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Three-Dimensional Fully-Coupled Electrical and Thermal Transport Model of Dynamic Switching in Oxide Memristors

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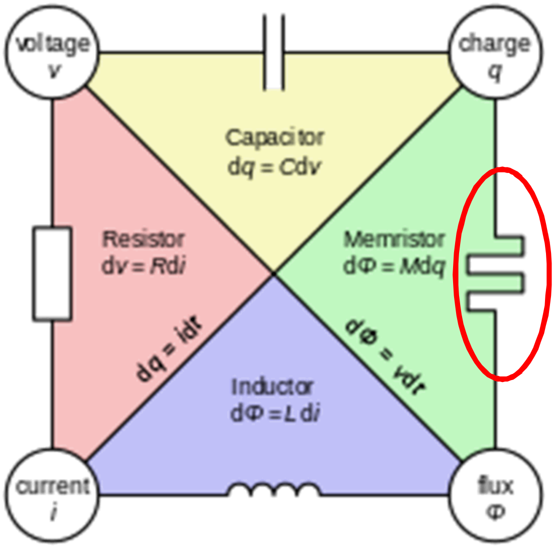
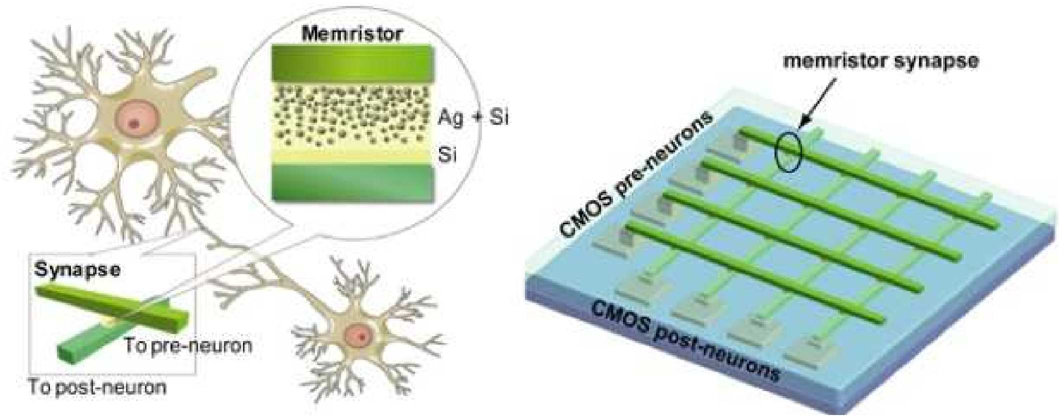
Memristor – New Research Frontier

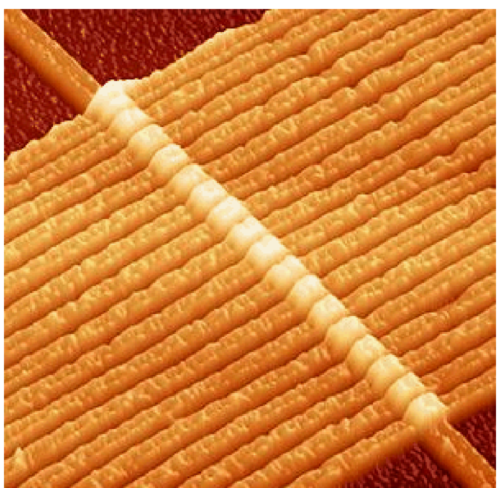


Brain-Inspired Computing

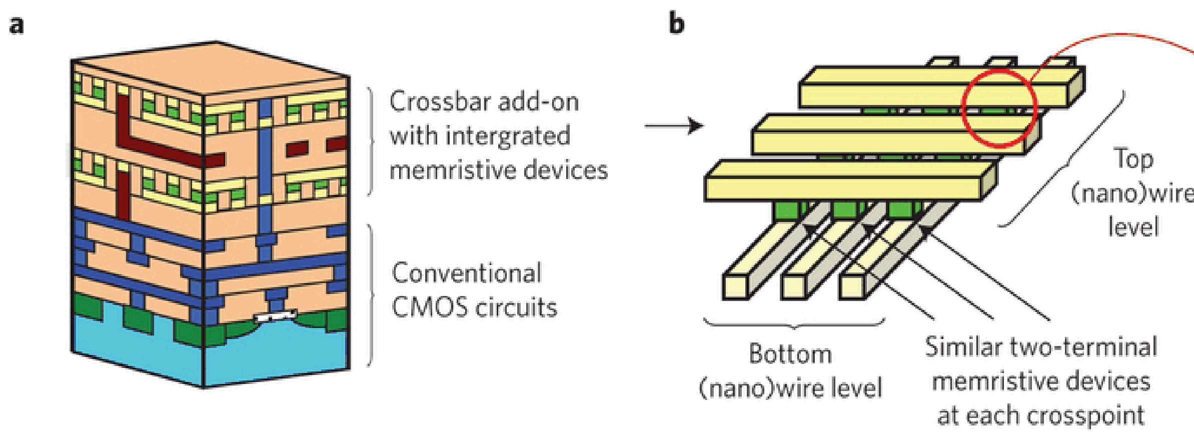
Using memristors as synapse to build computers like nature builds brains



