COMPREHENSIVE NUMERICAL MODELING OF FILAMENTARY RRAM DEVICE.

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COMSOL
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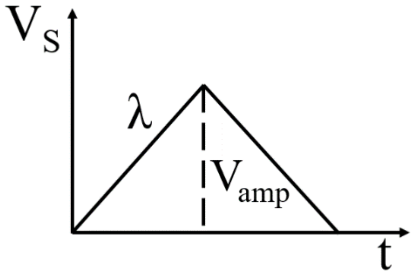
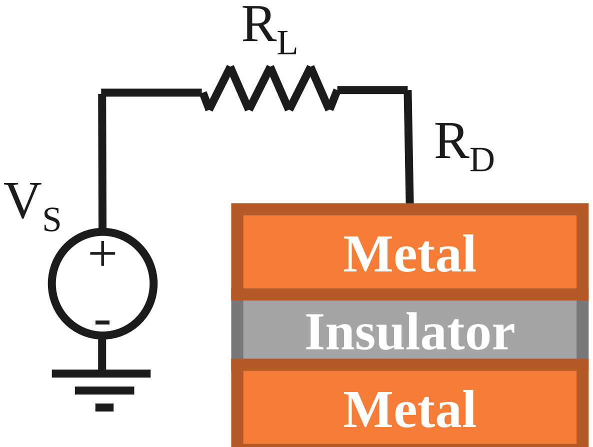
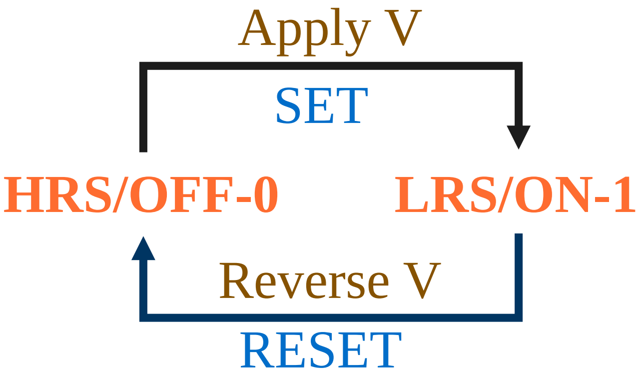
Research motivation:

Bipolar resistive switching in RRAM






Apply V

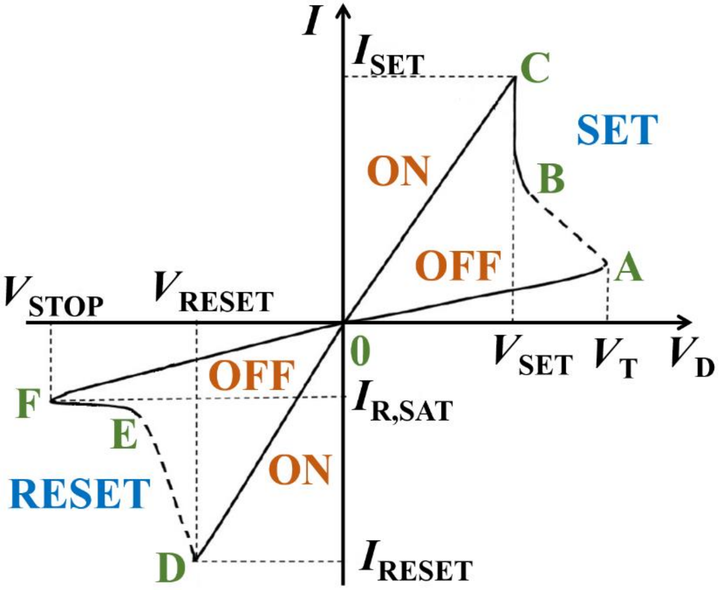
SET

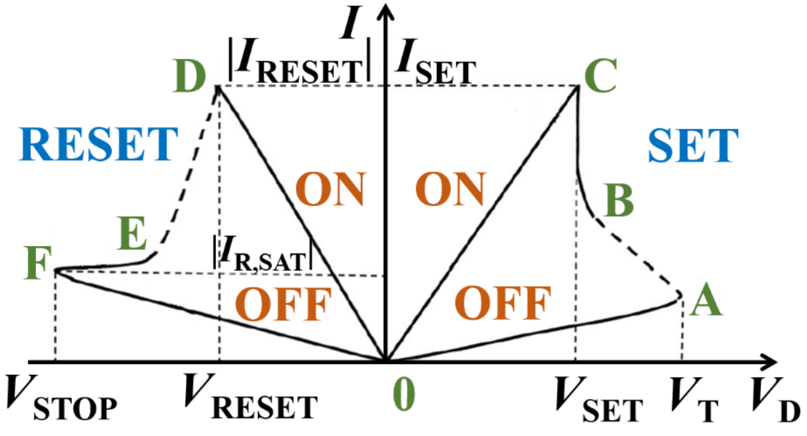
HRS/OFF-0

LRS/ON-1

Reverse V

RESET





Statement of goal

- Develop a physics based numerical model of bipolar filamentary RRAM operation
  - independent of microscopic structure details
  - RRAM characteristics expressed through material parameters
  - I-V characteristics exhibiting *ramp-rate* and *cycle-to-cycle variations*

