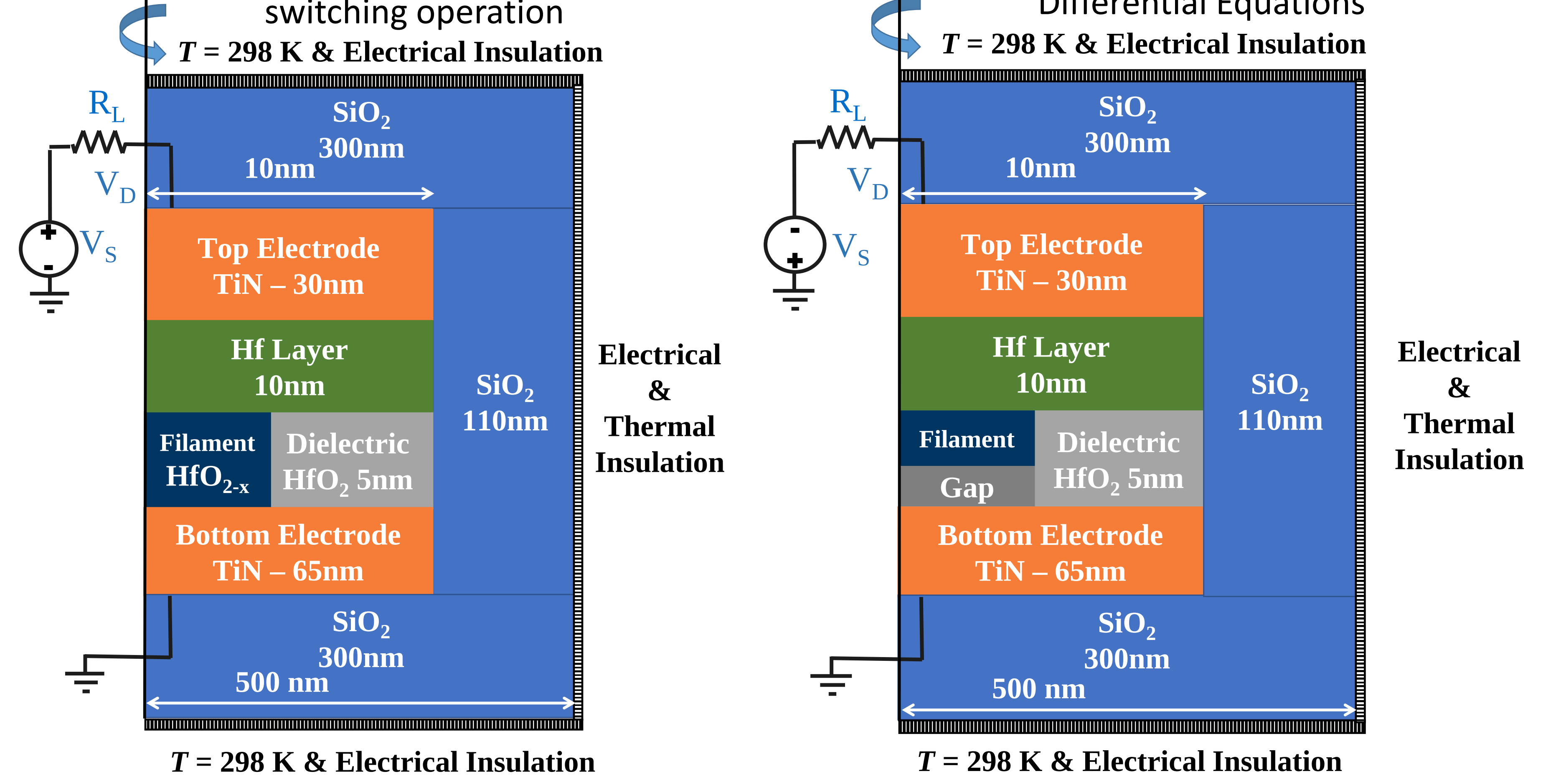


Figure 3. Schematic of the modeled RRAM device.[2] Left: ON and SET, Right: OFF and RESET. Note: the filament and gap in SET and RESET process grows with voltage ramping as dictated by thermodynamics.[3]

Material	σ_c[S/m]	κ[W/K.m]	C_P[J/kg.K]	ϵ_r	ρ[kg/m^3]
SiO_2	10^{-9}	1.38	703	3.9	2.2×10^3
TiN	Exp. $\sigma_c(T)^a$	$\sigma_c(T)TL$	545.33	-∞	5.22×10^3
Hf	Exp. $\sigma_c(T)^b$	$\sigma_c(T)TL$	144	-∞	13.3×10^3
HfO_2	10	0.5	120	25	10×10^3
HFO_{2-x}	$\sigma_{0f} exp(-\alpha_f \, ln(\tau/\tau_0)) exp(\sqrt{eV/kT})$	$\sigma_c(T)TL$	140	-∞	12×10^3
Gap	$\sigma_{0g} exp(-\alpha_g \, ln(\tau/\tau_0)) exp(\sqrt{eV/kT})$	$\kappa_{eff}\sigma_c(T)TL$	120	25	10×10^3

