RRAM Device Numerical Model Comsol/Matlab

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Acknowledgement

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CONTENTS

1.Introduction

- This text acts like a catalog to the numerical modeling software and is meant to present its construct, logic, and technical details.
- This text does not present the physics based on which the software is constructed. Please refer to Ref. [1] for the theoretical details.
- This software is constructed by implementing the Program in COMSOL and MATLAB package

[1] Dipesh Niraula and Victor Karpov, “Comprehensive numerical modeling of filamentary RRAM devices including voltage ramp-rate and cycle-to-cycle variations”, J. Appl. Phys. (In Press) 2018. https://arxiv.org/pdf/1806.01397.pdf

2.The PROGRAM

1. The Program models an RRAM device and simulates resistive switching in the device, yielding its electrical and thermal characteristics.
2. The Program requires a partial differential equation numerical solver to solve coupled electrodynamics and heat equations on a given device and a programming platform.
3. For this particular project, we have implemented the Program in MATLAB programming package that utilizes COMSOL Multiphysics package 5.3 as the numerical solver.
4. However, the logic of this program is independent of the choice of solver and programming package and any equivalent software can be used.
5. The most important and unique part of the program is the application of thermodynamics in quantifying the growth rate of filament during SET and gap during RESET process.

2.I Overview of the PROGRAM

a flowchart of the Program that simulates resistive switching in an RRAM device

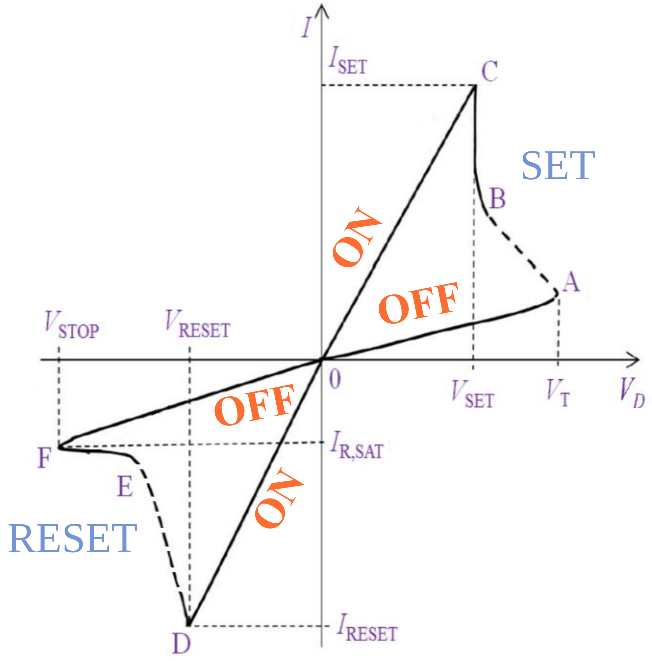
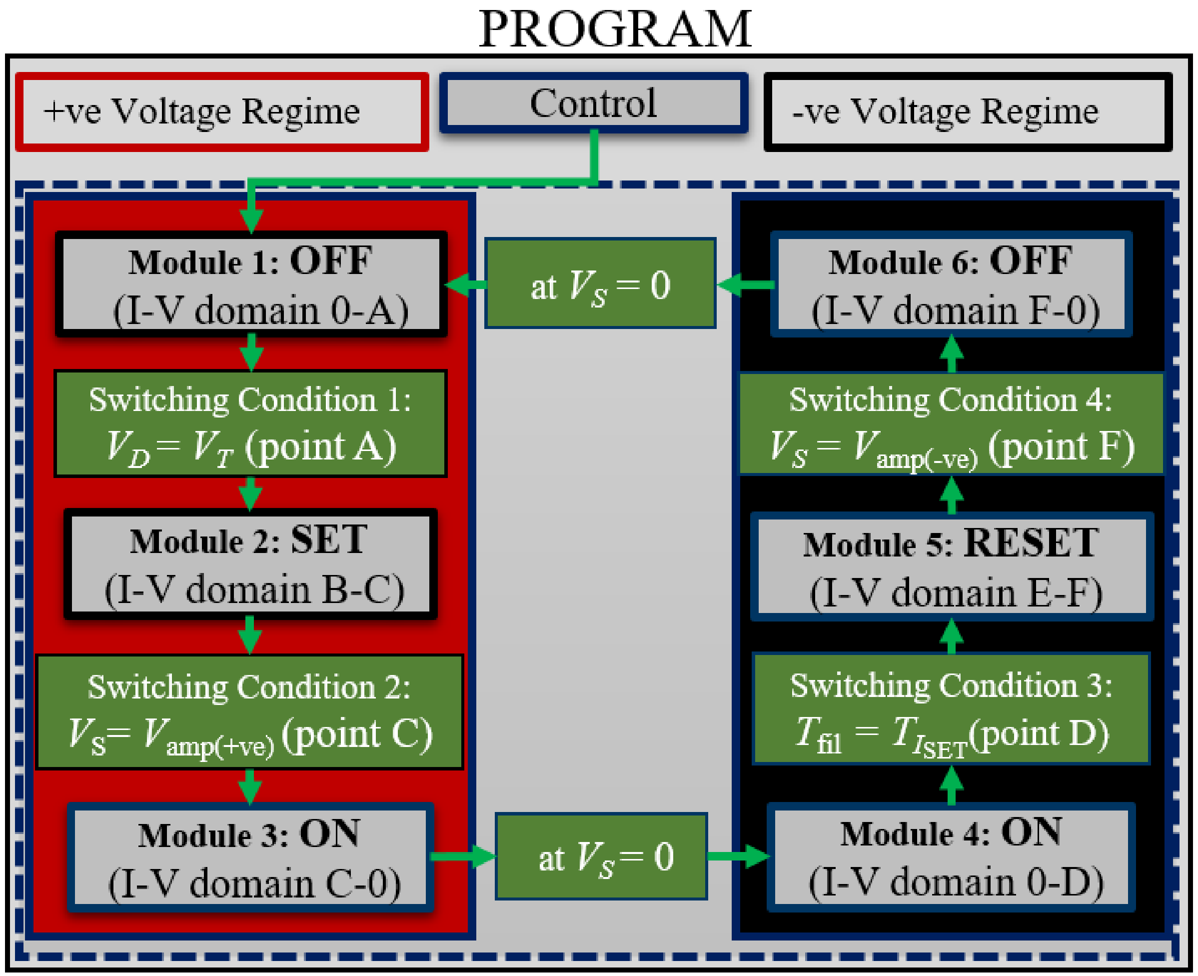


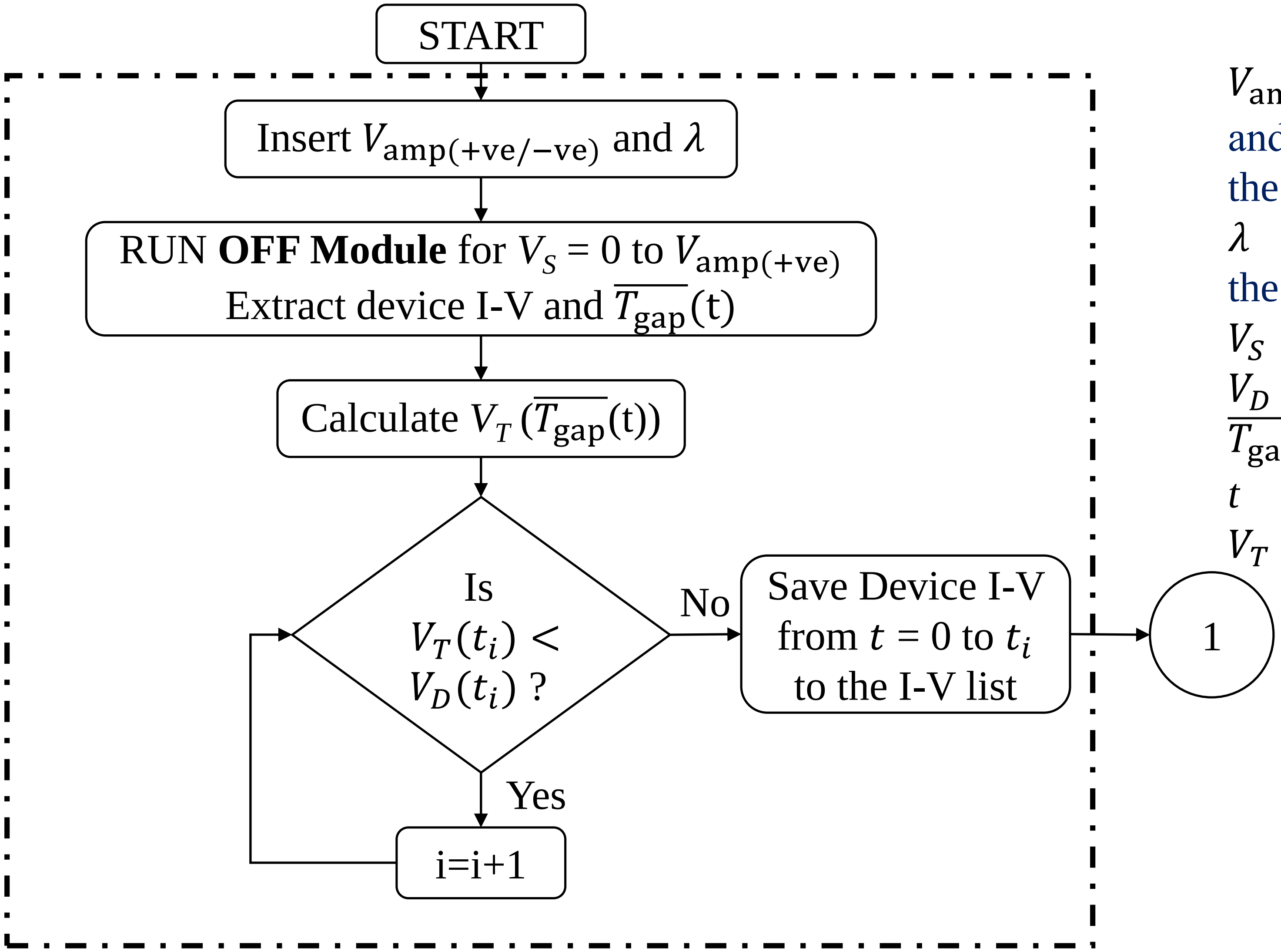
Fig: A typical RRAM device Current-Voltage Characteristics I-V characteristics