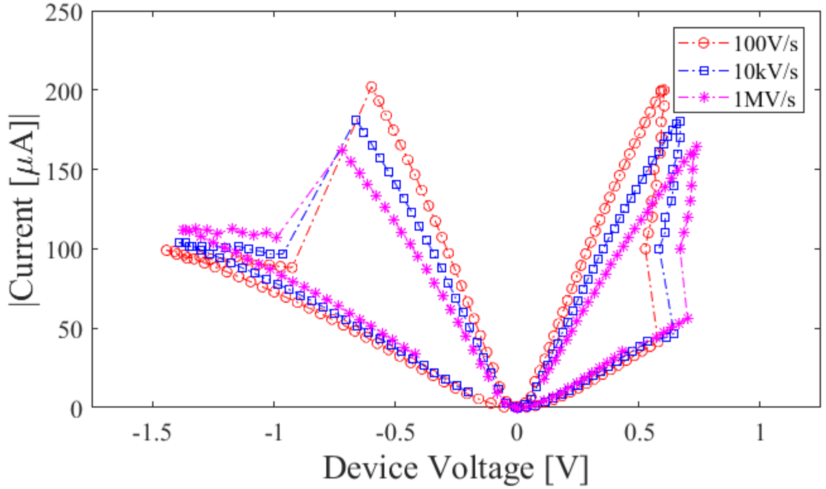
Showcasing our results

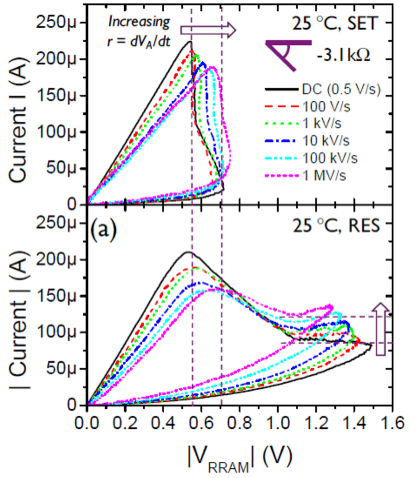
simulated I-V with ramp-rate and cycle-to-cycle variations

Simulated I-V

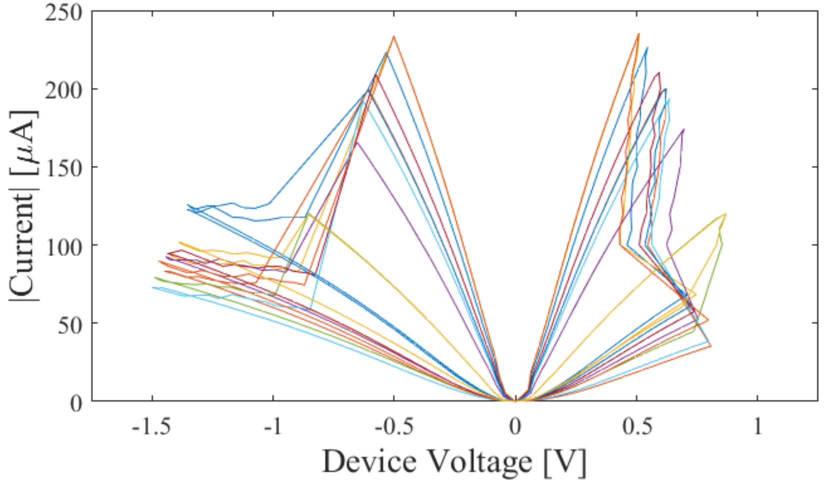
Experimental I-V

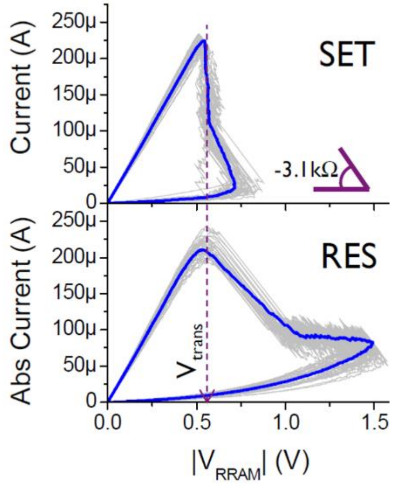
Increasing input voltage ramp-rate





Multiple switching cycles





A. Fantini, et al., IEEE IMW, Milan 2012.

Outline

- Physics of Device operation
- Numerical Modeling
  - Program: Modules and Switching Condition
  - Device Model
  - Conduction Mechanism: Electric and Thermal
- Variability of RRAM parameters
  - Average ramp-rate dependent effects
  - Cycle-to-cycle Variations