[a] E. Langereis et al., *J. Appl. Phys.* **100,** 023534 (2006).
[b] P. D. Desal, et al., *J. Phys. Chem. Ref. Data.* **3**, 1069 (1984).
[a, b] the experimental data points were inserted in COMSOL via *interpolation function*

Table 2: Utilized material parameters; additional parameters are presented in the paper.

RESULTS: The Program closely reproduces the observed [2] RRAM current-voltage (I-V) characteristics. As a unique feature, our numerical model incorporates the configurational disorder present in non-crystalline materials (HfO_{2-x} in our case) simulating the observed voltage ramp-rate dependency and cycle-to-cycle variation.

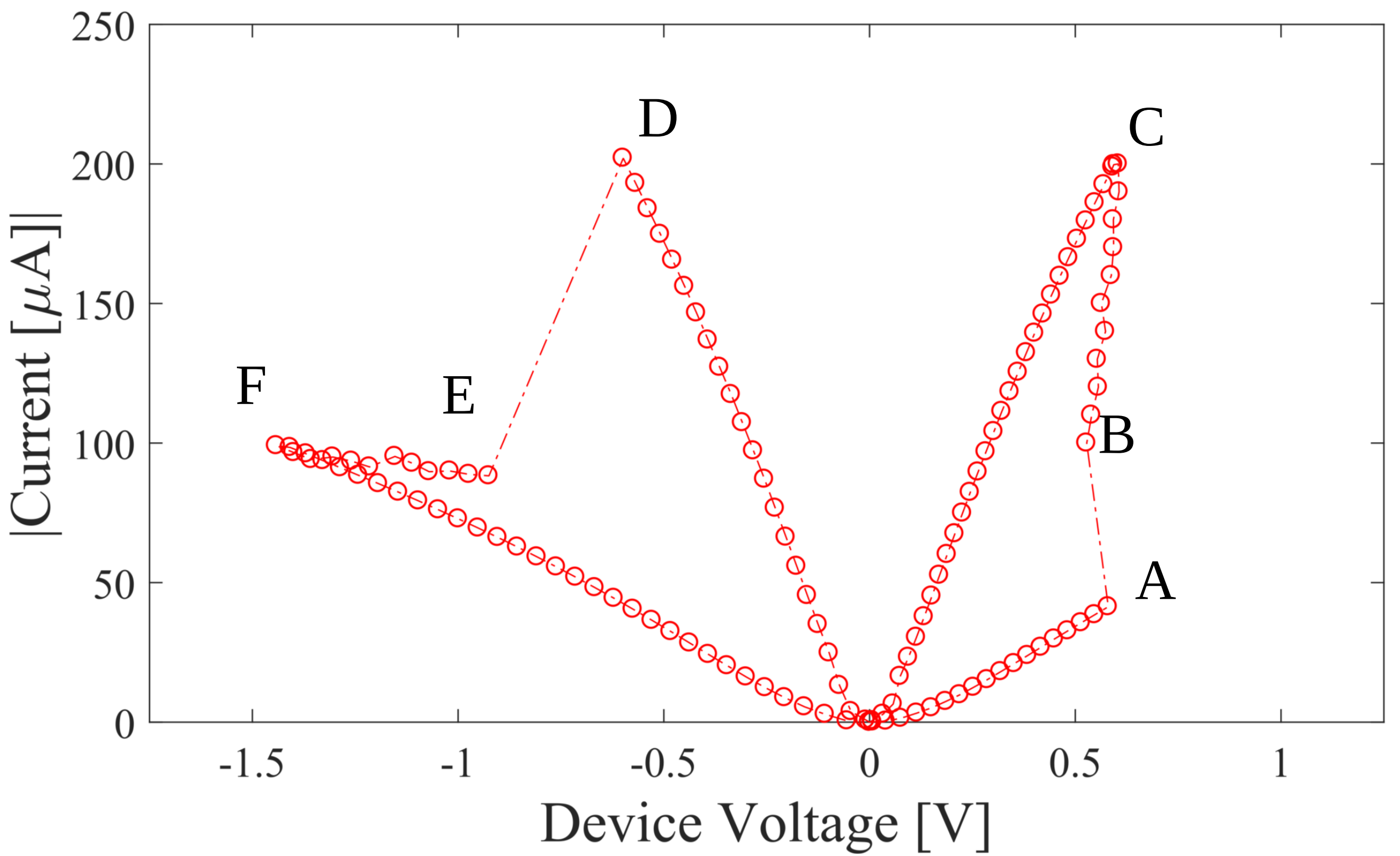


Figure 4. Simulated Current-Voltage characteristics of RRAM device for 100V/s source voltage ramp-rate

