NUMERICAL MODELING OF RESISTIVE SWITCHING IN RRAM DEVICE.

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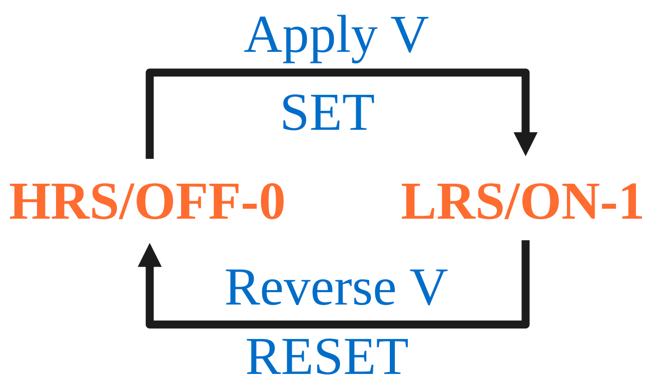
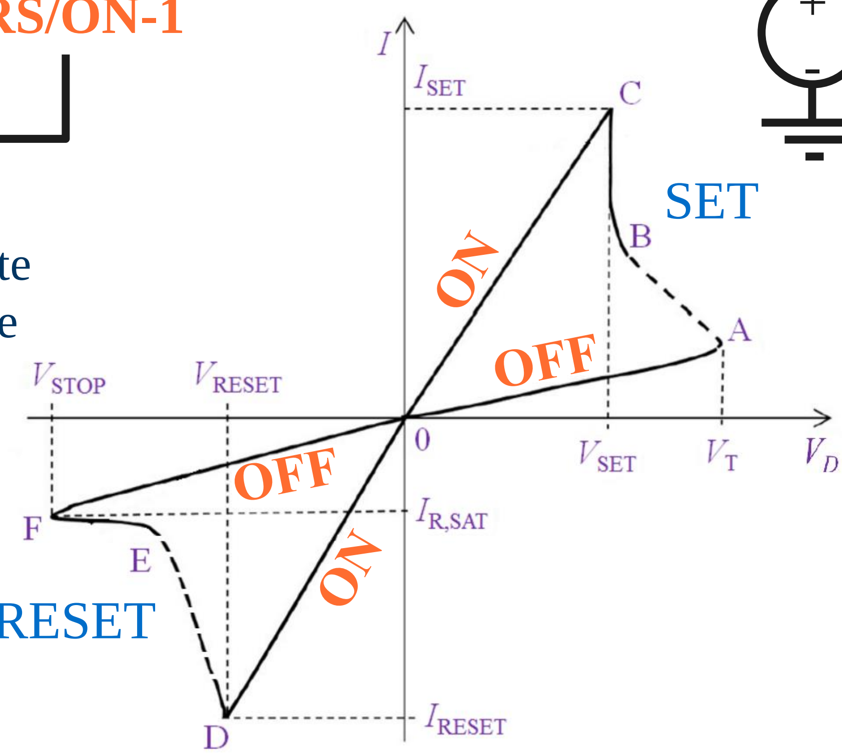
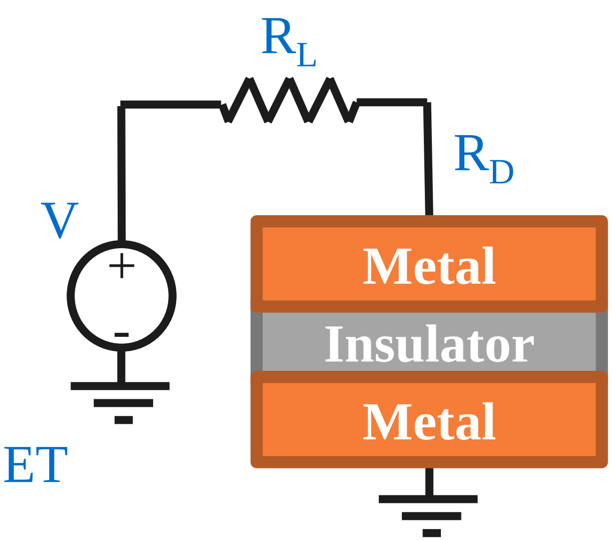
Research motivation:
Bipolar resistive switching



