Modeling of Memristive Devices (Memristors)

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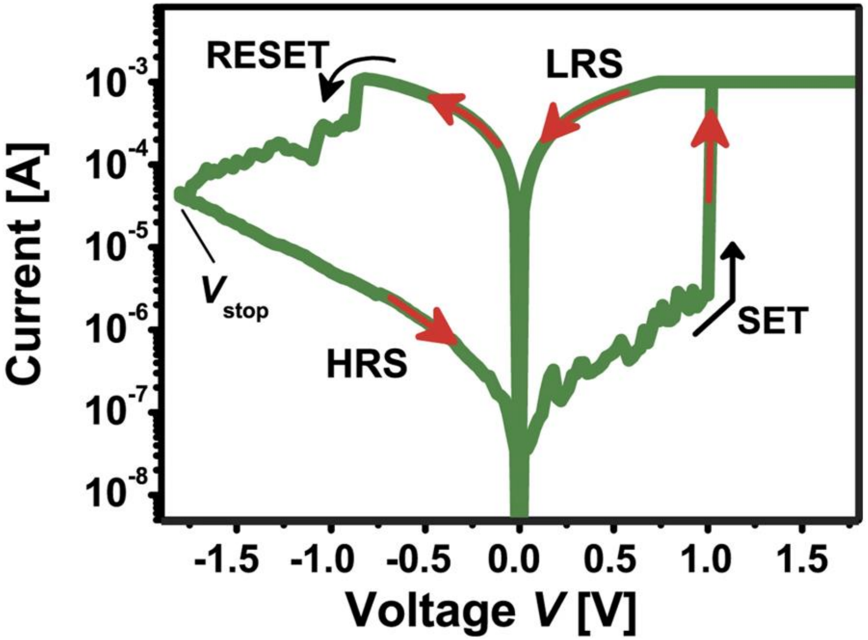
Memristors: Applications

- Memristors
  - Memristance *M*
  - Magnetic flux ϕ and electric charge *q*
  - Two-terminal passive device
  - State variable(s) that changes over time
  - LRS/HRS
  - NV-RAM
  - Programmable logic
  - Signal processing
  - Neuromorphic computing

$$d\varphi = M dq$$

$$v = \frac{d\varphi}{dt}$$

Ref 1



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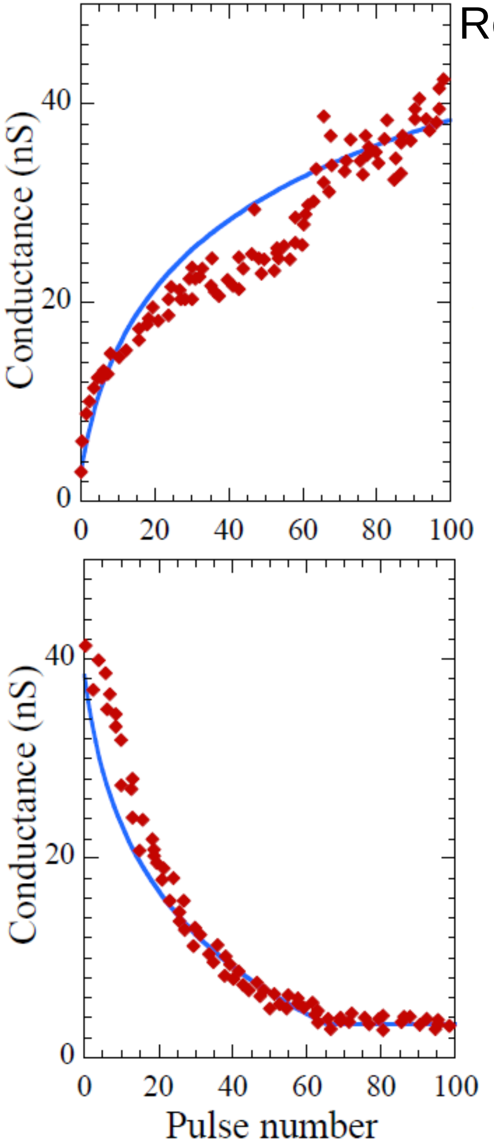

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2. D. Querlioz, et al. 2011 IEEE/ACM International Symposium on Nanoscale Architectures (NANOARCH), Jun 2011

Modeling of Memristors

❑ Critical roles – system-level and device-level?