Physics of Device operation:

device operation consists of Device States and Switching Processes

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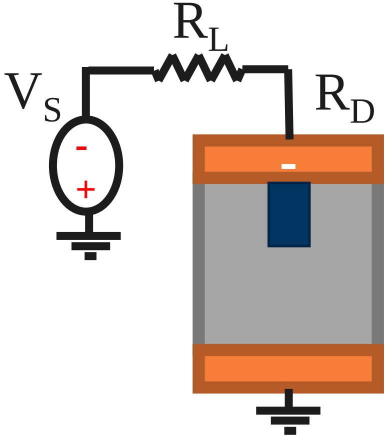
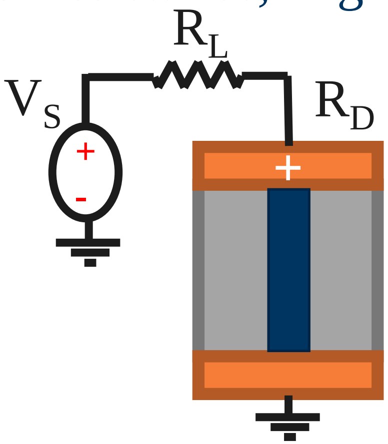
Device States (‘0’ or ‘1’)

OFF– Insulating State :
No or Partial Filament,
High Resistance, Low Current



ON– Conducting State:
Conducting Filament,
Low Resistance, High Current



Switching Processes (Write/Erase) :

structural change

SET : OFF→ON
Formation of
Conducting Filament

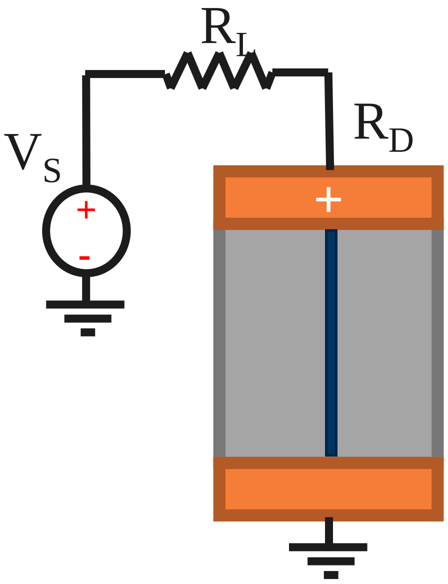
RESET : ON→OFF
Dissolution of
Conducting Filament

Physics Behind Switching Process:

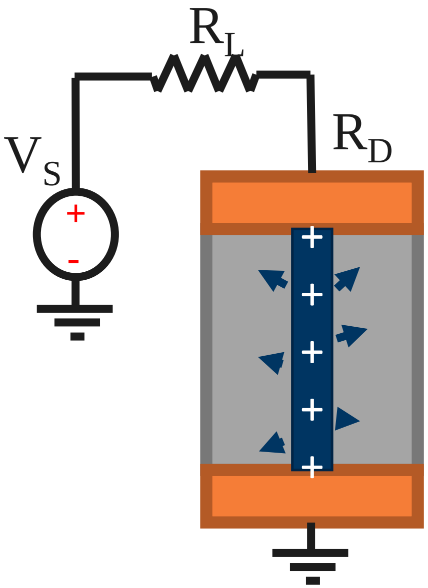
current carrying CF charges and produces strong radial field