HRS: High Resistance State
LRS: Low Resistance State





V_D: Device Voltage

Statement of goal

- Develop a numerical model of bipolar filamentary RRAM operation based on physical theory,
  - independent of microscopic structure details
  - RRAM characteristics described via material parameters
  - generates device I-V characteristics

Outline

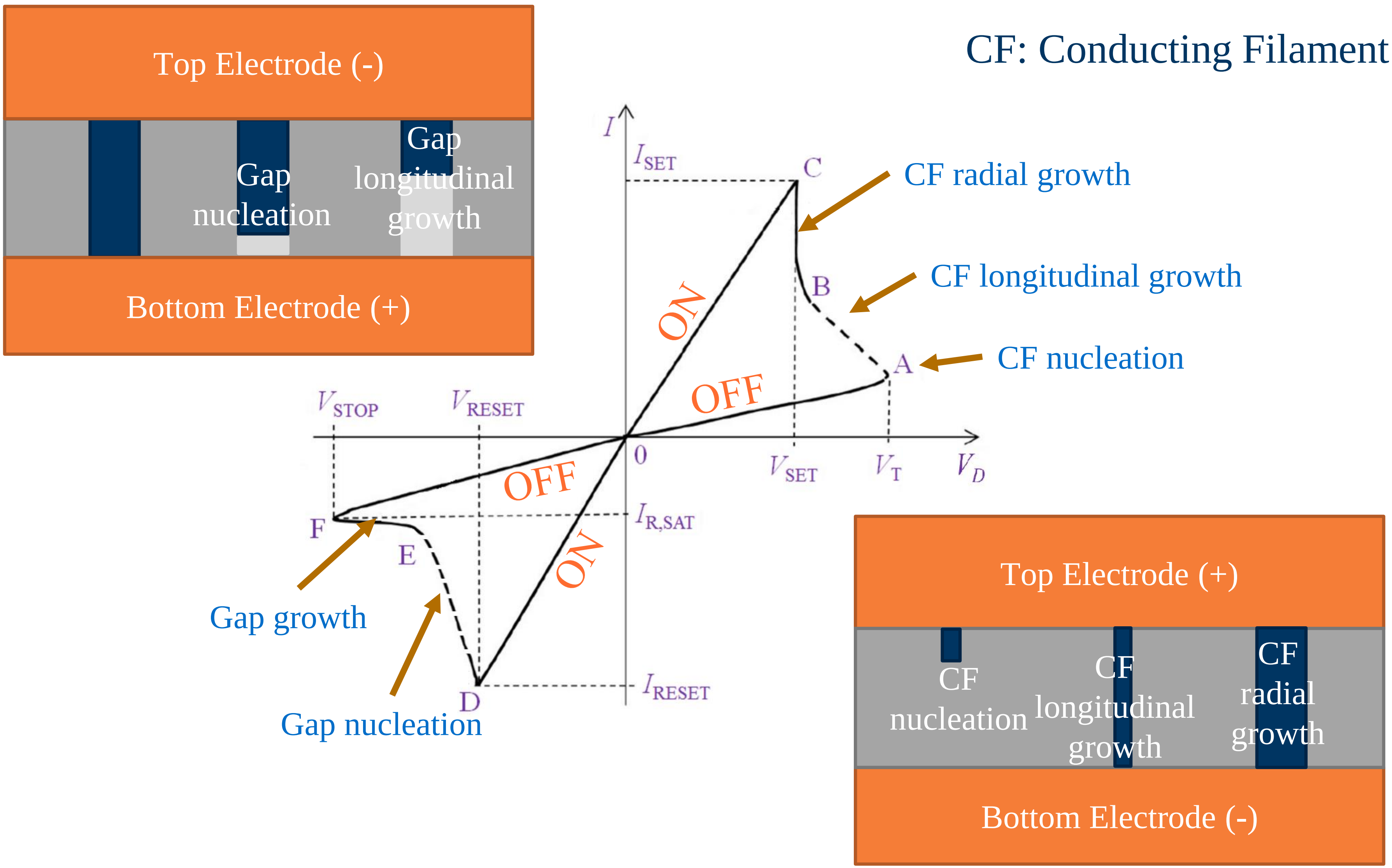
Thermodynamics theory of filament switching

- Mechanism of filamentary switching
- Physics behind switching
- Three Phase System
- Free energy