- Reduce design cycle time
- Build foundry models
- Optimize performance and yield
- Study basic physics

❑ Current modeling methods

- Circuit-based analytical ➔ Design computing systems, BUT no microscopic views
- Physics-based analytical➔ Reveal underlying physics, BUT no structural implications
- Physics-based FEM ➔ Multi-physics, BUT only for pre-determined geometries

❑ Review a few predominate modeling methods and introduce our approach – Phase field (PF)

- Circuit-based analytical
- Physics-based analytical/FEM
- Phase-field FEM ➔ atomistic characteristics

Circuit-based Analytical

❑ Formulation

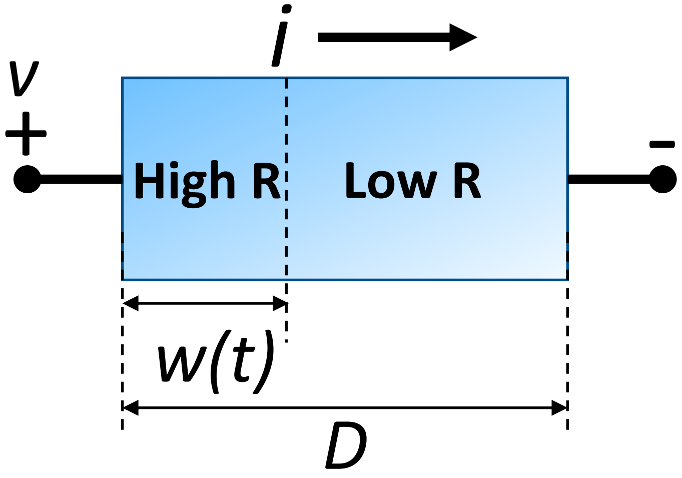
- Coupled variable-resistor
- State variable: *w*

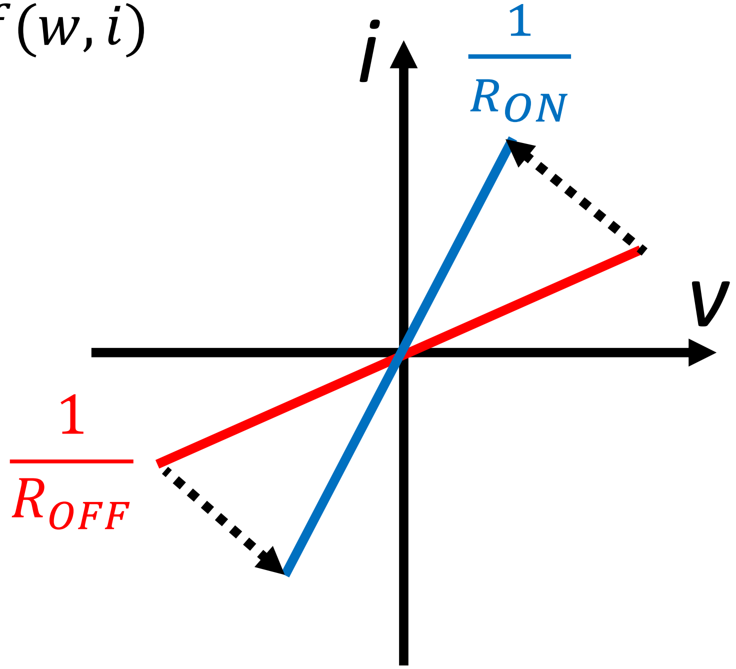
$$i = G(w, v)v$$

$$\frac{dw}{dt} = f(w, i)$$

❑ Examples

- Liner[1] or non-linear[2] charge drift
- Tunnel gap[3]
- SPICE[4]
- Benefits system design
- Provides no microscopic views





1. D. B. Strukov et al., Nature 453, 80 (2008)
2. Y. N. Joglekar, S. J. Wolf, Eur. J. Phys. 30, 661 (2009)
3. M. D. Pickett et al., J. Appl. Phys. 106, 074508 (2009)
4. H. Abdalla, M. D. Pickett, “SPICE modeling of memristors," 2011 IEEE International Symposium of Circuits and Systems (ISCAS), 2011, pp. 1832-1835

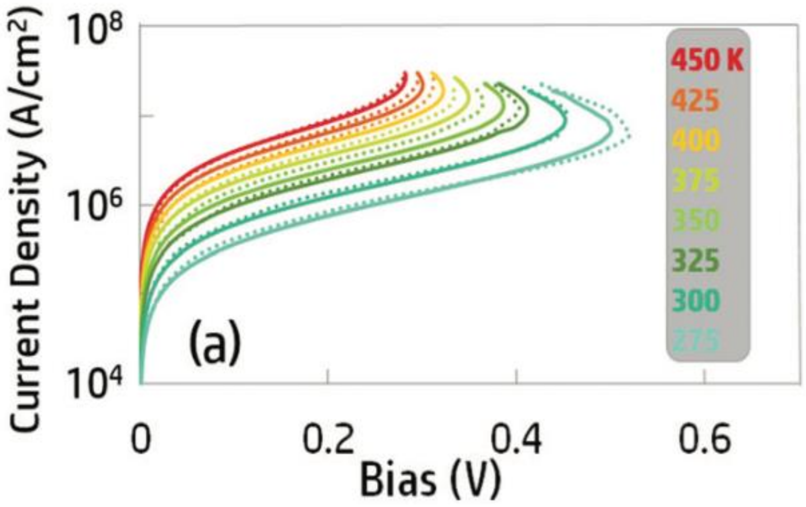
Physics-based Analytical

Flash Memory Summit

- **Formulation: Analytic descriptions for charge transport**
  - 3D Poole-Frenkel conduction
  - Frenkel defects – generation and recombination
  - Ion and vacancy diffusion