V_S : Source Voltage ($V_D + IR_L$)
V_D : Device Voltage
V_T : Threshold voltage
V_{SET} : Set Voltage
V_{STOP} : Stopping voltage
$V_{amp\ (+ve/-ve)}$: Input voltage amplitude for +ve and –ve voltage regime

Note: Compliance Current Absent
V_{amp} sets the current limit
I_{SET} corresponds to $V_{amp(+ve)}$
V_{STOP} corresponds to $V_{amp(-ve)}$



2.II Flow chart of the Program : OFF Module



$V_{\text{amp}(+\text{ve}/-\text{ve})}$: Input voltage amplitude for +ve and –ve voltage regime set by the user according to the experiment

λ : Ramp-rate set by the user according to the experiment

V_S : Source Voltage ($V_D + IR_L$)

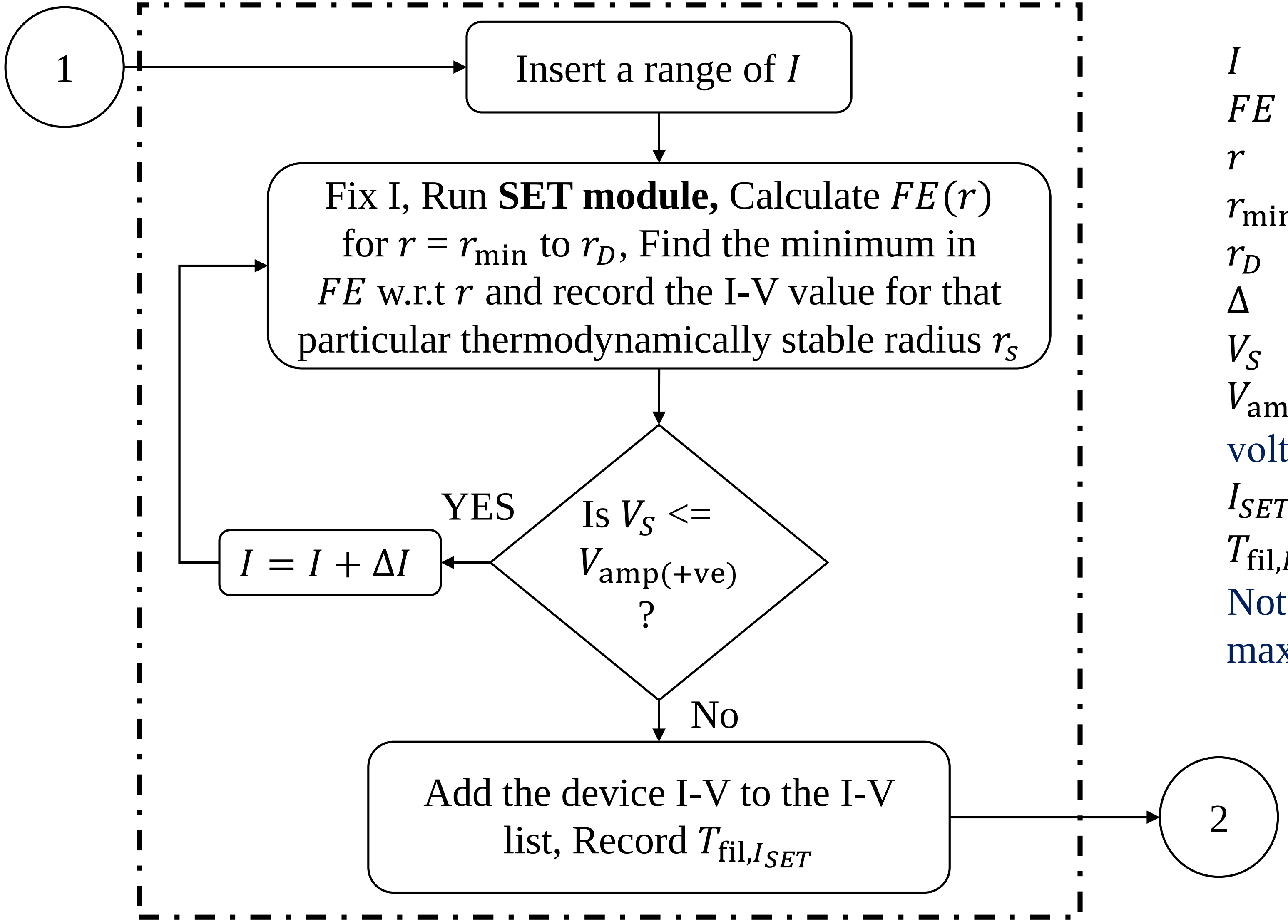
V_D : Device Voltage

$\overline{T_{\text{gap}}}$: Average Gap Temperature

t : Time

V_T : Threshold voltage

2.III Flow chart of the Program : SET Module



I : Current

FE : Free Energy

r : Filament radius

$r_{\min}$: minimum filament radius

r_D : Device Radius

Δ : step size increment

V_S : Source Voltage

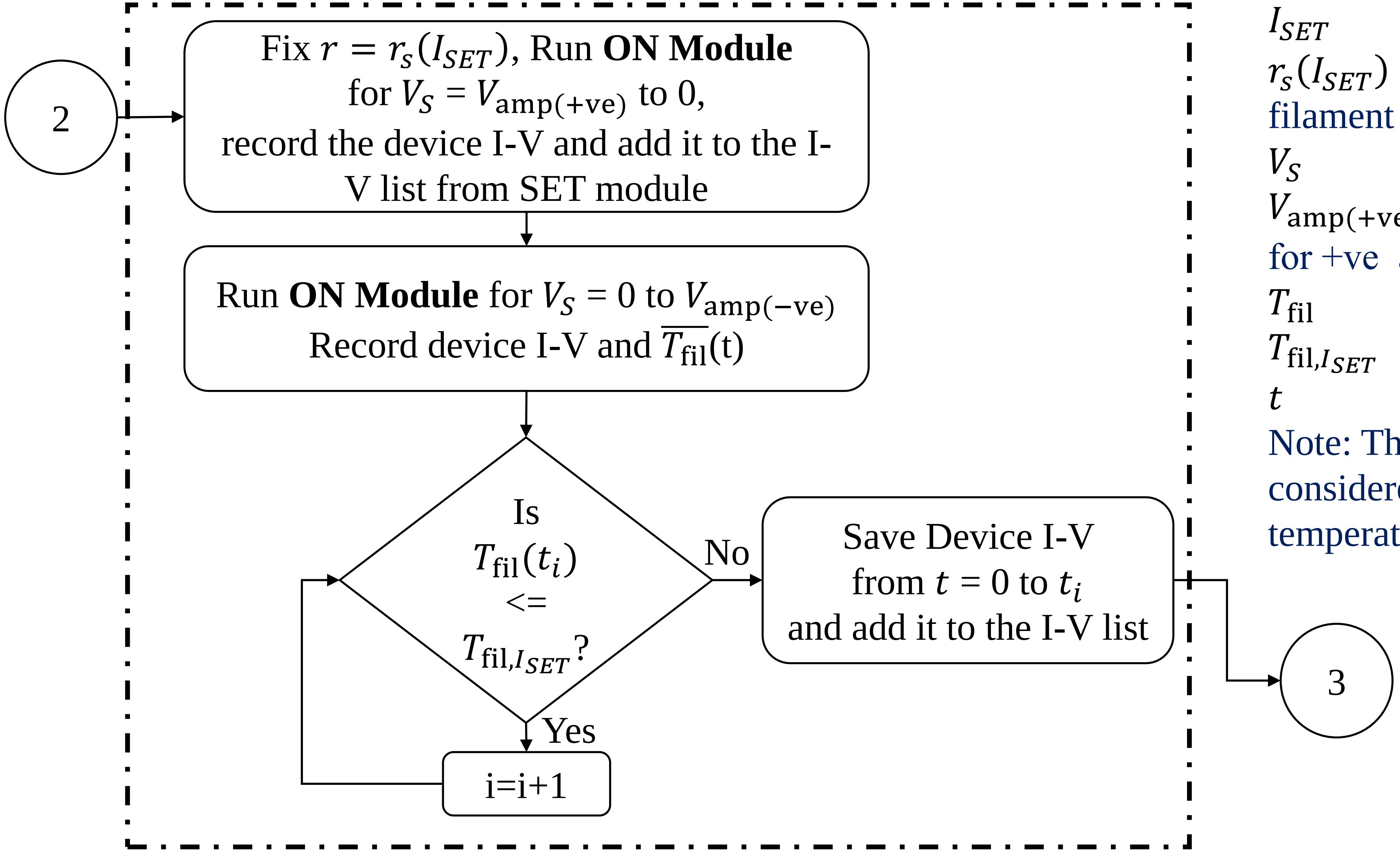
$V_{\text{amp}(+\text{ve})}$: Input voltage amplitude for +ve voltage regime