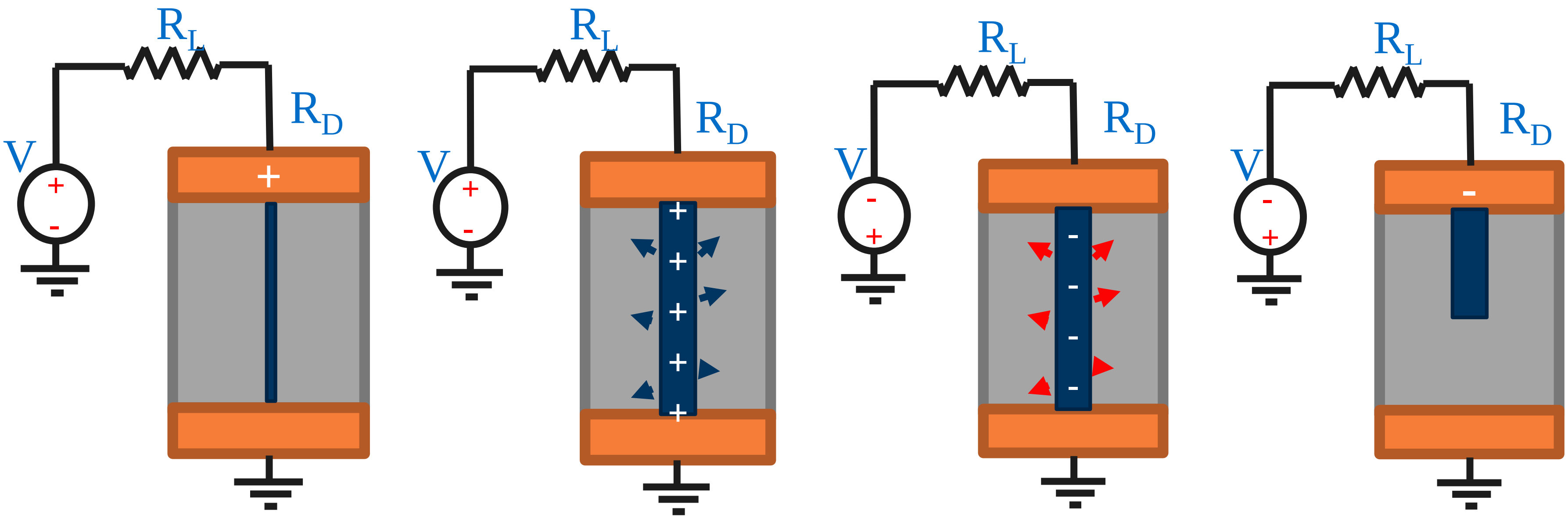
Numerical Modeling

- Partial Differential Equations
- Material Parameters and Boundary Conditions
- Workflow
- Free energy and I-V Characteristics

Mechanism of filamentary switching



Physics Behind Switching:
current carrying CF charges and produces radial field



Field Induced Nucleation then shunting ~1V/10nm = 10^8 V/m	CF charging polarizes insulating host matrix	Reversing Polarity charges CF unfavorable to the inherited polarization of the host	Charged CF produces a strong lateral field in its vicinity opposite to the host polarization, then dissolves