- **Examples**
  - Negative differential resistance (NDR) in NbO_2 selectors[1]
  - Kinetic Monte Carlo (cond. channel) + TCAD (device)[2]
  - *T* included, but no dynamic heat transport
  - Handles charge transport
  - Provides no microscopic structural views

$$j(F,T) = \sigma F = \sigma_0(T)\left(\frac{k_B T}{\beta}\right)^2 \left\{1 + \left(\frac{\beta\sqrt{F}}{a k_B T} - 1\right) e^{\frac{\beta\sqrt{F}}{a k_B T}}\right\} + \frac{\sigma_0(T)F}{2}, \qquad \sigma_0(T) = e\mu N_c \left(\frac{N_d}{N_t}\right)^2 e^{-\frac{E_d+E_t}{2k_B T}}$$



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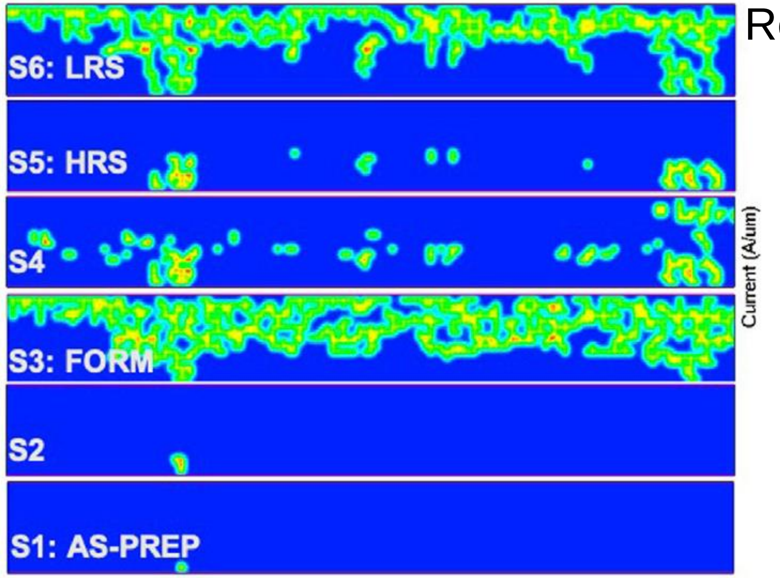

Ref 2

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2. A. Zeumault et al., Frontiers in Nanotechnology 3, 734121 (2021)

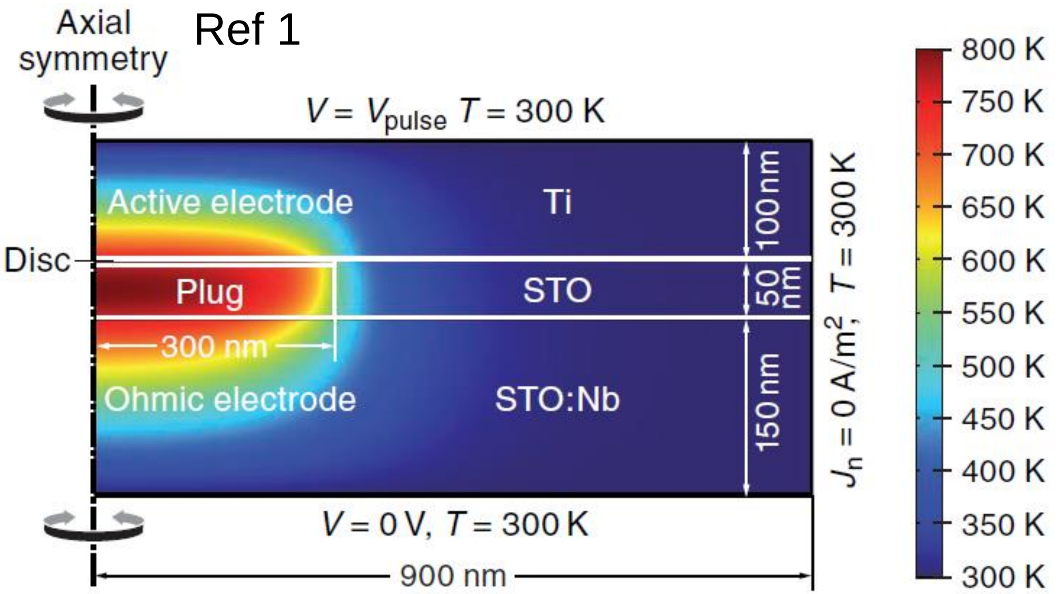
Physics-based FEM: Electrothermal

- Formulation: Expand physics-based analytical
  - Drift (electrons, holes, ions, defects)
  - Diffusion (electrons, holes, ions, point defects)
  - Temperature gradient (Soret effect)
  - Self-heating (e.g., Joule heating), heat transport
  - Poisson equation
  - Multi-physics

$$\frac{dw}{dt} = f(w, V, T)$$

- Examples
  - Diffusive[4] or non-diffusive[5] heat transport
  - Cylindrical "pre-formed" conducting channels[1,2,3] ➔ Major issue