I_{SET} : Current at $V_{\text{amp}(+\text{ve})}$

$T_{\text{fil},I_{SET}}$: Filament Temperature at I_{SET}

Note: Here, the filament temperature refers to the maximum filament temperature

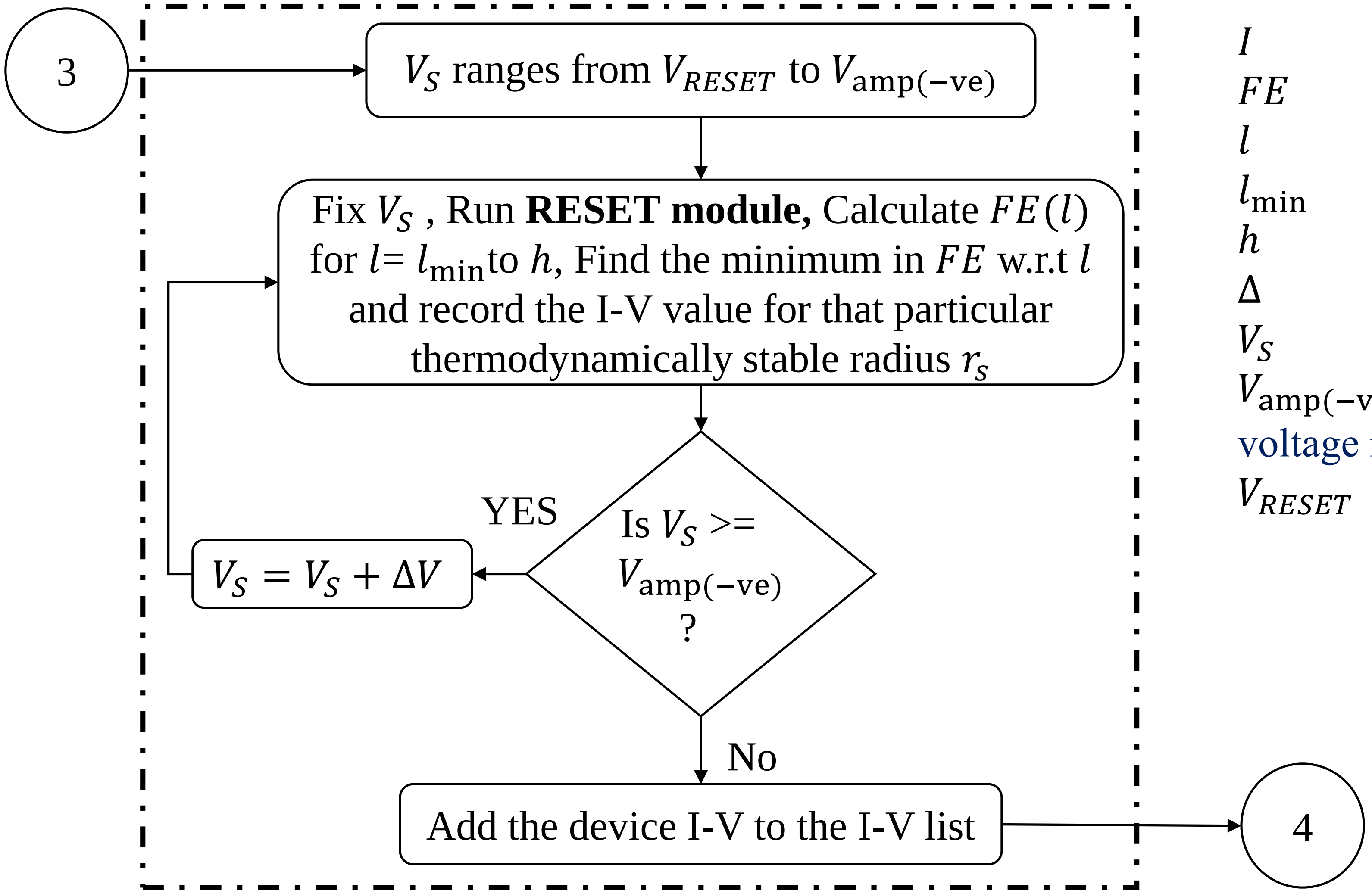
2.IV Flow chart of the Program : ON Module



I_{SET} : Current at $V_{\text{amp}(+\text{ve})}$
$r_s(I_{SET})$: Thermodynamically Stable filament radius at I_{SET}
V_S : Source Voltage
$V_{\text{amp}(+\text{ve}/-\text{ve})}$: Input voltage amplitude for +ve and −ve voltage regime
T_{fil} : Filament Temperature
$T_{\text{fil},I_{SET}}$: Filament Temperature at I_{SET}
t : time

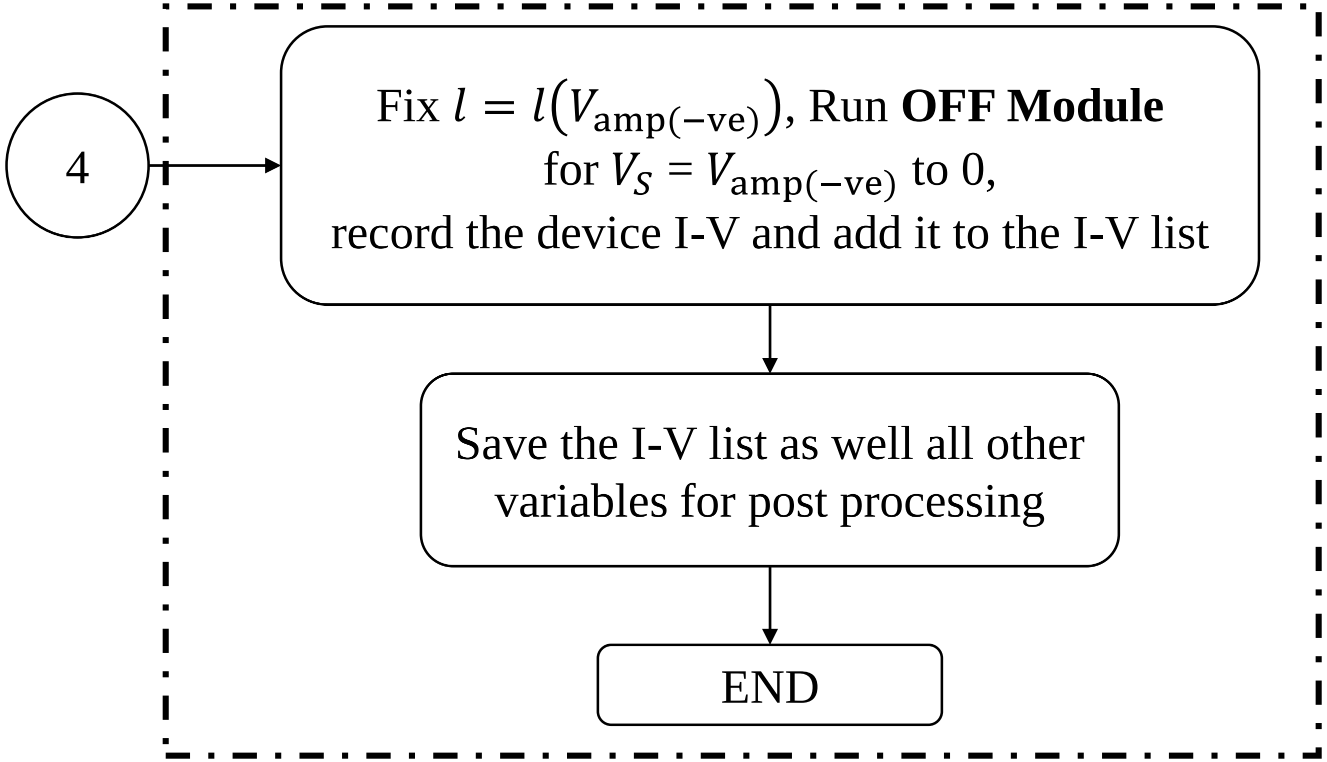
Note: The filament temperature is considered to be the maximum filament temperature for the simulation