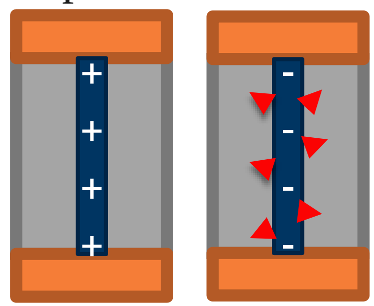
Note1: CF has finite capacitance

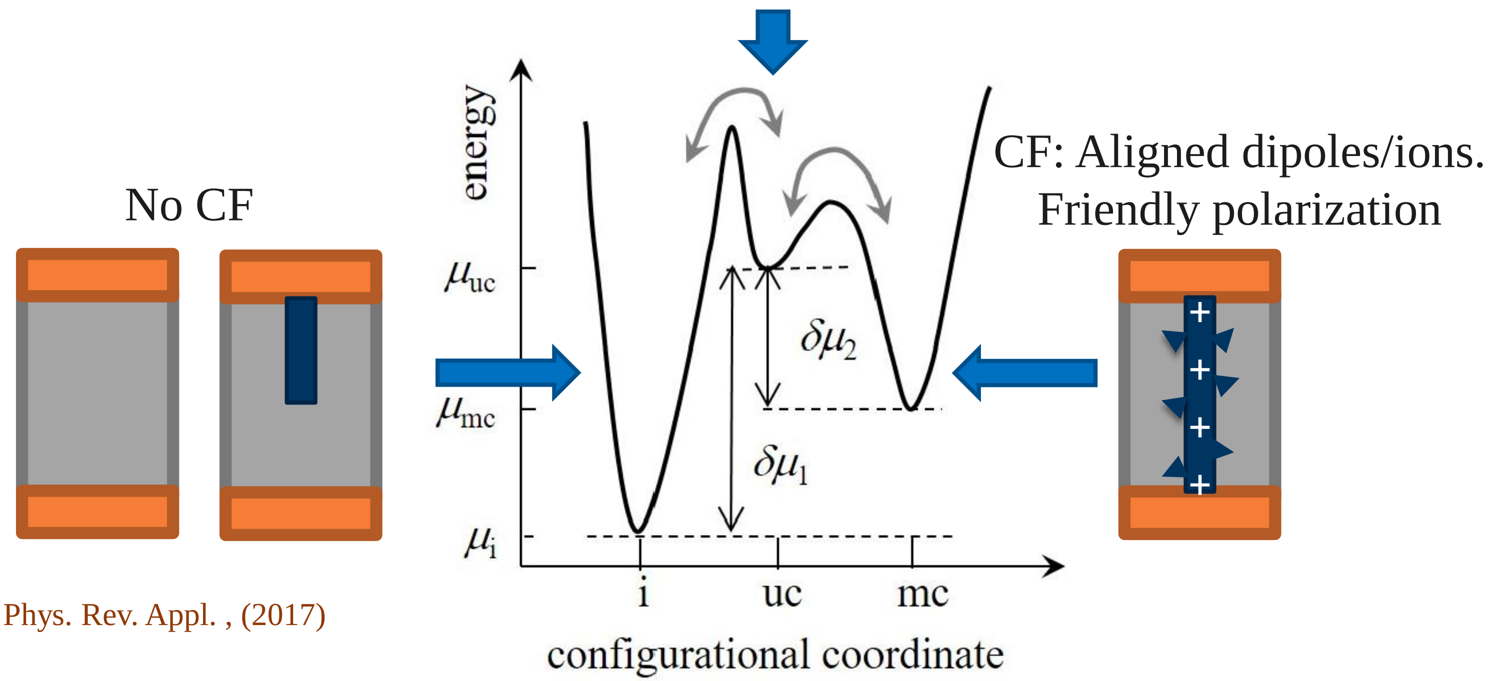
Note2: wire charging effect (due to Weber, 1852)
– overlooked in RRAM community

Phase Transformations:
thermodynamic analysis is possible due to fast thermalization, minimum of three phases required to describe IV

- Due to electric field and joule heat, the system makes transitions between three phases during SET and RESET process
  I. Insulating phase (i)
  II. Unstable conducting phase (uc)
  III. Metastable conducting phase (mc)

CF: No or misaligned polarization





V. Karpov et.al in press Phys. Rev. Appl. , (2017)
arXiv:1702.01480

Thermal and Electric energy driven phase transformation

Free Energy = Thermal + Electrostatic + Phase transition (Surface & Volume)

- The free energy of the ON state,

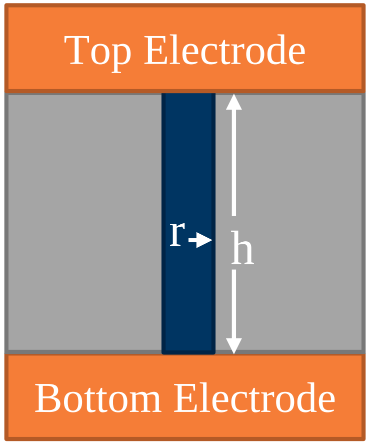
$$F = \int \rho C_p \delta T dx^3 + \frac{1}{2}\int \epsilon |E|^2 dx^3 + 2\pi r h \sigma + \pi r^2 h \delta\mu_1$$