Ref 1



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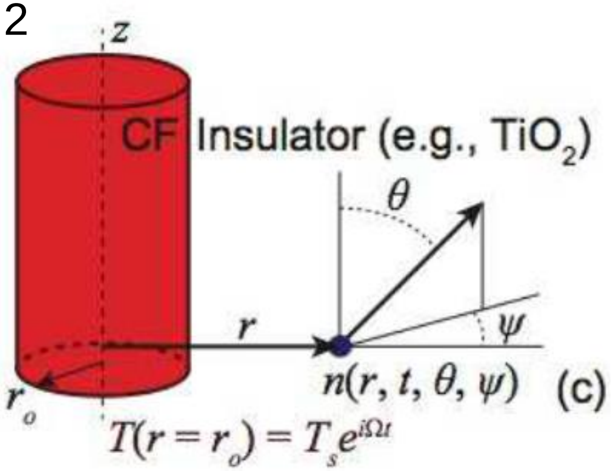

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2. Y. Zhao et al., IEEE Transactions on Electron Devices 65, 4290 (2018)
3. S. Kumar et al., IEEE Transactions on Electron Devices 69, 3124 (2022)
4. U. Russo et al., IEEE Transactions on Electron Devices 56, 1896 (2009)
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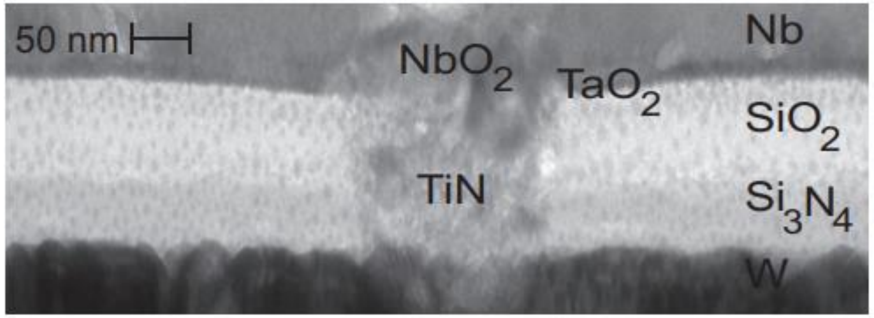
Physics-based FEM: Electroformation/Transient