2.V Flow chart of the Program : RESET Module



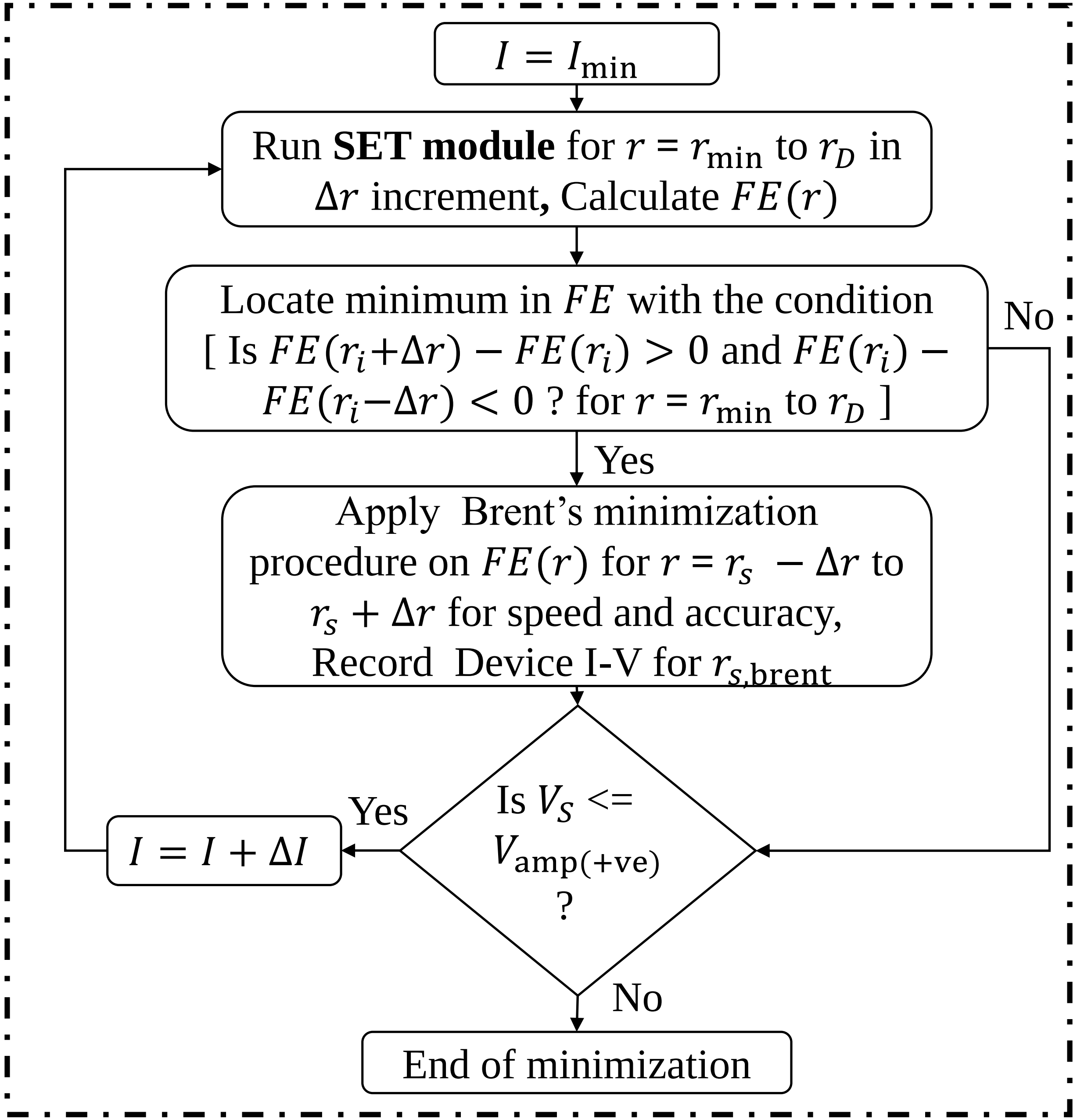
I : Current
FE : Free Energy
l : gap width
$l_{\min}$: minimum gap length
h : Insulator thickness
Δ : step size increment
V_S : Source Voltage
$V_{\mathrm{amp(-ve)}}$: Input voltage amplitude for −ve voltage regime
V_{RESET} : Voltage at which $T_{\mathrm{fil}} = T_{\mathrm{fil},I_{SET}}$

2.VI Flow chart of the Program : OFF Module



l : gap width
V_S : Source Voltage
$V_{\mathrm{amp}(-\mathrm{ve})}$: Input voltage amplitude for −ve voltage regime

2.VII Minimization Procedure: SET



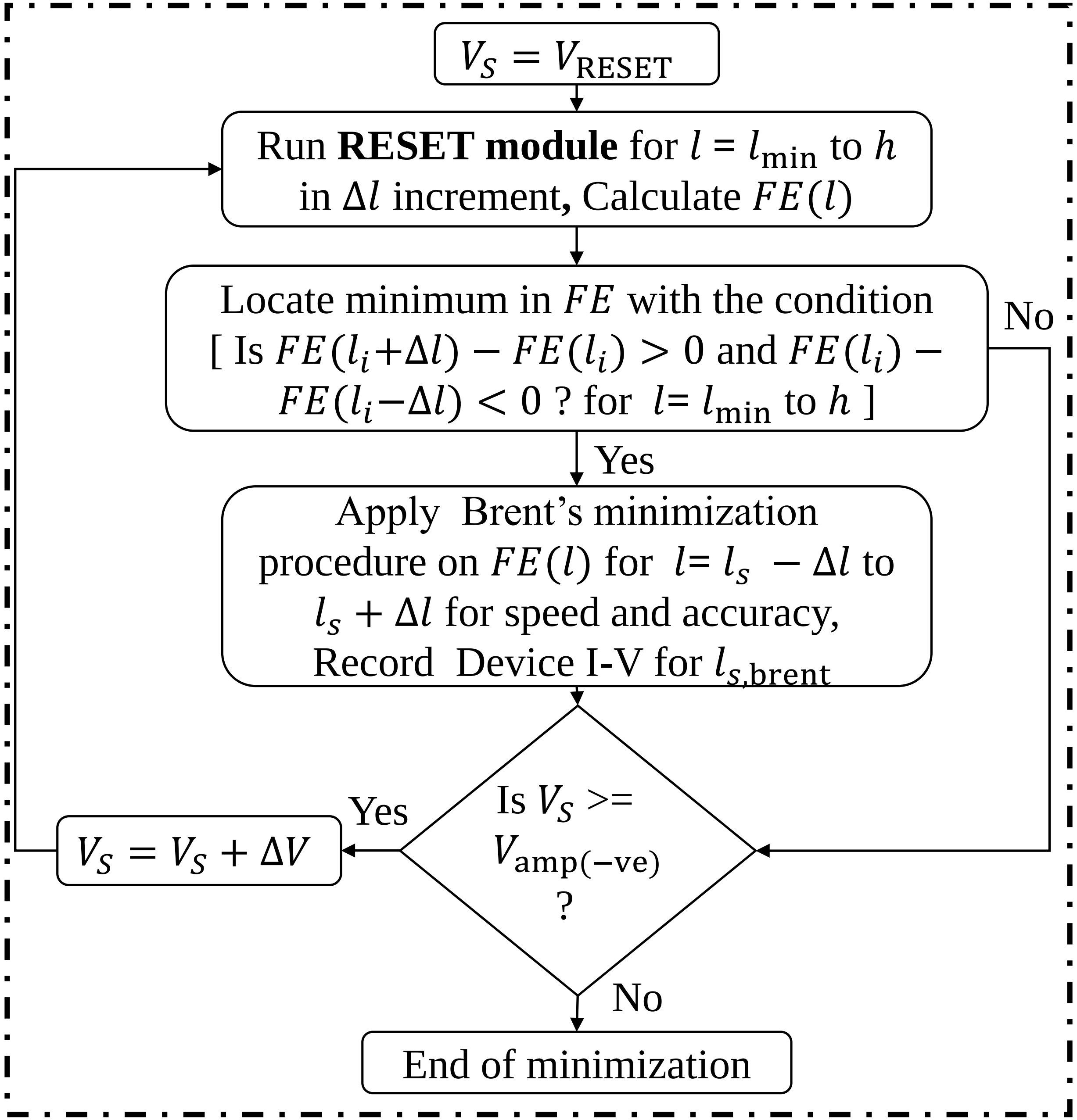
SET is current controlled process

Minimization in Two Step:

1. Locate minimum in $FE(r)$ using coarse Δr
2. If minima exist, use Brent's Minimization to find the minimum

I : Current
$I_{\min}$: Lower limit of the user input Current range
r : Filament radius
$r_{\min}$: Minimum filament radius
r_D : Device Radius
Δ : step size increment
FE : Free Energy
r_s : Thermodynamically stable filament radius
$r_{s,\mathrm{brent}}$: Thermodynamically stable filament radius obtained from Brent's Minimization
V_S : Source Voltage
$V_{\mathrm{amp(+ve)}}$: Input voltage amplitude for +ve voltage regime

2.VIII Minimization Procedure: RESET



SET is current controlled process

Minimization in Two Step:

1. Locate minimum in $FE(r)$ using coarse Δr
2. If minima exist, use Brent's Minimization to find the minimum

V_S : Source Voltage
V_{RESET} : Device voltage
l : Gap length
$l_{\min}$: Minimum gap length
h : Insulator thickness
Δ : step size increment
FE : Free Energy
l_s : Thermodynamically stable gap length
$l_{s,\mathrm{brent}}$: Thermodynamically stable gap length obtained from Brent's Minimization
$V_{\mathrm{amp}(-\mathrm{ve})}$: Input voltage amplitude for −ve voltage regime

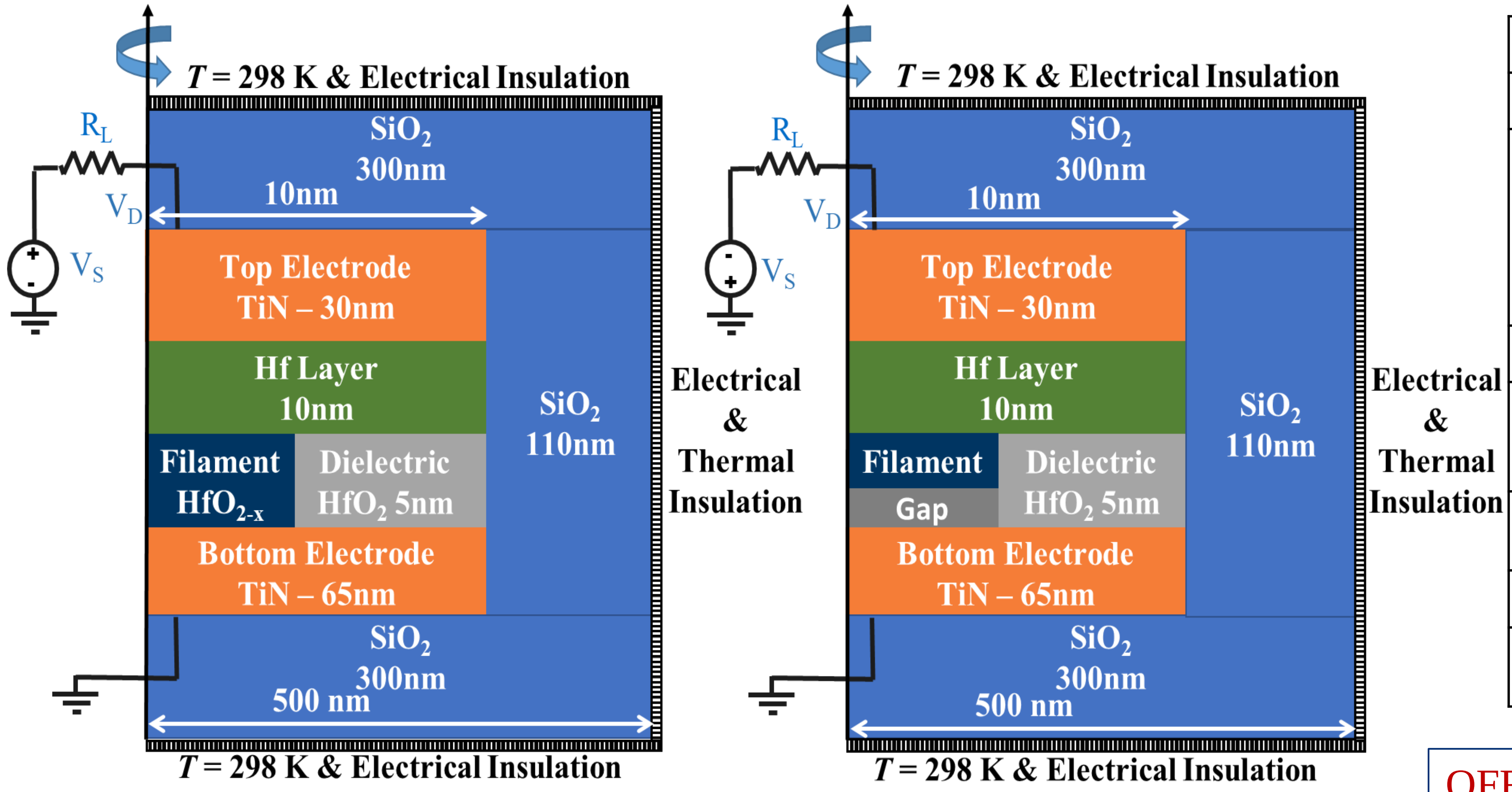
3 Implementation of the PROGRAM

1. As stated above, for this particular project, we have implemented the Program in MATLAB programming package that utilizes COMSOL Multiphysics package 5.3 as the numerical solver.
2. COMSOL solves partial differential equation via finite element numerical method. It can couple physics from different disciplines and has a good graphical user interface.
3. LiveLink for MATLAB is a COMSOL product which enables MATLAB to access COMSOL solver thus adding programming capabilities to COMSOL.
4. In this section, we present details to the COMSOL modeling and MATLAB programs

3.I Device model in COMSOL

device geometry, materials, circuitry, differential equations, and boundary conditions

ON/SET OFF/RESET



Utilized PDEs

OFF/ON	**SET/RESET**
Electric Currents COMSOL 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 COMSOL module	
$\rho C_P\frac{\partial T}{\partial t} - \nabla.(\kappa\nabla T) = Q_s$	$-\nabla.(\kappa\nabla T) = Q_s$
Multiphysics COMSOL module	
$Q_S = \boldsymbol{J}.\boldsymbol{E}$	$Q_S = \boldsymbol{J}.\boldsymbol{E}$
Electric Circuit module is utilized to create the circuitary	