1V/10nm = 1MV/cm

SET

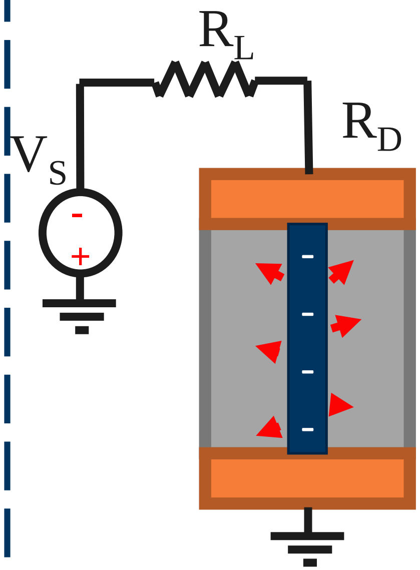


Field Induced Nucleation then shunting

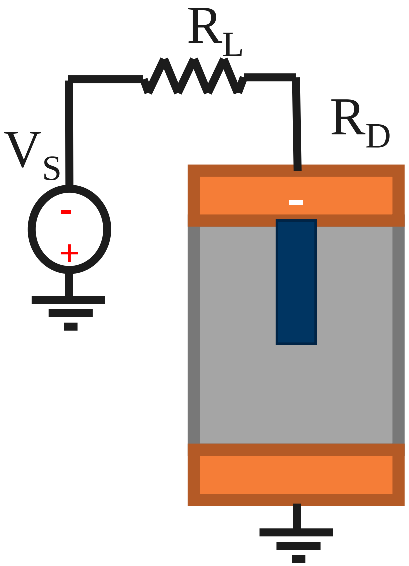


CF charging polarizes insulating host matrix

RESET



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

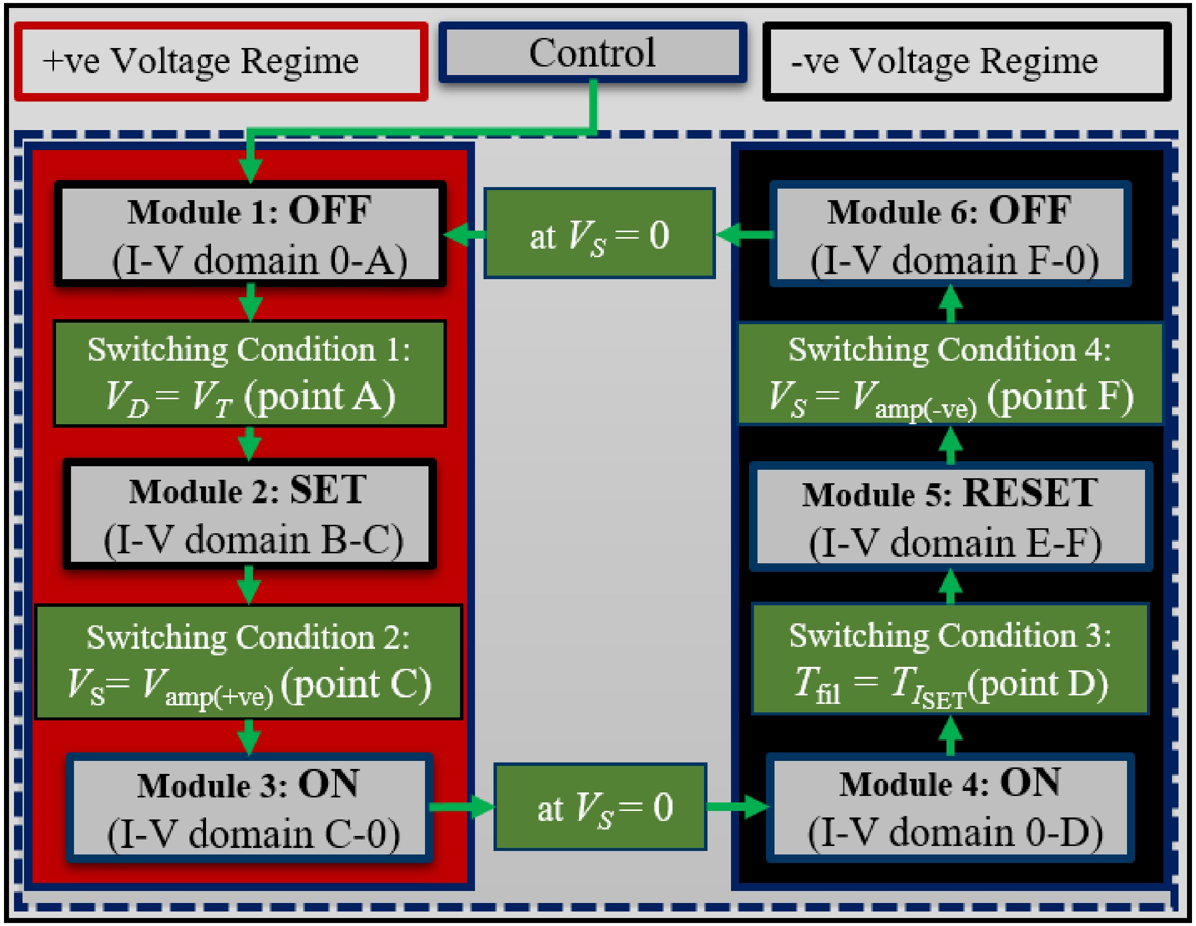
Note1: CF has finite capacitance

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

Numerical Modeling: Program

a MATLAB computer program is developed, consisting of 4 modules corresponding to the device states and switching processes executed sequentially mimicking actual device operation

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)

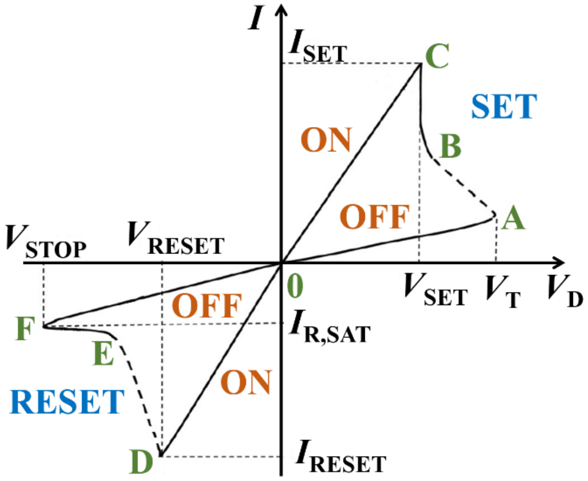
Switching Condition 3:
$T_{fil} = T_{I_{SET}}$ (point D)