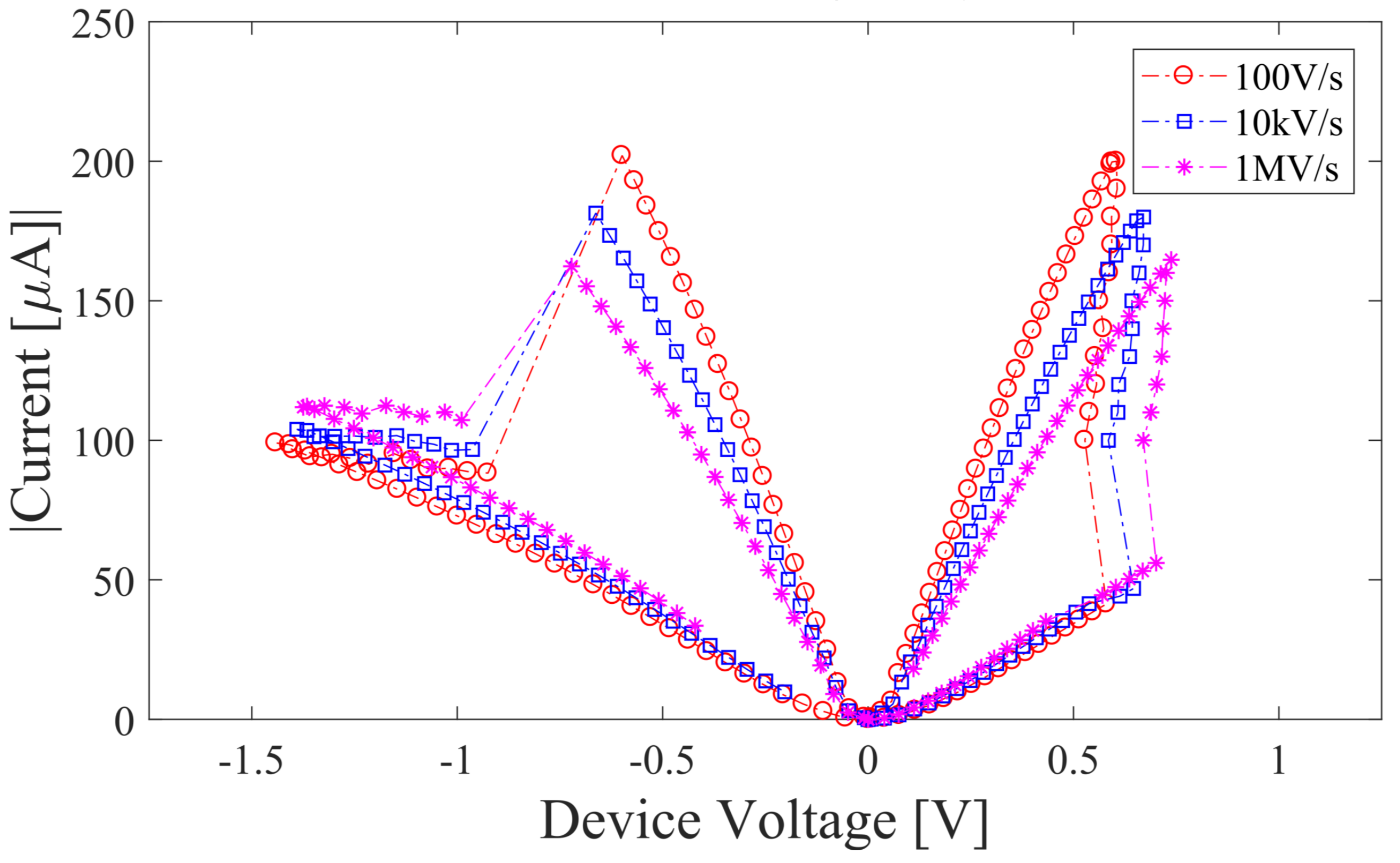


Figure 5. Simulated current-voltage characteristics of RRAM device for three source voltage ramp-rate depicting ramp-rate dependence.