A. Fantini et al, 2012 4th IEEE International Memory Workshop, Milan, pp. 1-4 (2012)

OFF/ON: the gap/filament remains intact

RESET/SET: the gap/filament grows

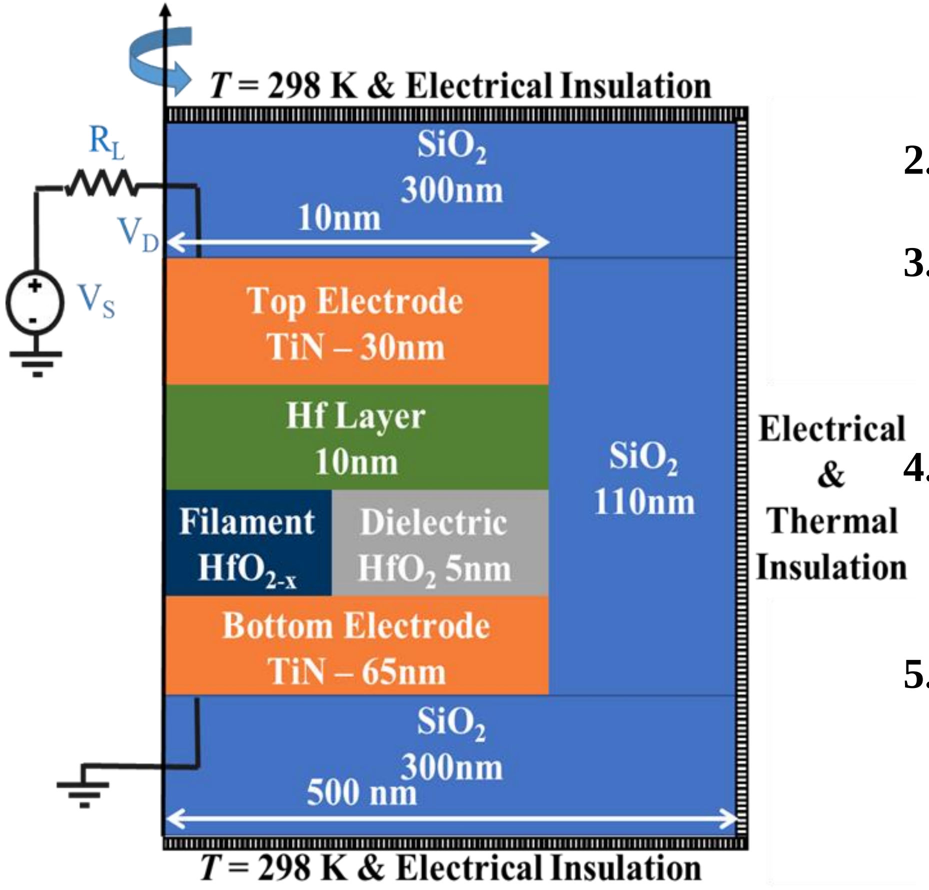
3.II Differential Equations

<table>
<tr><th>OFF/ON
(Time-dependent)</th><th>SET/RESET
(Stationary[1])</th></tr>
<tr><td colspan="2">Electric Currents COMSOL module
(Electrodynamics)</td></tr>
<tr><td>$\nabla . \boldsymbol{J} = 0 \quad (1)$
$\boldsymbol{J} = \sigma_c \boldsymbol{E} + \epsilon \frac{\partial E}{\partial t} \quad (2a)$
$\boldsymbol{E} = -\nabla V \quad (3)$</td><td>$\nabla . \boldsymbol{J} = 0 \quad (1)$
$\boldsymbol{J} = \sigma_c \boldsymbol{E} \quad (2b)$
$\boldsymbol{E} = -\nabla V \quad (3)$</td></tr>
<tr><td colspan="2">Heat Transfer in Solids COMSOL module
(Heat Transfer)</td></tr>
<tr><td>$\rho C_P \frac{\partial T}{\partial t} - \nabla . (\kappa \nabla T) = Q_s \quad (4a)$</td><td>$-\nabla . (\kappa \nabla T) = Q_s \quad (4b)$</td></tr>
<tr><td colspan="2">Multiphysics COMSOL module
(Electro-thermal Coupling (Joule Heat))</td></tr>
<tr><td>$Q_S = \boldsymbol{J} . \boldsymbol{E} \quad (5)$</td><td>$Q_S = \boldsymbol{J} . \boldsymbol{E} \quad (5)$</td></tr>
<tr><td colspan="2">[1] SET and RESET module calculates the rate of filament and gap growth utilizing standard thermodynamic approach, thus stationary equations are applied.</td></tr>
</table>

Eq. (1) is the Current Conservation Law,
Eq. (2) is the Ohms Law
Eq. (3) is the relation between Electric Field and Potential due to Maxwell's law.
Eq. (4) is the Fourier Heat Law where the heat source is represented by the Joule heat of Eq. (5).

In the above equations, the symbols have following meaning	
$\boldsymbol{J}$: Current Density,	ρ: Mass Density
σ_c : Electrical Conductivity,	C_P: Specific Heat Capacity
$\boldsymbol{E}$: Electric Field,	κ : Thermal Conductivity
ϵ: Dielectric Permittivity	T: Temperature
t: Time	Q_S : Heat Source
V : Electric Potential	

3.III Boundary Conditions



1. **Electric Insulation** ($\boldsymbol{n}.\boldsymbol{J} = 0$) and **Thermal Insulation** ($\boldsymbol{n}.\boldsymbol{q} = 0$)
   All three boundaries of the SiO_2 domain are electrically insulated and only the boundary of the side SiO_2 was thermally insulated. Here $\boldsymbol{n}$ is the unit vector normal to the surface boundary.
2. **Ground** ($V = 0$)
   Interface common to the bottom electrode and SiO_2 substrate is grounded.
3. **Terminal** ($V = V_\mathrm{D}$ or $I = I_S$)
   Interface common to the top electrode and SiO_2 superstrate is connected to the power-source and load resistor in series. Terminal handles both voltage source and current source.
4. **Temperature** ($\mathrm{T} = 298\mathrm{K}$)
   Free surfaces of both SiO2 layers are placed at room temperature, assuming they are in contact with a larger body which acts as a heat sink and maintains room temperature. Also, all three boundaries of the SiO_2 domain are at room temperature.
5. **Diffusive Surface** ($-\boldsymbol{n}.\boldsymbol{q} = \sigma_B(T_{\mathrm{amb}}^4 - T^4)$)
   All the interface of the device loses heat through radiation governed by Stefan-Boltzmann law. Here $\boldsymbol{q}$ is the power radiated per surface area, σ_B is the Stefan-Boltzmann constant, and T_{amb} is the ambient temperature (298 K).

Note: Strictly speaking, surface-to-surface, instead of surface-to-ambient radiation heat transfer must be applied to the inner surfaces for a more accurate result. The surface-to-surface radiation condition was not available in the basic COMSOL package and had to be purchased separately (Heat Transfer Module), thus we couldn’t apply it. However, since conductive heat lost is the major contributor, the error due to radiation is negligible.

3.IV Parameters

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

[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).
[c] Relative Permittivity
[d] Wiedemann-Franz-Lorenz Law
[e] Assumed value such that it lies in between Hf and HfO_2
[f] -10^6 was used instead of $-\infty$ for practical purpose
[g] Assumed to be equal to that of HfO2

Parameter	Value
Circuitry	
R_L	3.1 kΩ
$V_{\mathrm{amp(+ve)}}$, $V_{\mathrm{amp(-ve)}}$	1.25 V, -1.75 V
λ	100 V/s, 10 kV/s, 1 MV/s
Filament Nucleation	
h	5 nm
W_0	2.5 eV
Λ	6.6
r_c	2.9 nm
$r_{\min}$	0.5nm
α	$r_{\min}/r_c$
Electric Conductivity	
σ_{0f}	5 kS/m
σ_{0g}	3 kS/m
α_f	-0.05
α_g	0.05
τ	V_{amp}/λ
$\tau_0(\tau_{\min})$	0.1 ps

Parameter	Value
Chemical Energy	
σ	0.01 J/m^3
$\overline{\delta\mu_1}$	10 GJ/m^3
$\overline{\delta\mu_2}$	6.5 GJ/m^3
β_1	0.35 GJ/m^3
β_2	0.5 GJ/m^3
ΔW_{Buc}	1.0 eV
ΔW_{Bi}	0.1eV
ΔW_{Bmc}	0.3eV
Static Disorder	
σ_{0f}	rand(2, 8) kS/m[h]
σ_{0g}	rand(1, 5) kS/m[h]
α_f	rand(-0.07, -0.03)[h]
α_g	rand(0.03, 0.07)[h]
$\overline{\delta\mu_1}$	rand(8.5, 11.5) GJ/m^3[h]
$\overline{\delta\mu_2}$	rand(5.5, 7.5) GJ/m^3[h]
W_0	rand(2.4, 2.6) eV[h]
Thermal Conductivity	
κ_{eff}	10

[h] function rand(x, y) produces uniformly distributed random number between x and y

M.A. Panzer, et al, *IEEE El. Dev. Lett.*, 30, pp. 1269-1271 (2009)
B. Govoreanu, et al., *IEEE Trans. El. Dev.*, 60, pp. 2471-2478 (2013)
E. Hildebrandt, et al., *Appl. Phys. Letts.*, 99, pp. 112902, (2011)
M.K. Samani, et al., *Thin Solids Films*, 573, pp. 108-112, (2013)
Carl L. Yaws. *The Yaws Handbook of Physical Properties for Hydrocarbons and Chemicals*, 2nd ed. (2015)