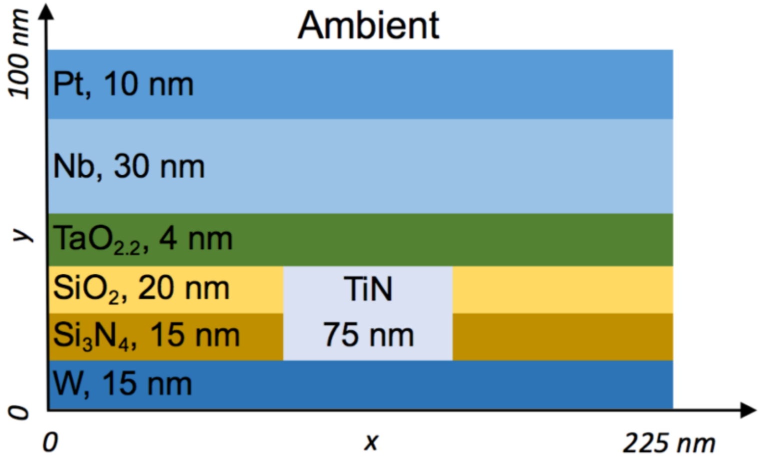


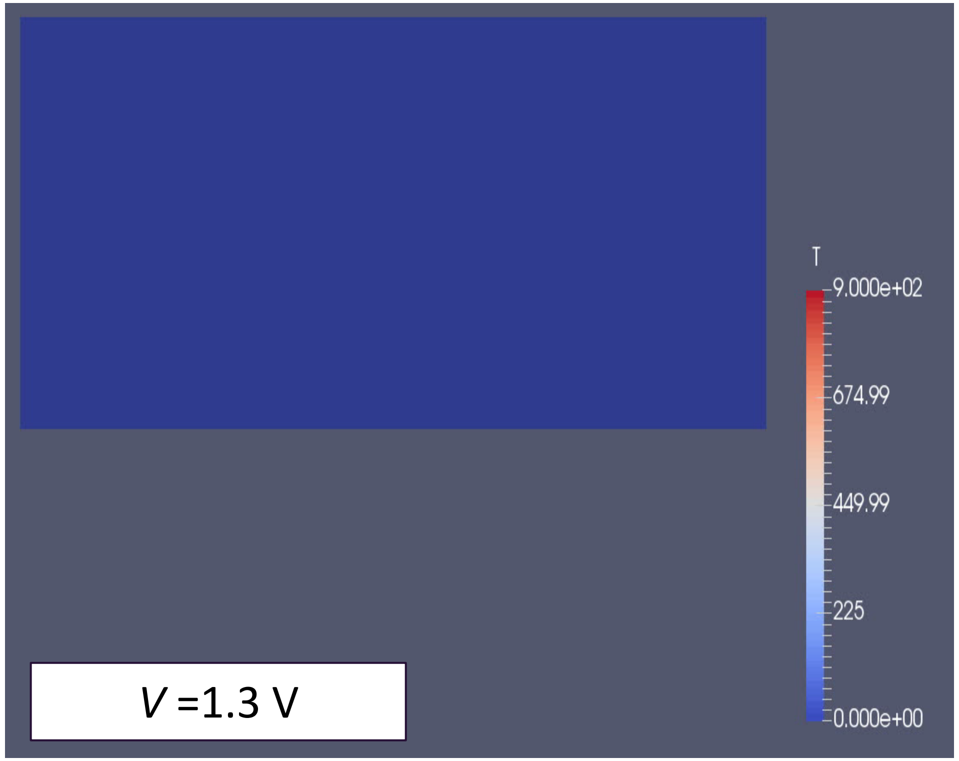
Frenkel defects
Oxygen vacancies $\Rightarrow \dfrac{\partial n}{\partial t}$

$$\nabla \cdot \sigma(\vec{r}, T)\nabla V(\vec{r}, t) = 0$$

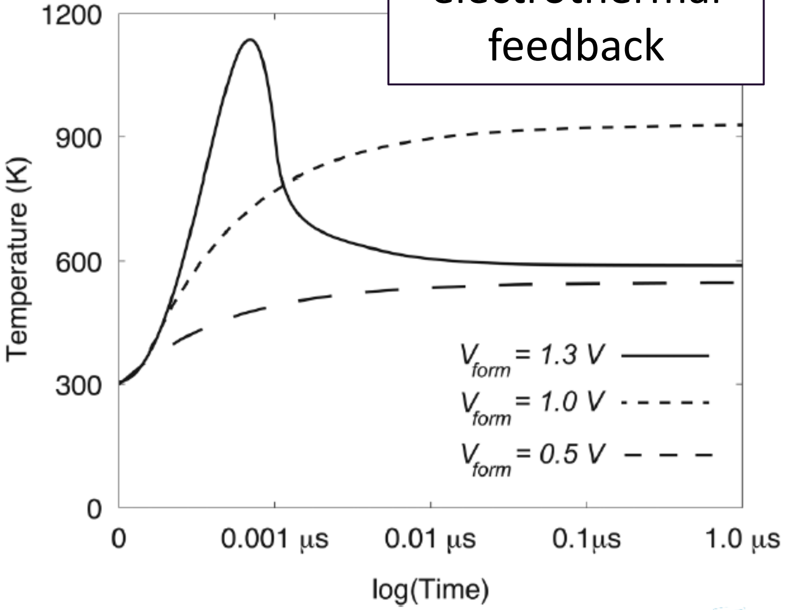
Diffusive heat transport
Joule heating $\Leftarrow \sigma(\mathbf{r}, n, T) \Rightarrow \dfrac{\partial T(\mathbf{r}, t)}{\partial t}$

n: normalized charge density
t: time; σ: elec. cond.
T: temperature
r: 2D coordinates





spontaneous electrothermal feedback



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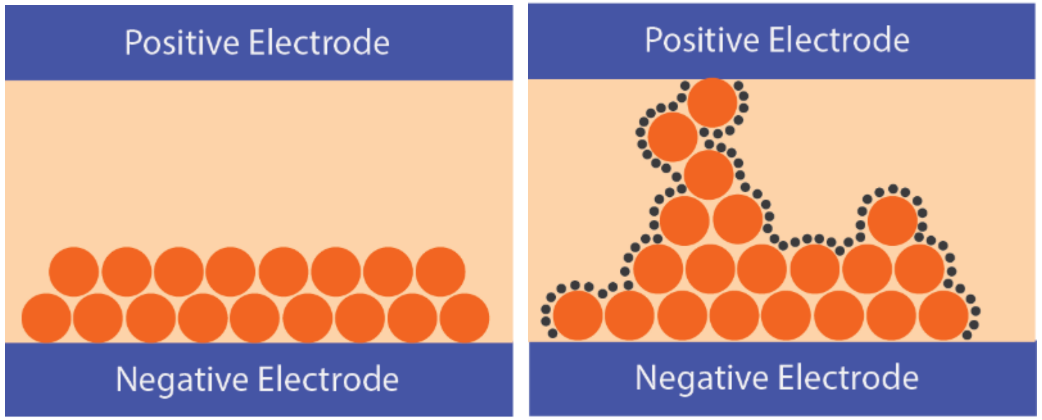
Phase-Field (PF) + FEM

The bases: Thermodynamic formulation that accounts for the gradients in thermodynamic properties in heterogeneous systems.



a) Pristine state. b) Formed state.