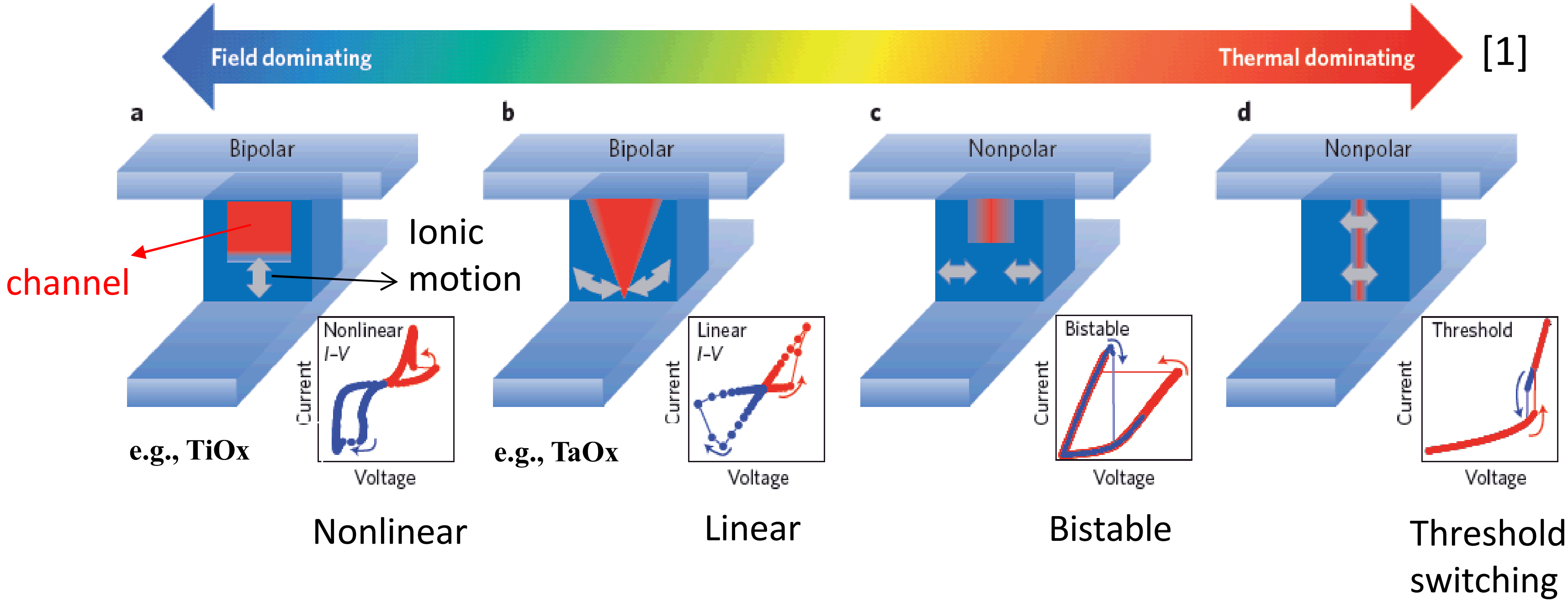
Non-volatile Memory



Hybrid CMOS/Memristor 3D Circuits



Memristor – Complex Switching Process



Complex switching behavior - governed by temporally and spatially intertwined electrical and thermal processes of electrons , holes, and mobile vacancies:

- Field drift
- Fick diffusion
- Soret effect
- Joule heating
- High-order effects

NO existing models have captured all these processes and their couplings for **electrons, holes, and mobile vacancies simultaneously** in 3D device structures !

[1] J. J. Yang, D. B. Strukov, and D. R. Stewart, Nature Nanotechnology **8**, 13 (2013).

Fully-Coupled Transport Model

We solve, **simultaneously**, the five coupled differential equations:

Poisson (P): $\nabla \bullet \varepsilon \nabla(\phi) = -q(p - n + C + z_V N_V)$ → include all charge species

Electron (E): $q\frac{\partial n}{\partial t} = \nabla \bullet \vec{J}_n - qR_{net}$

Hole (H): $q\frac{\partial p}{\partial t} = -\nabla \bullet \vec{J}_p - qR_{net}$

Vacancy (V): $q\frac{\partial N_V}{\partial t} = -\nabla \bullet \vec{J}_V$

(E), (H), (V): time-dependent continuity equations for all carriers

Temperature (T): $\frac{\partial}{\partial t}(c_L T) - \nabla \bullet (\kappa_L \nabla T) = H$

Auxiliary relations:

$$\vec{J}_n = qn\mu_n \vec{E} + qD_n \nabla n + k_B n \mu_n \nabla T$$

$$\vec{J}_p = qp\mu_p \vec{E} - qD_p \nabla p - k_B p \mu_p \nabla T$$

$$\vec{J}_V = qN_V \mu_V \vec{E} - qD_V \nabla N_V - qD_V S_V N_V \nabla T$$

Field drift (first terms), Fick diffusion (second terms), Soret effect (third terms)

$$H = (\vec{J}_n + \vec{J}_p + \vec{J}_V) \bullet \vec{E} + R_{net}(E_g + 3k_B T)$$