3.V Step-by-Step Process of building RRAM in COMSOL

1. Open **Model Wizard**
2. Select **2D Axisymmetric** as **Space Dimension**
3. Select **AC/DC module** and add **Electric Currents** and **Electrical Circuit** submodules
4. Select **Heat Transfer module** and add **Heat Transfer in Solids** submodule
5. Select **Done**
6. Create **Geometry** of the device as in the Figure
7. Create **Blank Materials** in the **Materials** node and add material parameters from Table 1.
8. To add the experimental temperature dependent electric conductivity,
   - from **Definitions** node, select **Functions** then **Interpolation**, and then insert temperature and corresponding conductivity values in the given table
   - Select **Linear** in both **Interpolation** and **Extrapolation** option
9. To add the temperature and voltage dependent hopping conductivity,
   - from **Definitions** node, select **Variables**, add the formula from Table 1, and then select the corresponding domain.
   - Note: the argument of the exponential and logarithm function must be unitless
10. Assign the materials to the corresponding domain.
11. In **Electric Currents** submodule,
    - add **Terminal** boundary condition, select the top boundary of the top electrode, and then select **Circuit** as the **Terminal type**
    - add **Ground** boundary condition and select the bottom boundary of the bottom electrode
    - Note: **Electric Currents** submodule has four necessary default subnodes

3.V Step-by-Step Process of building RRAM in COMSOL

12. In **Electric Circuit** submodule,
    - add **Resistor** and insert the value of load resistance,
    - add **External I Vs. U** from **External Coupling** and select **Terminal voltage** from **Electric potential** option
    - add **Voltage Source** for OFF, ON, and RESET modules and **Current Source** for SET module
    - select **DC-Source** as **Source type** for SET and RESET modules then insert the source current or voltage value
    - select **Pulse source** as **Source type** for ON and OFF modules and dene the pulse length according to the different ramp-rate as listed in Table. 2
    - Note: every component has positive **p** and negative **n** node names under **Node Connections** which enables to position a component in the circuit. For example, **Ground Node** is **0** by default; to ground the voltage source, insert **0** in the **n** node name
    - Note: **Electric Circuit** submodule has one necessary default subnode

13. In **Heat Transfer in Solids** submodule,
    - add **Temperature** boundary condition, select the top boundary of the SiO2 superstrate and bottom boundary of the SiO2 substrate, and choose 298K in the user defined temperature section.
    - add **Diffusive Surface** boundary condition, select all the inner boundaries, and then choose 298K in the user dened temperature section and 0.9 in the user defined **Surface emissivity** section
    - Note: **Heat Transfer in Solids** submodule has four necessary default subnodes

14. In **Multiphysics** node, to couple the **Electric Currents** and **Heat Transfer in Solids** submodule,
    - select all the domains and boundaries in **Electromagnetic Heating** sub-node
    - select **Heat Transfer in Solid** as **Source** and **Electric Currents** as **Destination** in **Temperature** sub-node

3.V Step-by-Step Process of building RRAM in COMSOL

15. Create **Mesh**
    - either automatic **Physics-controlled mesh** or manual **User-controlled mesh** can be selected
    - **Free Triangular** meshes of different sizes were manually defined for our simulation : to define the mesh size, add **Size** in **Free Triangular** mesh, then use either the **Predefined** or the **Custom** option
    - select **Build All**
16. Select **Study** type
    - select **Time Dependent** study for ON and OFF modules and then add **Times** corresponding to the pulse lengths
    - select **Stationary** study for SET and RESET modules
17. Select **Compute**
18. Obtain results in desired form from the **Results** node

3.VI List of the MATLAB files

The 4 modules are

1. RRAM_OFF.m (RRAM_OFF.mph)
2. RRAM_ON.m (RRAM_ON.mph)
3. RRAM_SET.m (RRAM_SET.mph)
4. RRAM_RESET.m (RRAM_RESET.mph)

Note .m are the Matlab files and .mph are the COMSOL equivalent

There are 3 Control Files

1. Complete_I_V_avg.m
2. Complete_I_V_ramprate.m
3. Complete_I_V_C2C.m

which generates average I-V characteristics, ramp-rate dependent I-V characteristics, and I-V characteristics with cycle-to-cycle variations.

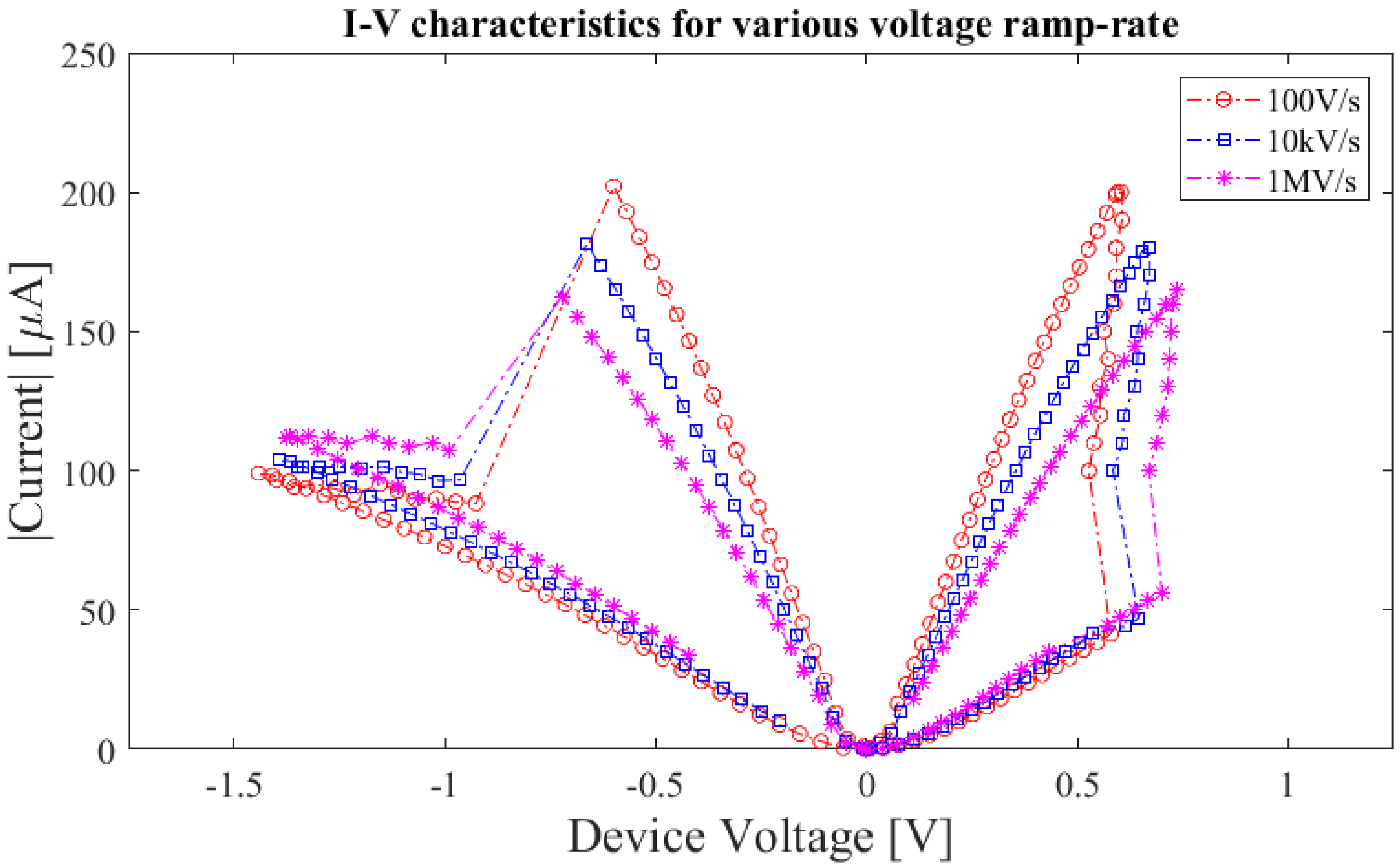
3.VII Guide on Running the files

- Run COMSOL Multiphysics 5.3 with MATLAB (livelink to matlab)
  - This opens MATLAB and simultaneously links it to COMSOL solver
- Store all the files in a folder and then in MATLAB change the Current Folder to that folder
- Open and run the desired Control file in MATLAB
  - The control file will produce following information during SET and RESET module in the MATLAB Command Window helpful in tracking the progress
  - During SET – Ramp-Rate(V/s)|Source Voltage(V)|Device Resistance(Ω)|Current (μA)|Device Voltage(V)|Filament radius (nm)|Maximum Filament Temperature(K)|Average Dielectric Temperature(K)|Chemical Potential (J/m^3)
  - During RESET – Ramp-Rate(V/s)|Source Voltage(V)|Device Resistance(Ω)|Current (μA)|Device Voltage(V)|Gap length(m)|Average Filament Temperature(K)|Average Gap Temperature(K)|Chemical Potential (J/m^3)
- When the program completes it saves all the generated data in <filename>_DATA.mat MATLAB Variable
- Open the MATLAB Variable to obtain the I-V as well other electrical and thermal properties