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 $V_S = 0$

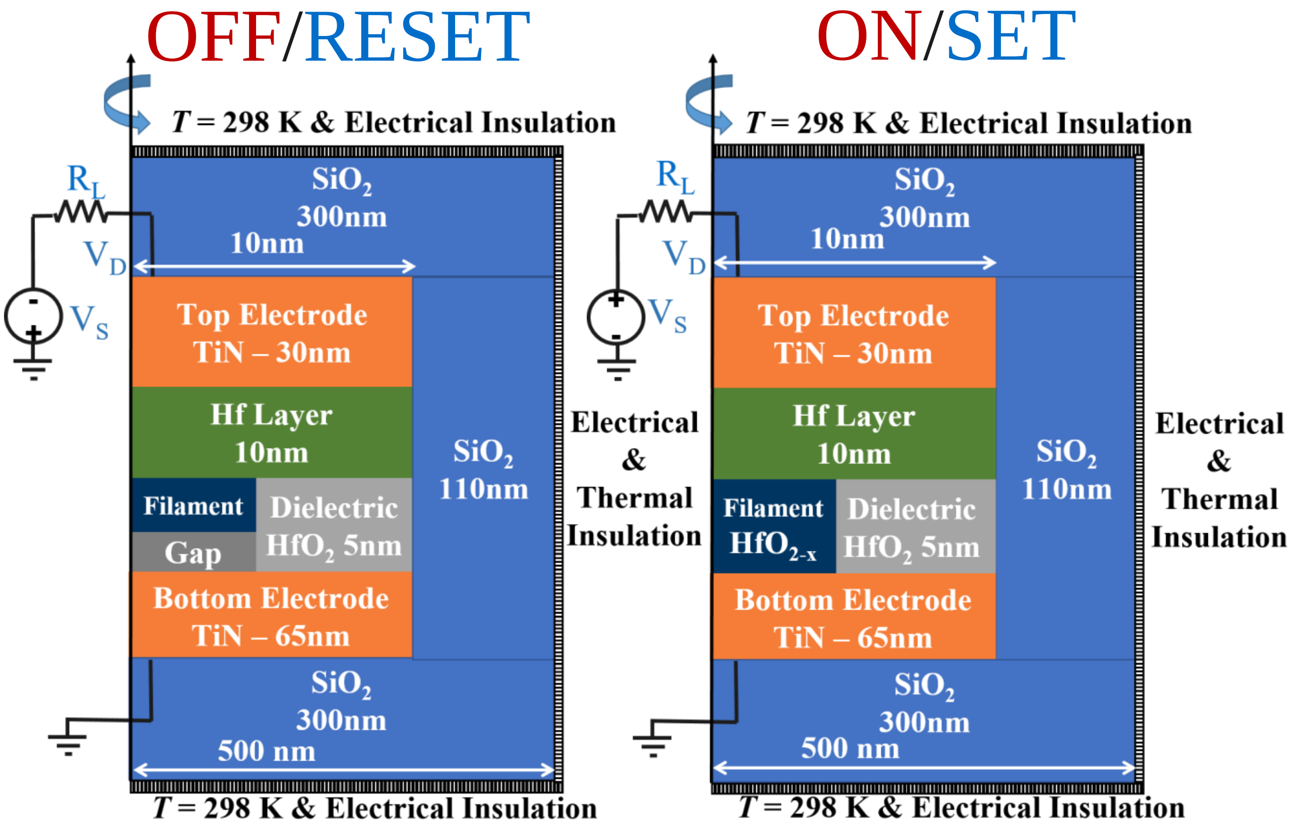


Device State: determined by conduction mechanism and filament dimensions

Switching process: governed by thermodynamics: (minimizing free energy by transforming phase)

Device Model:

TiN/Hf/HfO$_2$/TiN multilayered RRAM device is modeled in COMSOL



Utilized PDEs

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	
$Q_S = \boldsymbol{J} . \boldsymbol{E}$	$Q_S = \boldsymbol{J} . \boldsymbol{E}$
Electric Circuit module is used to define the circuitry	

OFF/ON: the gap/filament remains intact

RESET/SET: the gap/filament grows following the free energy minimum

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

The thermal and electrostatic energies are obtained by solving coupled heat-electromagnetic PDE in COMSOL

Device Model:

material and various other 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	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).