- Does not deal with particles
- Provides dynamic behavior of the boundary
- Evolving boundaries as *F* is reduced
- Boundary conditions that change over time
- Diffuse interface

$$F = \int_R \left[f_{bulk}(c) + \frac{\kappa}{2}\nabla^2 c(\vec{r},t) + g_{elec}(c,V) \right] d\vec{r}$$

$$J_{PF} = M \times \nabla \frac{\delta F}{\delta c}$$

$$\frac{\partial c(\vec{r},t)}{\partial t} = \nabla \cdot J_{PF}$$ Eq. 1 (PF PDE)

$$\frac{\partial T(\vec{r},t)}{\partial t} = S_T(\vec{r}) + S_J(\vec{r})$$ Eq. 2 (Heat PDE)

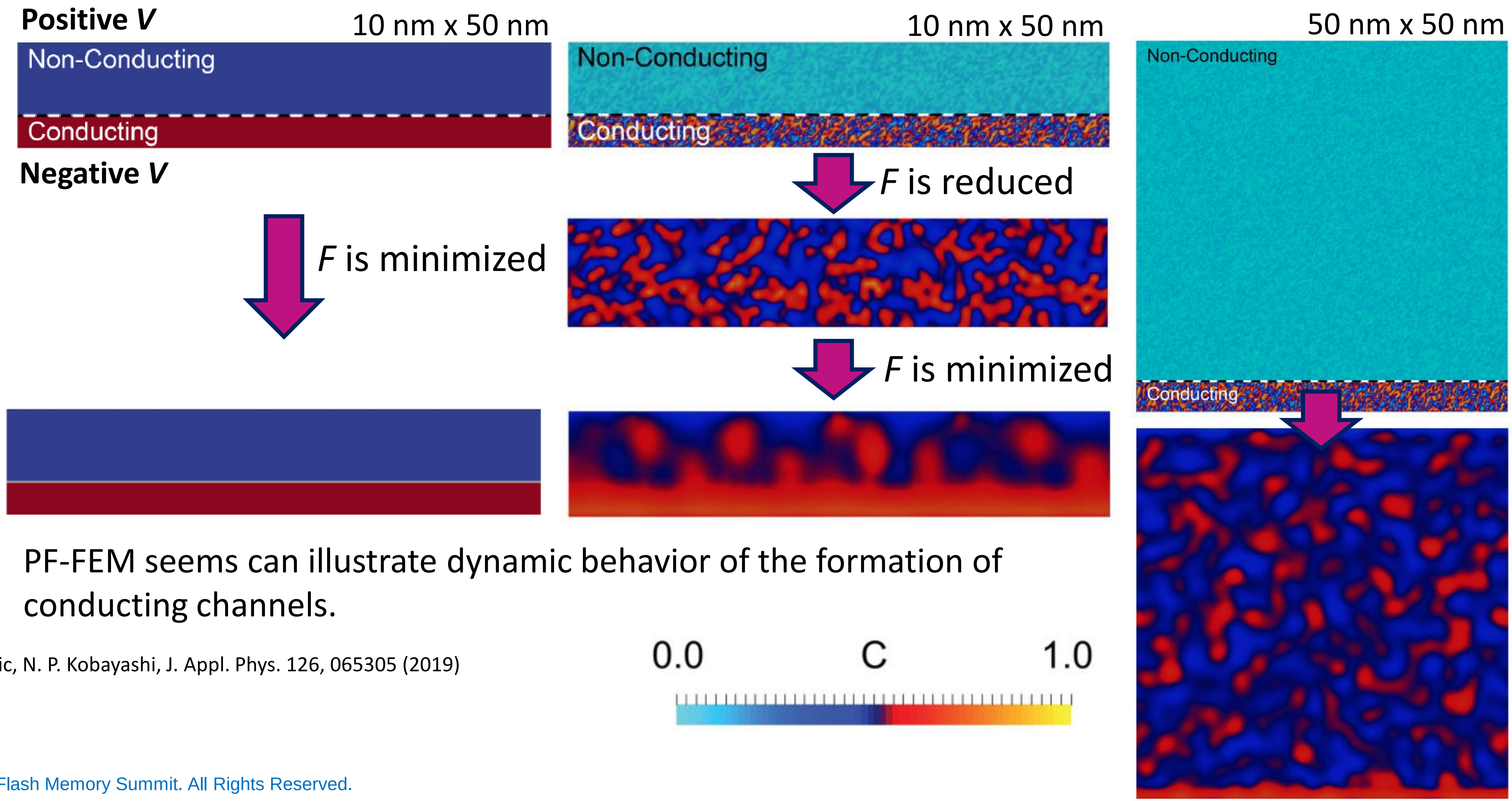
$$\nabla \cdot \sigma(\vec{r},T)\nabla V(\vec{r},t) = c(\vec{r},t)$$ Eq. 3 (Charge PDE)