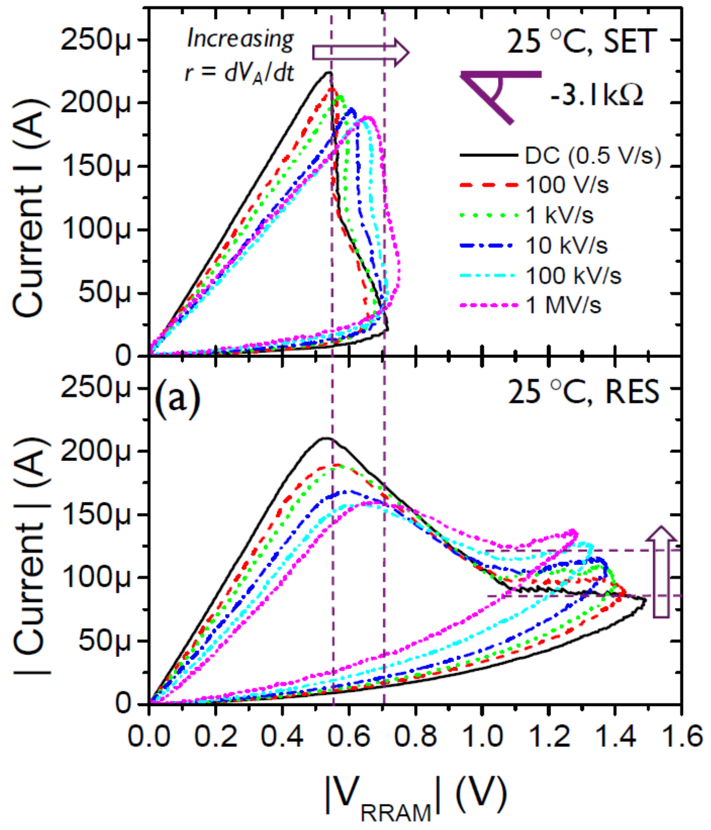
3.VIII Other Technical Details

- Since the program runs with OFF module, filament radius and gap length for the first cycle has to be user input which in general is not the thermodynamically stable dimension. Following two tricks can be exercised
  1. Run the control file for two cycle:
     during the first cycle the program finds the thermodynamically stable dimension, then use the data from the second cycle
  2. Start the Program from SET module and end at OFF module:
     the program obtains the thermodynamically stable filament radius from SET module then goes to ON, during RESET the program finds the stable gap length for the stable filament radius; this trick only requires running of 1 cycle.
- We have placed lower limit on Chemical Potential, a function of temperature and ramp-rate, to be 10^7 J/m^3

3.IX Results: Simulated I-V Characteristics Ramp-rate dependence

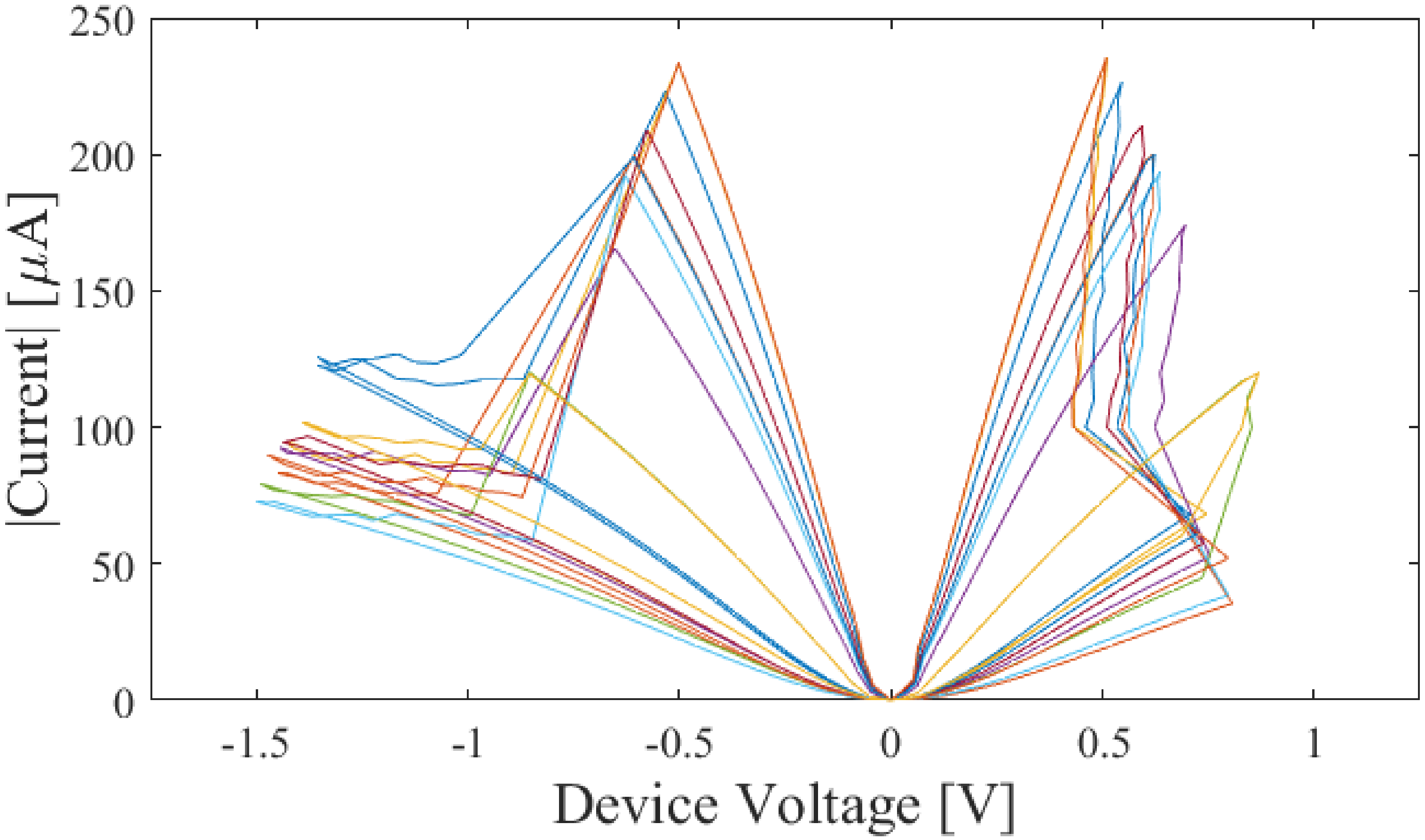


Simulated I-V curve from the numerical modeling for three different voltage ramp-rate.

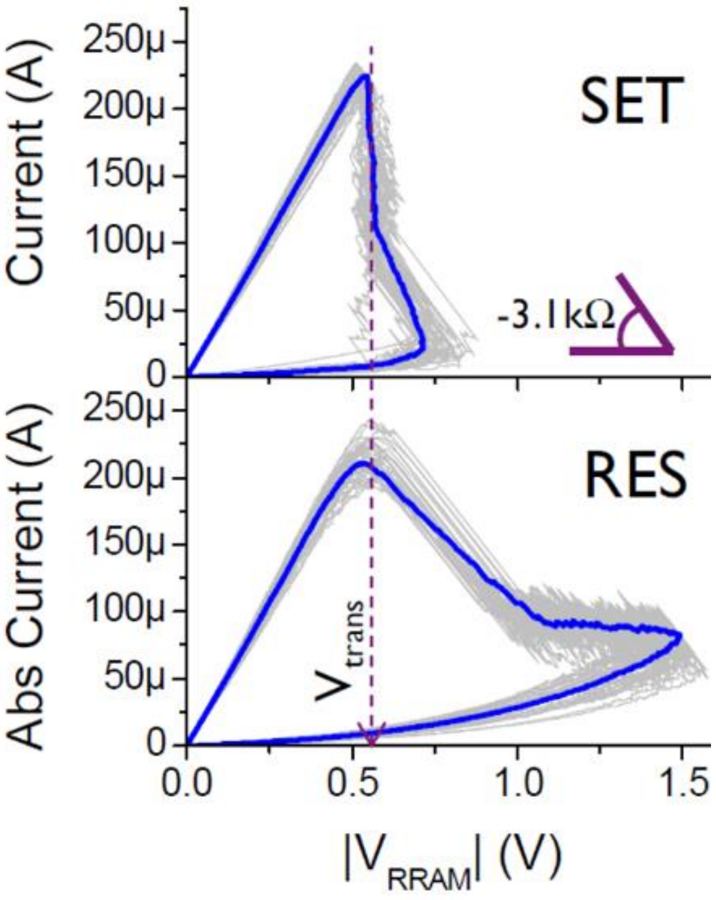


A. Fantini, et al., IMEC IMW 2012

3.IX Results: Simulated I-V Characteristics Cycle-to-Cycle Variation



Simulated I-V curve from the numerical modeling showing cycle-to-cycle variations.



A. Fantini, et al., IMEC IMW 2012