- The free energy of the OFF state,

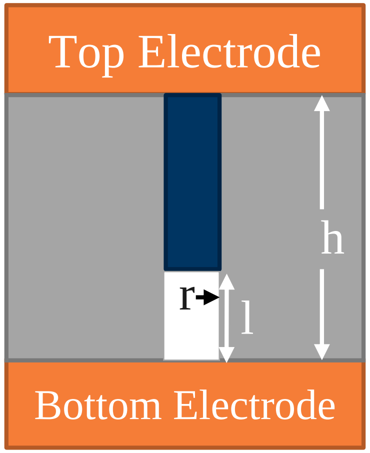
$$F = \int \rho C_p \delta T dx^3 + \frac{1}{2}\int \epsilon |E|^2 dx^3 + 2\pi r l \sigma + \pi r^2 l \delta\mu_2$$

ρ is material density
C_P is specific heat capacity at constant pressure
ϵ is the permittivity
σ is the interfacial energy
$\delta\mu_1, \delta\mu_2$ is the difference in the chemical potential between insulating and unstable conducting phase, and metastable and unstable conducting phase

- Equations to solve
  - Maxwell equation : Electric field distribution
  - Fourier Law : Temperature distribution



r varies from 1nm to device radius for a fixed Source voltage



l varies from 0.5nm to *h* for fixed *r* and for a fixed source voltage

PDE Solver: COMSOL Multiphysics®

- COMSOL uses finite element method to solve PDEs and has an excellent graphical user interface
- Solves following PDE to calculate the field and temperature distributions

Electrical Currents	*Heat Transfer in Solids*	*Multiphysics*
$\vec{\nabla}.\vec{J} = 0$ $\vec{J} = \sigma_c \vec{E}$ $\vec{E} = -\vec{\nabla} V$	$-k\vec{\nabla}.\vec{\nabla}T = Q_s$	$Q_S = \vec{J}.\vec{E}$

- COMSOL also performs the necessary integration for free energy

Material parameters and Boundary Conditions

Table.1. Material Parameters

Material	κ [W/(Km)]	σ_c [S/m]	C_P [J/(kgK)]	ε	ρ[kg/m^3]
TiN	11.9	10^6	545.33	-10^6	5.22×10^3
HfO_2	0.5	10^{+}	120	25	10×10^3
HfO_{2-x}	0.65	2×10^4	140*	-10^6*	12×10^3*
Hf	23	5×10^6	144	-10^6	13.3×10^3
SiO_2	1.38	10^{-14}	703	3.9	2.2×10^3
Air	0.015	5×10^{-15}	1000	1	1.225

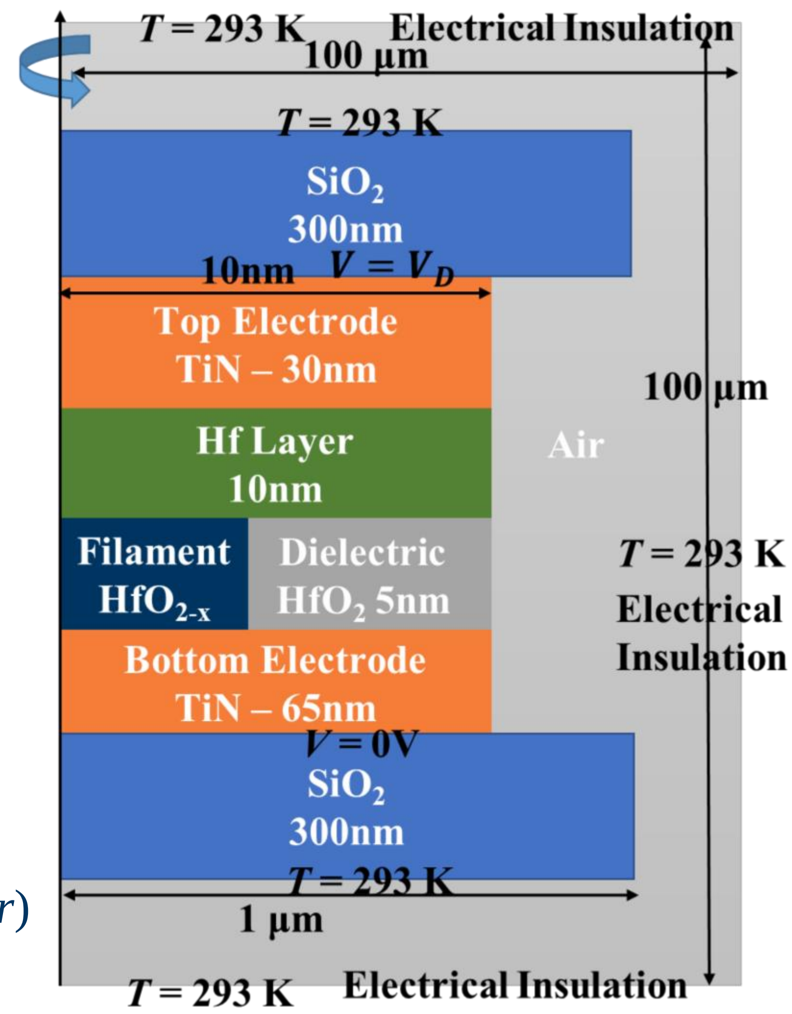
*Assumed values, lies in between Hf and HfO_2