[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

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)

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
$\tau_0(\tau_{\mathrm{min}})$	0.1 ps

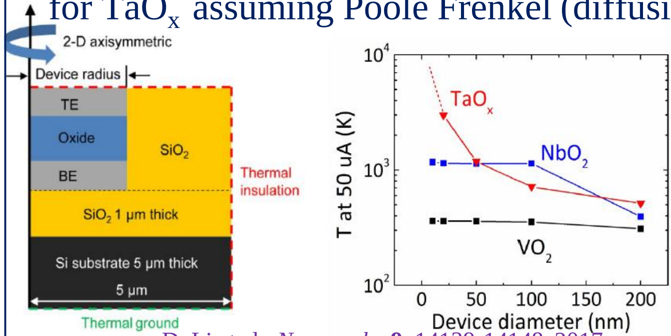
Parameter	**Value**
Chemical Energy	
σ	0.01 J/m^3
$\overline{\delta\mu_1}$	10 GJ/m^3
$\overline{\delta\mu_2}$	6.5 GJ/m^3
β_1	0.35 GJ/m^3
β_2	0.5 GJ/m^3
ΔW_{Buc}	1.0 eV
ΔW_{Bi}	0.1 eV
ΔW_{Bmc}	0.3 eV
Static Disorder	
σ_{0f}	rand(2, 8) kS/m[g]
σ_{0g}	rand(1, 5) kS/m[g]
α_f	rand(-0.07, -0.03)[g]
α_g	rand(0.03,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

Conduction Mechanism:

no consensus in RRAM community; we eliminate diffusion based mechanisms on the basis of unphysical device temperature

- Conduction mechanisms proposed: Poole-Frenkel, trap-assisted tunneling, Schottky emission, space charge limited current, variable range and nearest neighbor hopping
- All provide equally acceptable fits: non-indicative

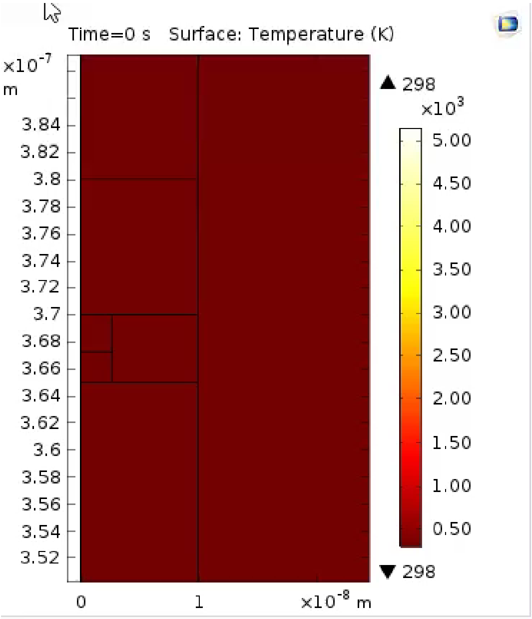
Similar temperature observed independently for TaO_x assuming Poole Frenkel (diffusive)



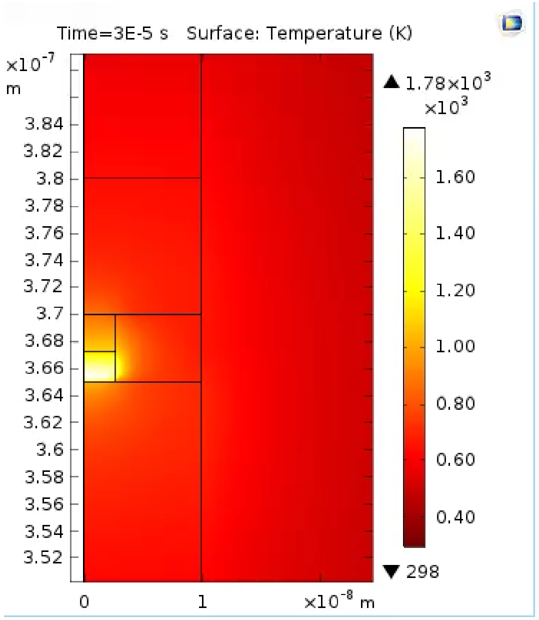
D. Li et al., *Nanoscale*, **9**, 14139-14148, 2017.

- Diffusion transport yields unphysical gap temperature ~ 4500K
- Electrons ballistically travels through ~2nm gap
- Correction term κ_{eff} introduced in thermal conductivity
- $\kappa_{\text{eff}} = \frac{\lambda_{\text{bal}}}{\lambda_{\text{diff}}} \approx \frac{10nm}{1nm}$
- $\kappa_{\text{gap}} = \kappa_{\text{eff}}\kappa_{\text{diff}}$
- λ is the mean free path

Diffusive heat Transport



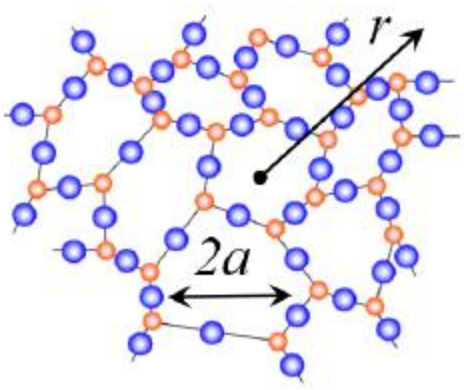
With Correction



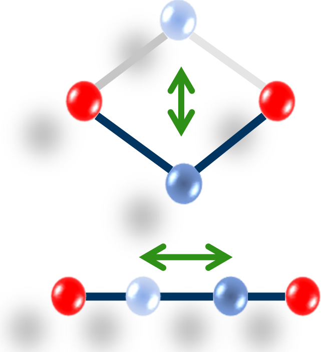
Variability of RRAM parameters:

HfO_2 is amorphous: some atoms retain mobility represented by random Double Well Potentials (DWP)

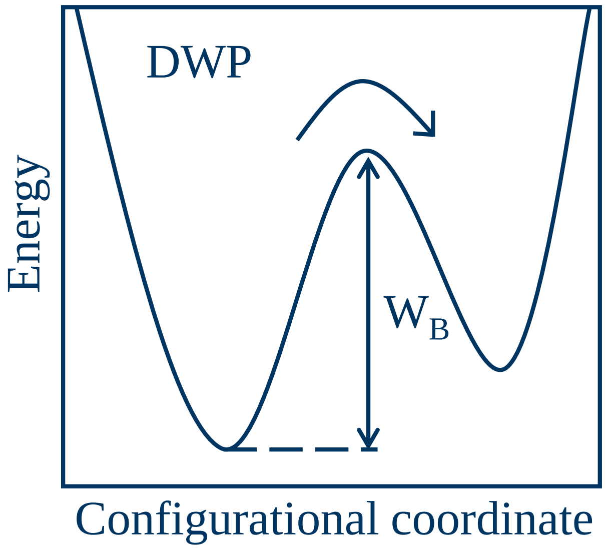
Disordered system: HfO_2



Blue Atom can reside in either position



In noncrystalline structures some atoms retain mobility moving in random **Double Well Potentials**



Known since 1971 due to *Anderson, Halperin, Varma*

Verified via effects on:

Specific heat, Thermal expansion, Thermal conductivity, Sound absorption, Sound propagation, IR absorption, Light propagation, Point contact resistance, Electronic noises, High pressure behavior...more

Universal in noncrystalline metals, semiconductors, and dielectrics

Transition time $\tau = \exp\left(\frac{W_B}{kT}\right)$

Probability density $g(\tau) = \frac{1}{\tau}$

Cumulative density $\propto \ln \tau$

Average ramp-rate dependent effects

DWP affecting the electric conduction and energetics of filament and gap

The structural changes affects

- Electrical Conduction; the deformation due to DWP distorting the mobility edge and conduction;
- Chemical potential contribution

To Quantify

- the input voltage activates DWPs with transition time smaller than pulse time $(\tau < \tau_P)$
- Average fraction of activated DWP

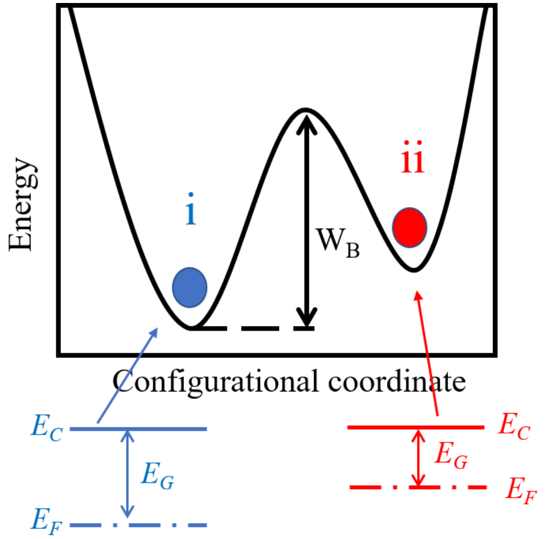
$$f(\tau_P) = \frac{kT}{\Delta W_B} \ln\left(\frac{\tau_P}{\tau_0}\right)$$