F : Free energy
$f_{bulk}(c)$: Bulk free energy density
κ: Interface energy
$g_{elec}(c, V)$: Interaction f_{bulk} and V
M: Mobility of the phase field flux in phase space

V: Electric potential
c: Charge density (Normalized)
S_T: Diffusive heat transport
S_J: Joule heat generation

J. F. Sevic, N. P. Kobayashi, J. Appl. Phys. 126, 065305 (2019)

PF-FEM: Initial Trial (Isothermal)



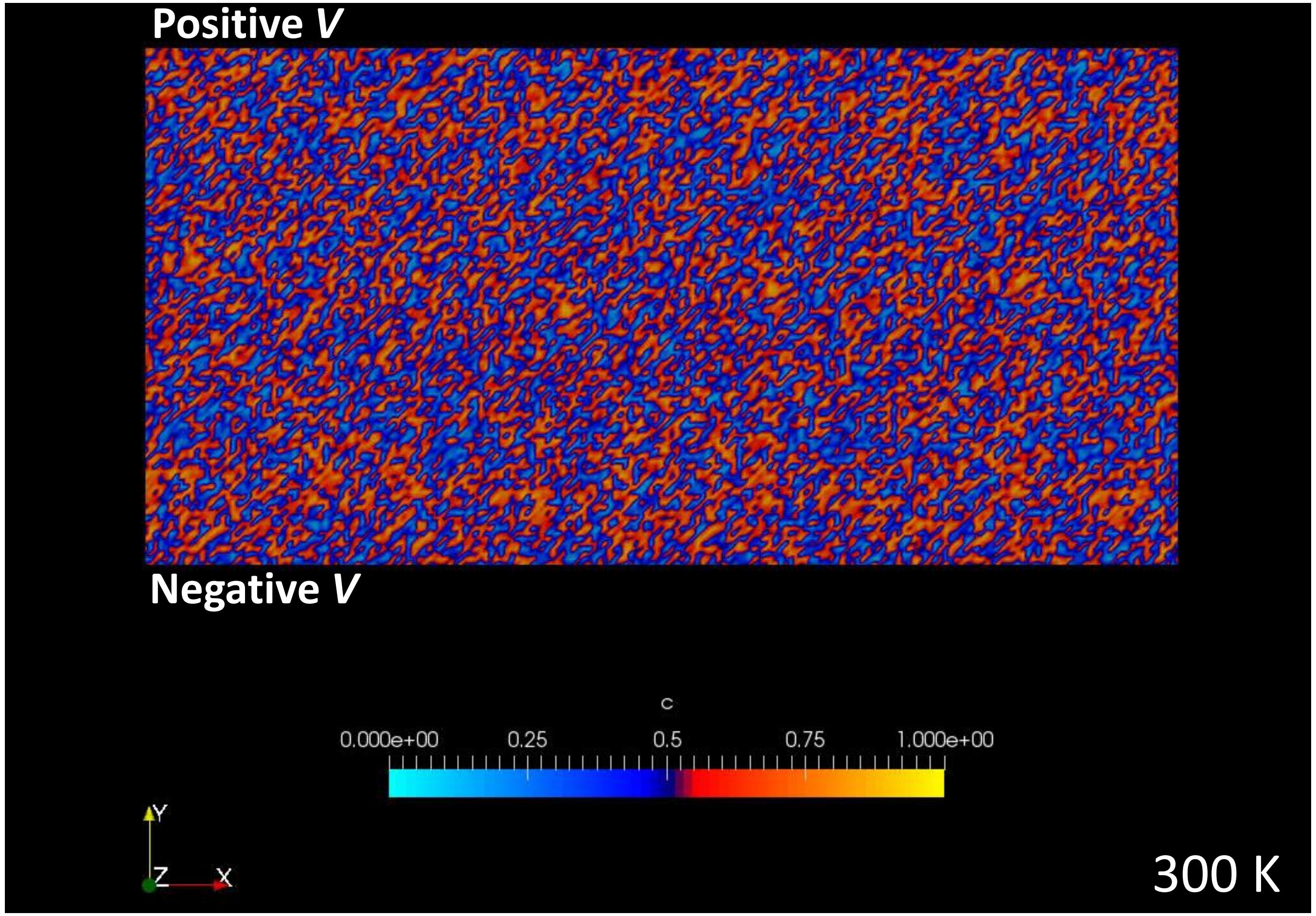
PF-FEM seems can illustrate dynamic behavior of the formation of conducting channels.