Joule heating due to all carriers

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Vacancy Mobility Model

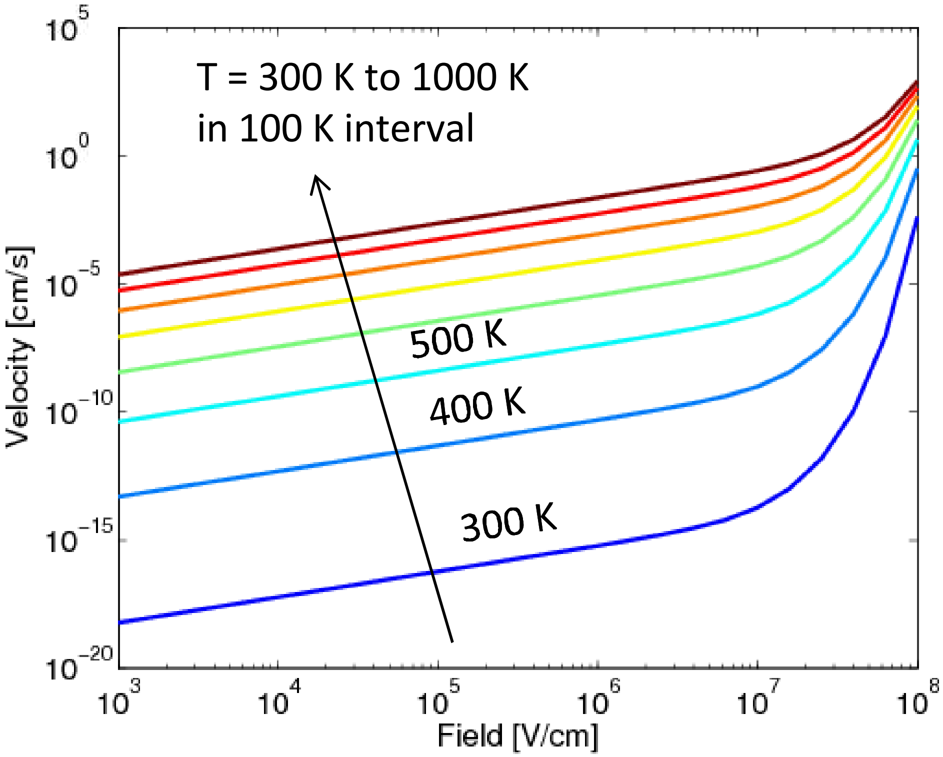
Rigid Point Ion Model (RPI)

Vacancy activation energy

Electric field

Vacancy velocity $v_V = 2 \cdot f \cdot a \cdot \exp\left(\frac{-E_a}{kT}\right) \cdot \sinh\left(\frac{qaE}{kT}\right)$

Vacancy diffusion $D_V = f \cdot a^2 \cdot \exp\left(\frac{-E_a}{kT}\right)$



- Vacancy motion exponentially depends on temperature, and field when the field exceeds a critical value

Charon Device Simulator

The fully-coupled equations are implemented in Charon.

Sandia TCAD code

Charon

Trilinos

ParaView

Cubit for geometry and mesh creation

https://cubit.sandia.gov/

Open-source suite:

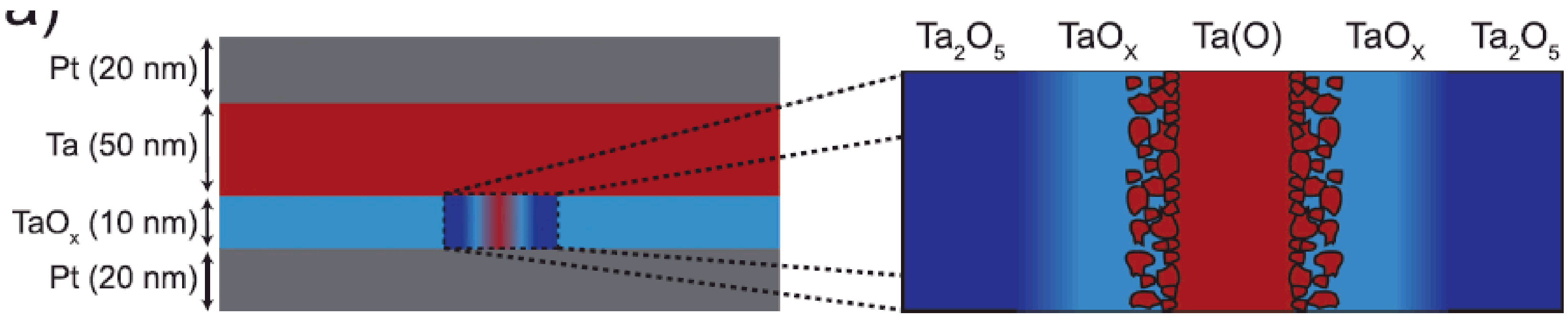
- Discretization (FE, FV)
- Nonlinear & linear solvers
- MPI parallel
- Automatic differentiation
- Many more…