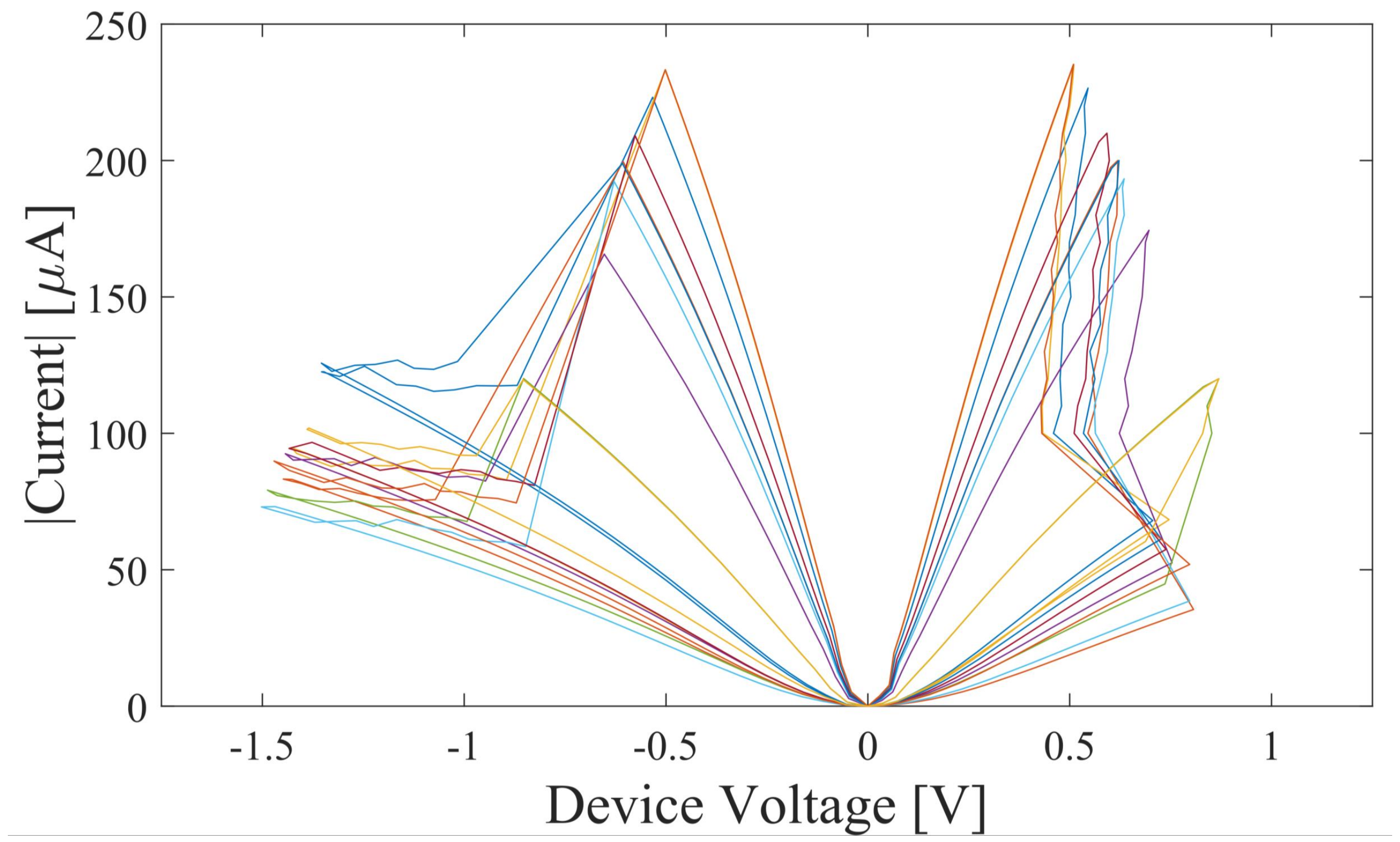


Figure 6. Simulated current-voltage characteristics of RRAM device for 10 switching cycle depicting cycle-to-cycle variation.

CONCLUSIONS: (1) We have developed a numerical model of RRAM device in COSMOL® based on the thermodynamic description as a significant simplification to the kinetic treatment. (2) Our approach will aid the industry in technological advancement. (3) The non-trivial feature of our modeling lie in the overlap of (a) the device smallness and (b) its disordered structure accounted for through the random double well atomic potential characteristic of amorphous materials. (4) Future work includes tuning the Program for particular systems and conditions.

REFERENCES:

1. V. G. Karpov, et al., Thermodynamics of phase transitions and bipolar filamentary switching in resistive random-access memory, *Phys. Rev. Appl.*, **8**, 024028 (2017).
2. A. Fantini, et al., Intrinsic Switching Behavior in HfO_2 RRAM by Fast Electrical Measurements on Novel 2R Test Structures, *2012 4th IEEE International Memory Workshop, Milan*, pp. 1-4 (2012).
3. D. Niraula, et al., Comprehensive numerical modeling of filamentary RRAM devices including voltage ramp-rate and cycle-to-cycle variations, *J. Appl. Phys*. (2018) (Submitted) arXiv:1806.01397 [cond-mat.mes-hall].

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