J. F. Sevic, N. P. Kobayashi, J. Appl. Phys. 126, 065305 (2019)

PF-FEM: Work in Progress

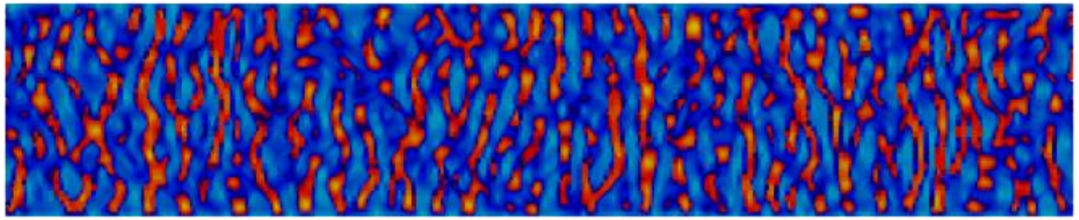
Isothermal

30 nm x 50 nm

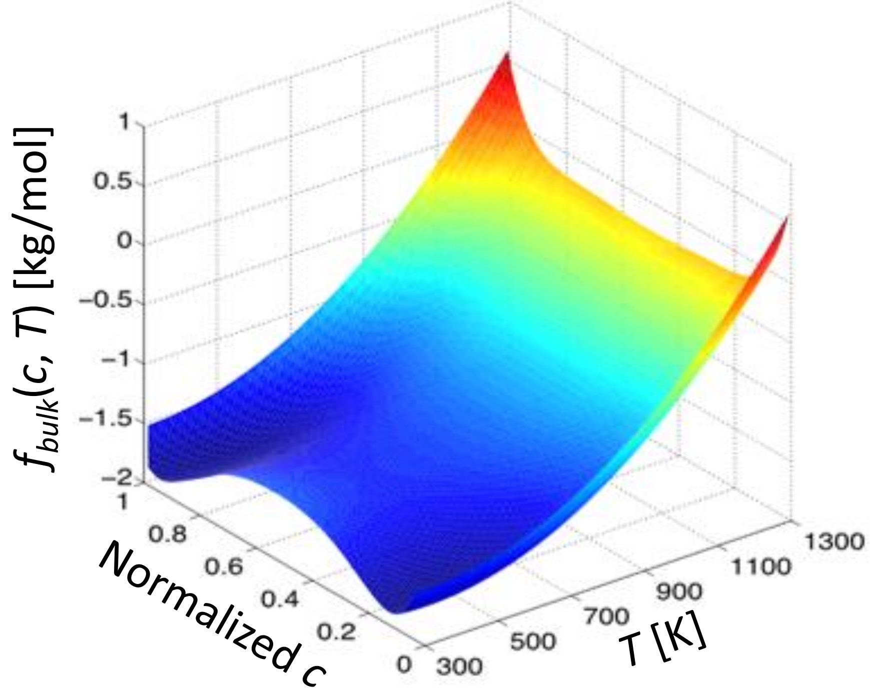


Joule Heating

10 nm x 50 nm



$$F = \int_R \left[\boxed{f_{bulk}(c)} + \frac{\kappa}{2}\nabla^2 c(\vec{r}, t) + g_{elec}(c, V) \right] d\vec{r}$$



Comparison of Modeling Methods

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Capability	Circuit/Physics	Physics-based analytical FEM	PF-FEM
Ideal for neuromorphic computing applications	Yes	No	No
Ideal for circuit-level NV-RAM simulation	Yes	No	No
Ideal for physics-level NV-RAM simulation	No	Yes	Yes
Full treatment of SET and RESET processes	No	Yes	Yes
Parameter extraction	Easy	Moderate	Difficult
Atomic Phase Change Formulation	No	No	**Yes**
Scales to Nanoscale Geometries	No	Difficult	**Yes**
Transient SET-RESET Evolution	Yes	Yes	**Yes**
Electroforming	No	Possible	**Yes**
Does not require a pre-existing current filament model	No	No	**Yes**

microscopic natures of underlying physics

35 YEARS OF NAND FLASH MEMORY INNOVATION

Summary

Flash Memory Summit

- ❑ Circuit-based analytical
  - System-level design (e.g., neuromorphic computing)
  - Simple model generation and coding
  - SPICE
- ❑ Physics-based analytical FEM
  - FEM➔Multi-physics
  - Conducting channels with a specific geometry
  - TCAD
- ❑ Phase-field FEM (Microscopic view)
  - Complex (PDEs/weak form and multi-physics)
  - Electroforming and SET-RESET through the formation/annihilation of conducting channels
  - Realistic description for various energy terms (In progress)