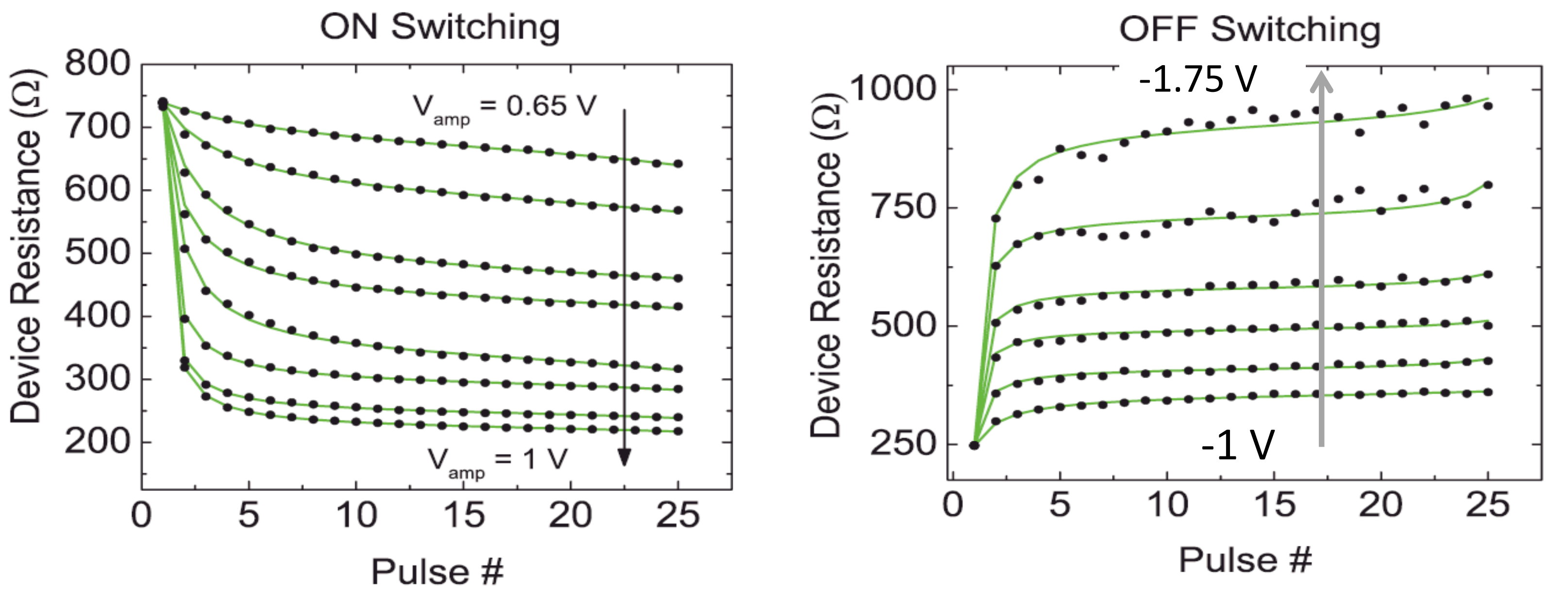
http://trilinos.org/

Data analysis and visualization

http://www.paraview.org/

Experimental Resistance





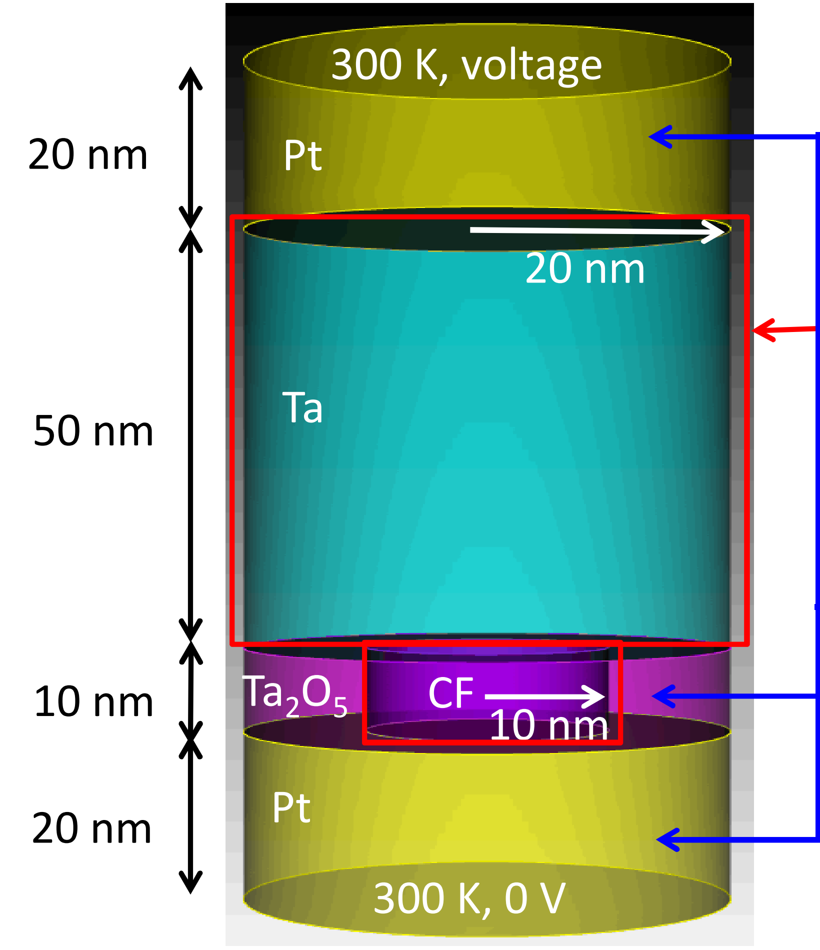
- **Experimental ON-resistance decreases with time and increasing voltage**
- **Experimental OFF-resistance increases with time and increasing voltage**