Table.2. Various Parameters

Parameters	Value
σ	0.01 [J/m^2]
$\delta\mu$	3×10^9[J/m^3]
R_L	15 kΩ
TBR HfO_2	3[m^{2}K/GW]
TBR TiN	5[m^{2}K/GW]

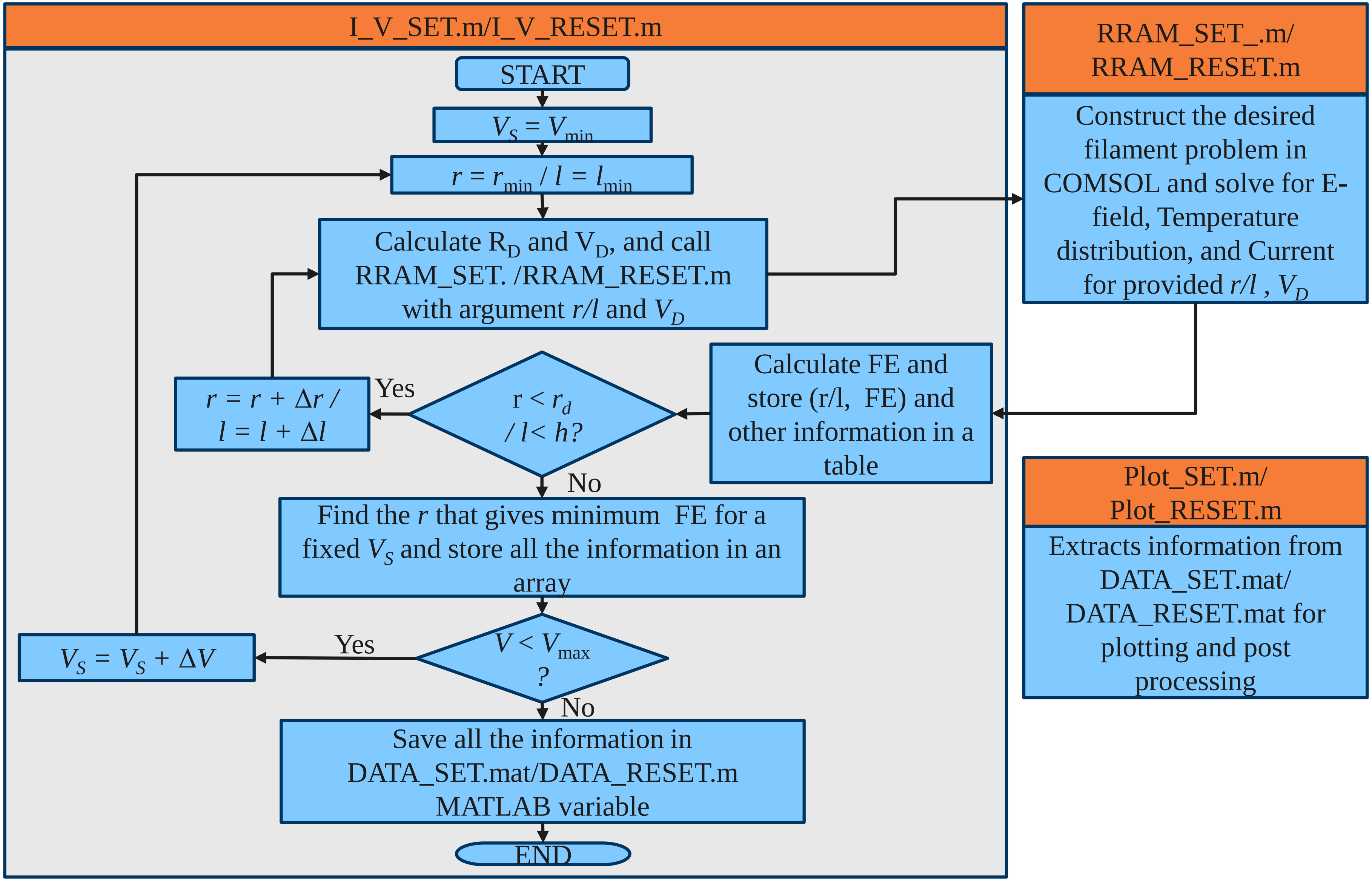
Additional Boundary Condition

- Thermal Boundary Resistance (*Thin Layer*)
- Heat lost by Radiation (*Diffusive Surface*)