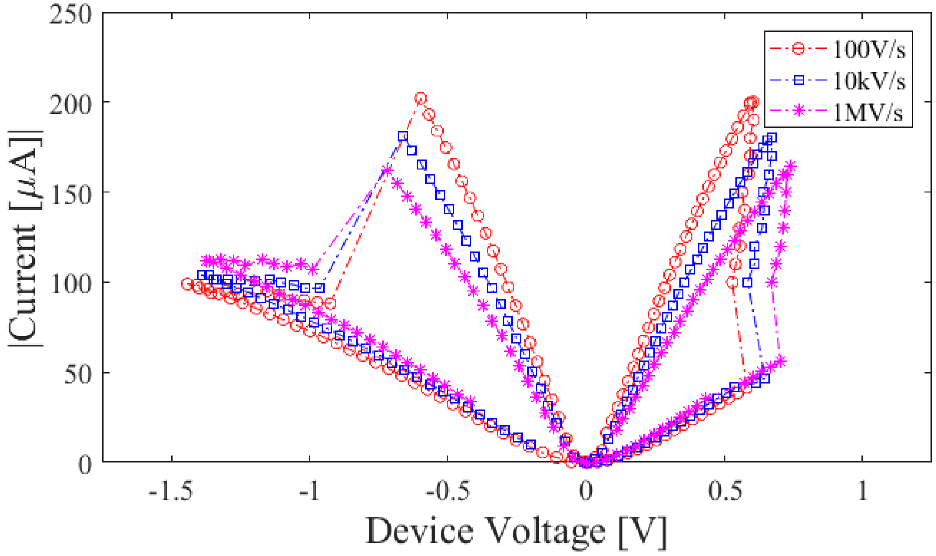
- Rate dependent Conduction

$$\sigma \sim \exp\left(\alpha \ln\left(\frac{\tau_P}{\tau_0}\right)\right), \text{ where } \alpha = \frac{u_0 D}{kT}$$

- Rate dependent Chemical Potential

$$\delta\mu = \overline{\delta\mu} + \beta kT\left(\frac{1}{\Delta W_{uc}} - \frac{1}{\Delta W_i}\right) \ln\left(\frac{\tau_P}{\tau_0}\right)$$

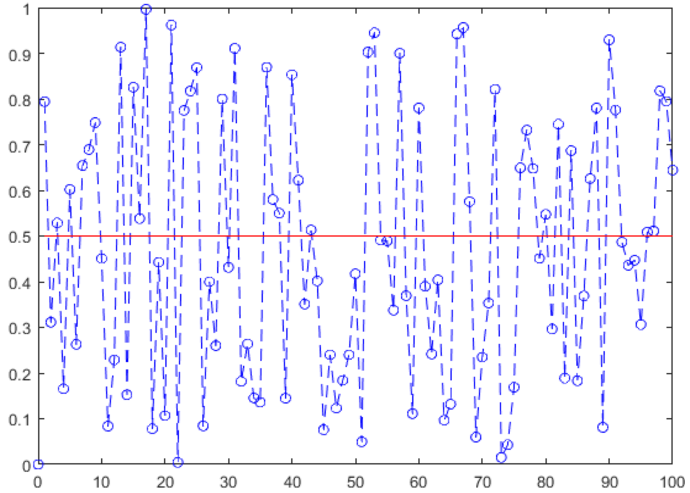




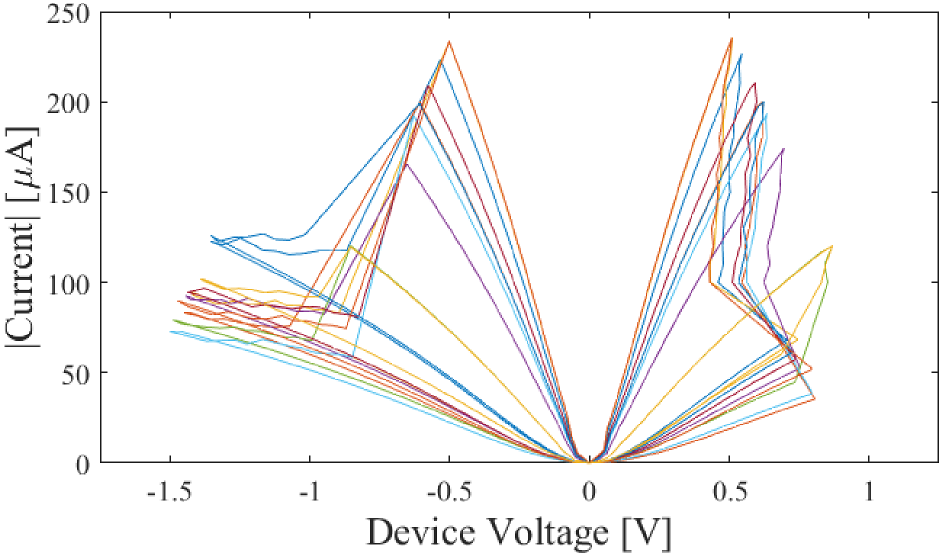
Cycle-to-cycle Variations

due to smalless of RRAM, the number of DWPs not enough to provide the statistical self-averaging

- Each switching cycle yields different structure
- The difference cause variation in DWP barrier heights, chemical potentials, and deformation potentials
- Applied random number generator to randomly vary DWP ensembles from once cycle to another



Uniformly distributed random number from 0 to 1



CONCLUSIONS

1. Developed physics based numerical model of RRAM including voltage ramp-rate and cycle-to-cycle variations
2. Established and incorporated the ballistic nature of electron transport
3. Included structural disorder of amorphous HfO_2 via double well atomic potentials modeling the observed variations between nominally identical RRAM devices
4. Developed a thermodynamic description of nano-sized modern RRAM and its numerical algorithm dramatically simpler than the kinetic approach

Acknowledgement

- This work was supported in part by Semiconductor Research Corporation (SRC) under Contract No.2016LM-2654.
- Collaborators
  - Ilya V. Karpov (Component Research, Intel)
  - Roza Kotlyar (Process Technology Modeling, Intel)