[2] Patrick R. Mickel et al., A physical model of switching dynamics in tantalum oxide memristive devices, APL **102**, 223502 (2013).

Modeling Goal

- Demonstrate qualitatively the **resistance increases with time and increasing voltage** during OFF switching in a TaOx memristor
- Demonstrate qualitatively the **resistance decreases with time and increasing voltage** during ON switching in a TaOx memristor
- Demonstrate qualitatively the **current-voltage hysteresis** under triangular voltage sweep in a TaOx memristor

TaOx Device Structure



- Solve **P+E+V+T** equations
- V is limited to Ta and CF

- Solve **P+E+T** equations
- No mobile vacancies
- Ohmic contact for electron

[2] Patrick R. Mickel et al., A physical model of switching dynamics in tantalum oxide memristive devices, APL **102**, 223502 (2013).

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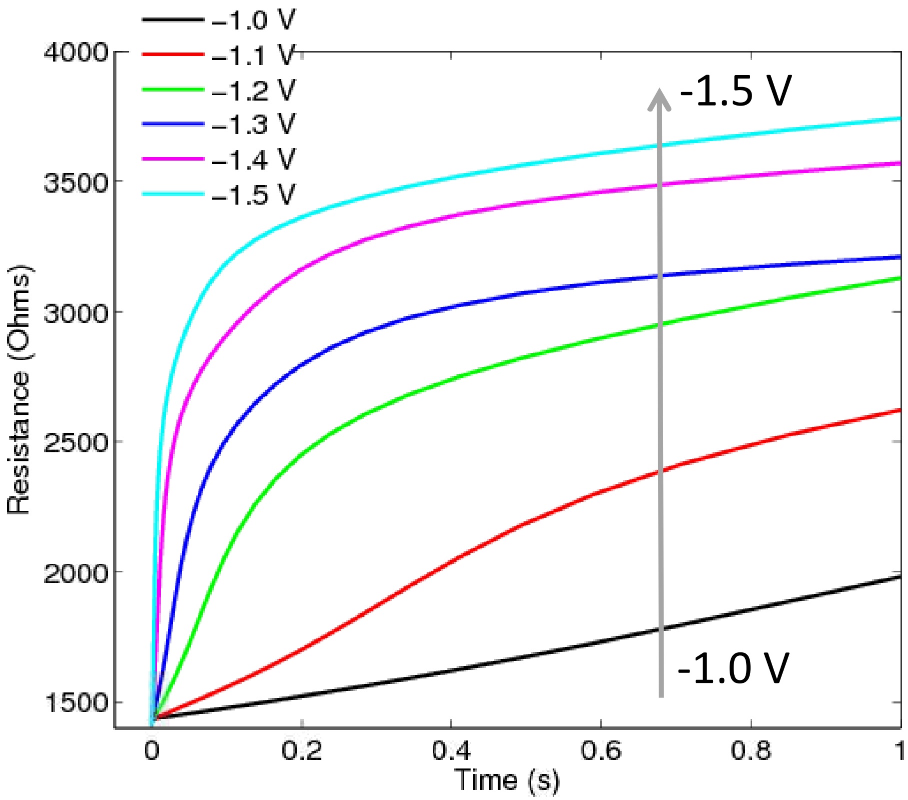
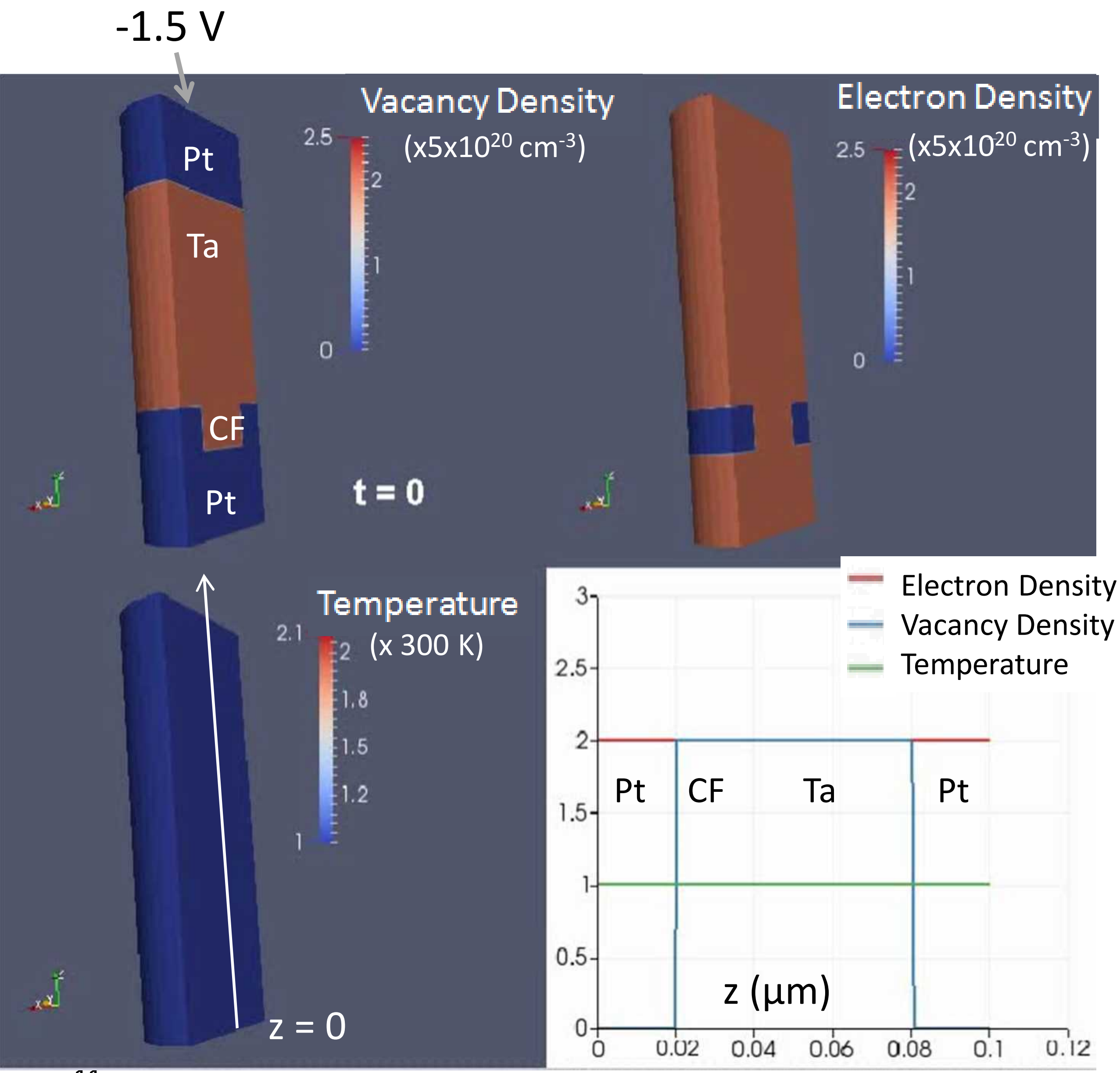
OFF-Switching Resistance Evolution