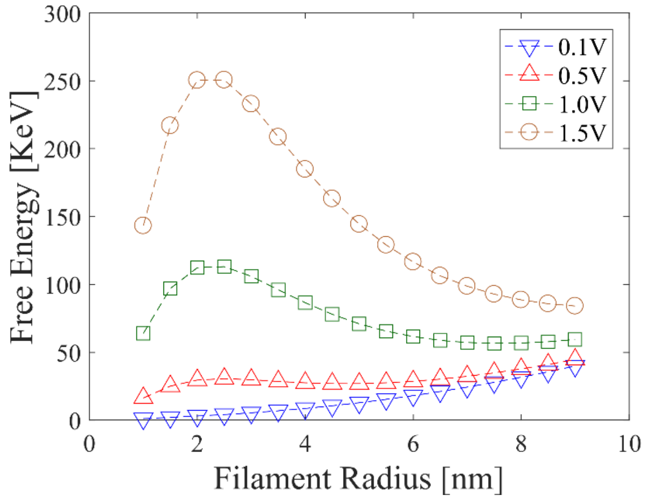


Work Flow between MATLAB® scripts:

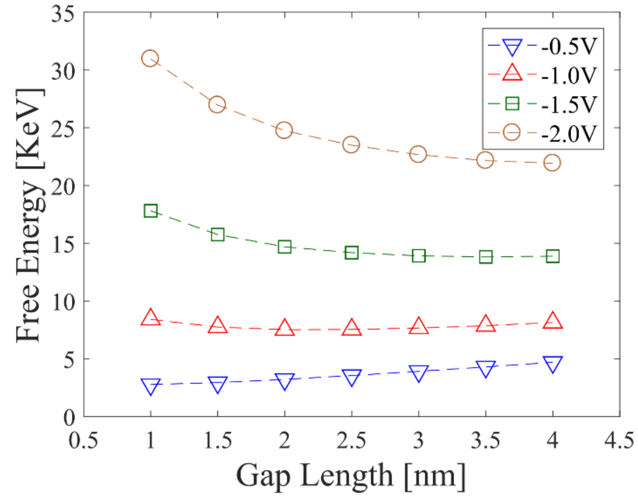
MATLAB talks to COMSOL Multiphysics® via LiveLink™ to MATLAB®, utilized to find minimum in Free Energy



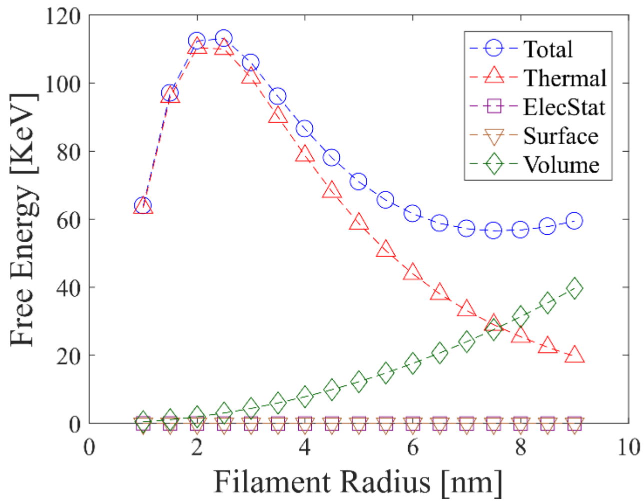
Free Energy Plots:
system evolves through minimum energy points



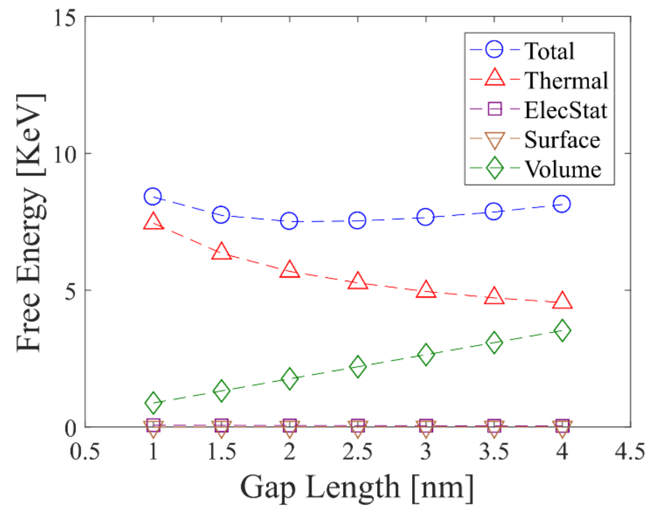
Free Energy vs CF radius for different source voltages.



Free Energy vs gap length for different source voltages.

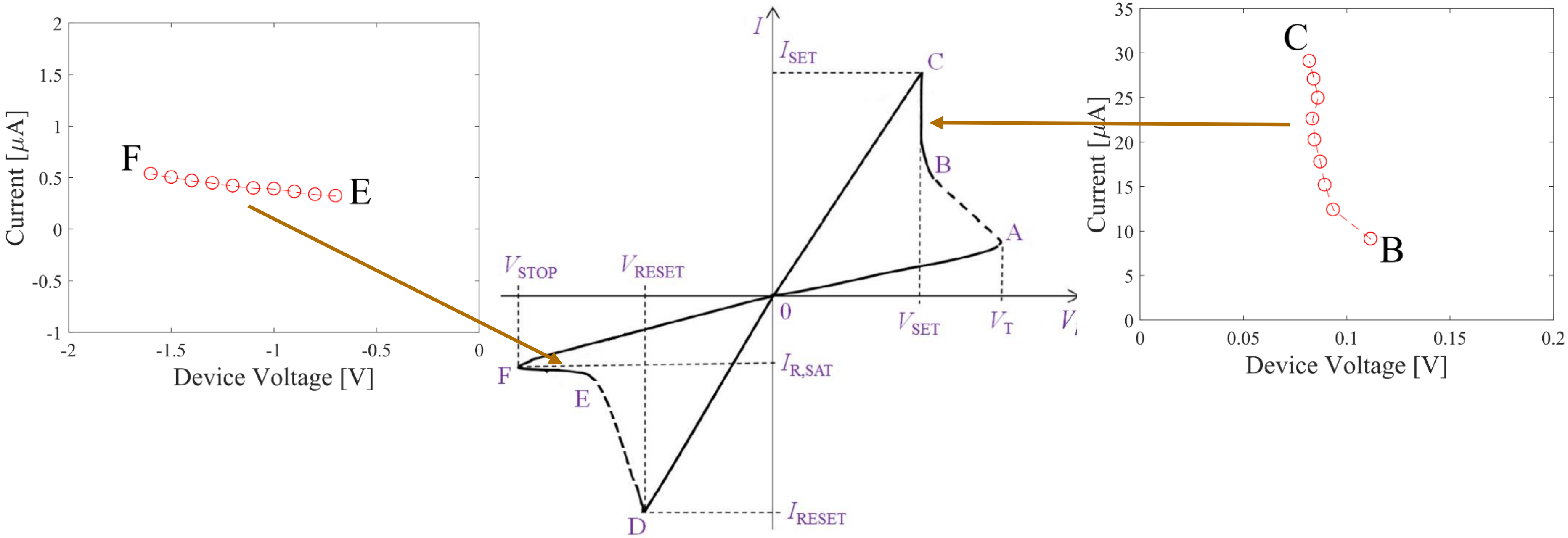


Free energy contribution vs CF radius for **1.0V** source voltages.



Free energy contribution vs gap length for **-1.0 V** source voltages.

Simulated I-V Characteristics:
corresponds to the stable radius and gap lengths



CONCLUSIONS:

- COMSOL/MATLAB model verifies thermodynamic model
- Discrepancy in V_{SET} and $I_{R,SAT}$ values
  - Optimization of material parameters
  - Further refinement of filament description
- Modeling full I-V characteristics in progress

Acknowledgement

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