- Resistance increases with time and increasing voltage during OFF-switching, consistent with experimental observation

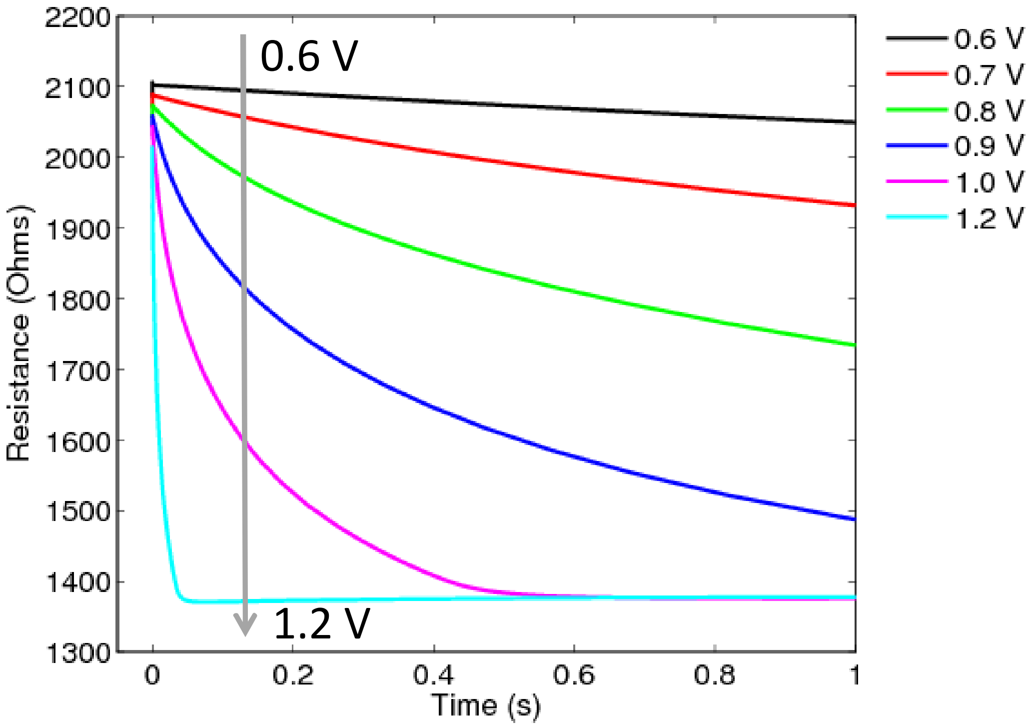
What Happens During OFF-Switching



OFF-Switching:

- Initial temperature increase occurs on the order of 100 ps, and initial heating is broad in space
- Vacancies near the peak temp. start to move around μs, and move away from CF into Ta
- CF first has a density gap formed, and eventually is depleted of vacancies, resulting in OFF state
- As CF becomes more resistive, heating is more localized in CF

ON-Switching Resistance Evolution

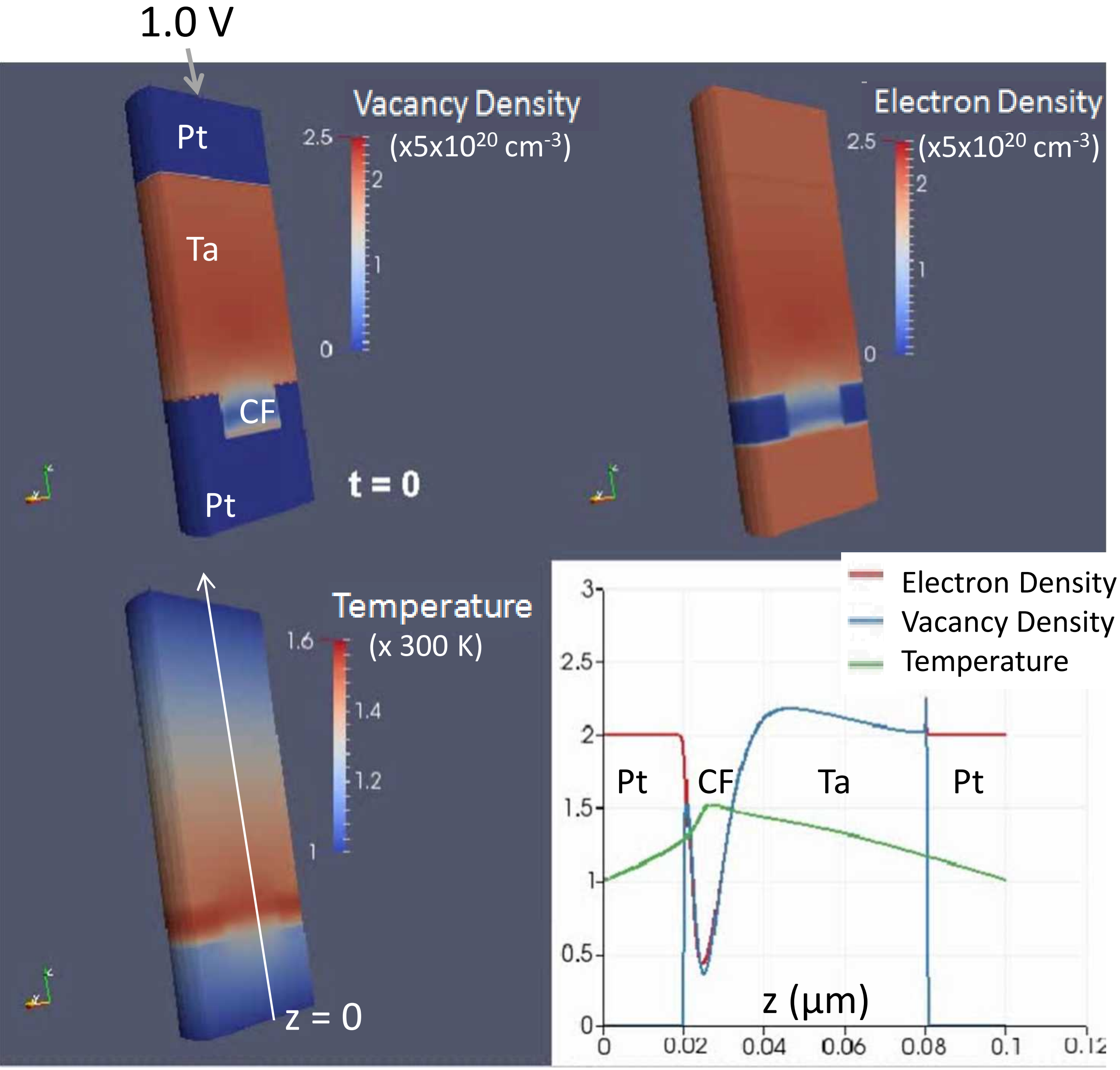


During ON-switching, vacancy diffusion is increased with vacancy density to avoid unphysical piling-up:

$$D_V = \frac{D_{rpi}}{1 - \frac{N_V}{N_{max}}}$$

- ON-resistance decreases with time for a given voltage, and decreases faster with time for higher voltage, consistent with experimental observation

What Happens During ON-Switching



ON-Switching:

- Starting with an OFF-state, temp. increases on the order of 100 ps
- Vacancies move from Ta into CF to fill in the gap according to RPI model
- As CF becomes more conductive, heating is more spread in space

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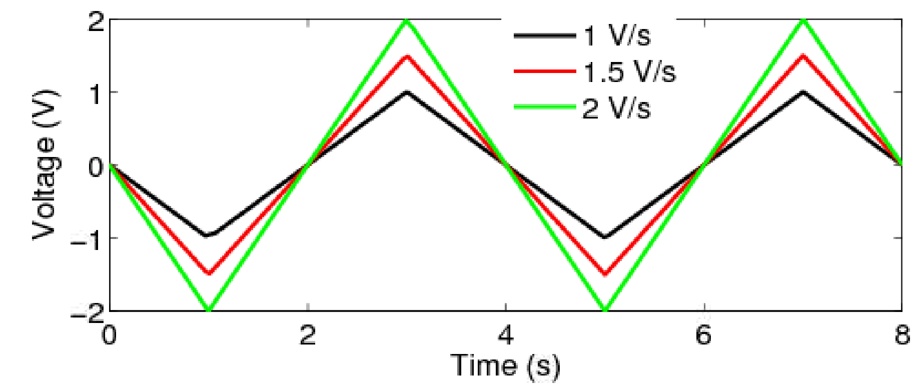
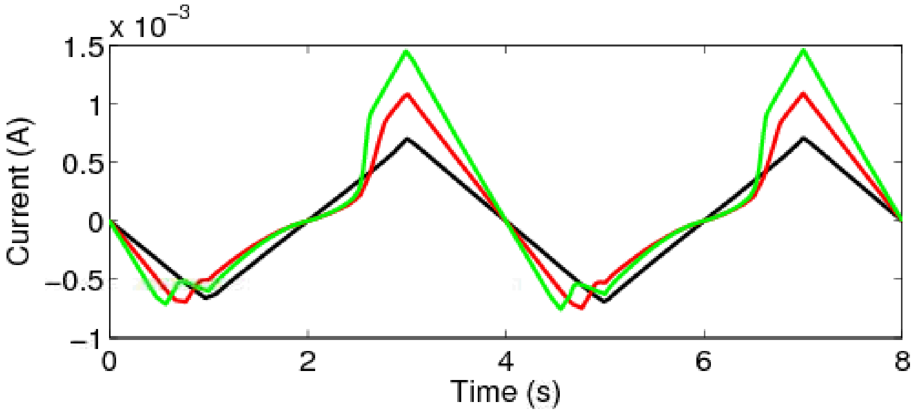
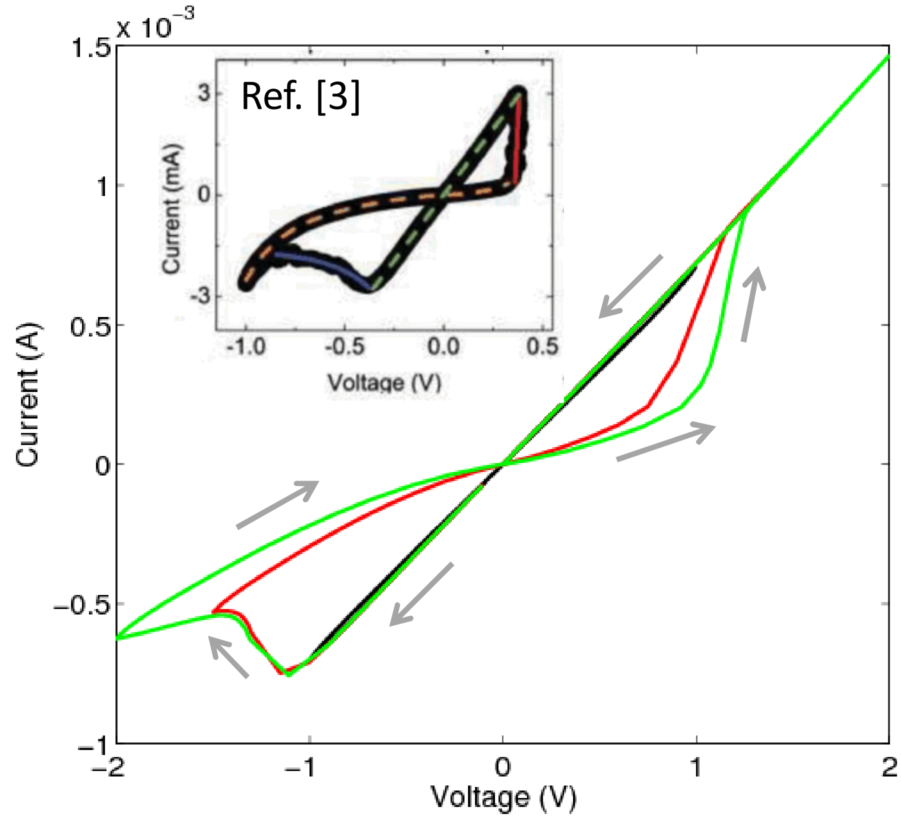
Current-Voltage Hysteresis



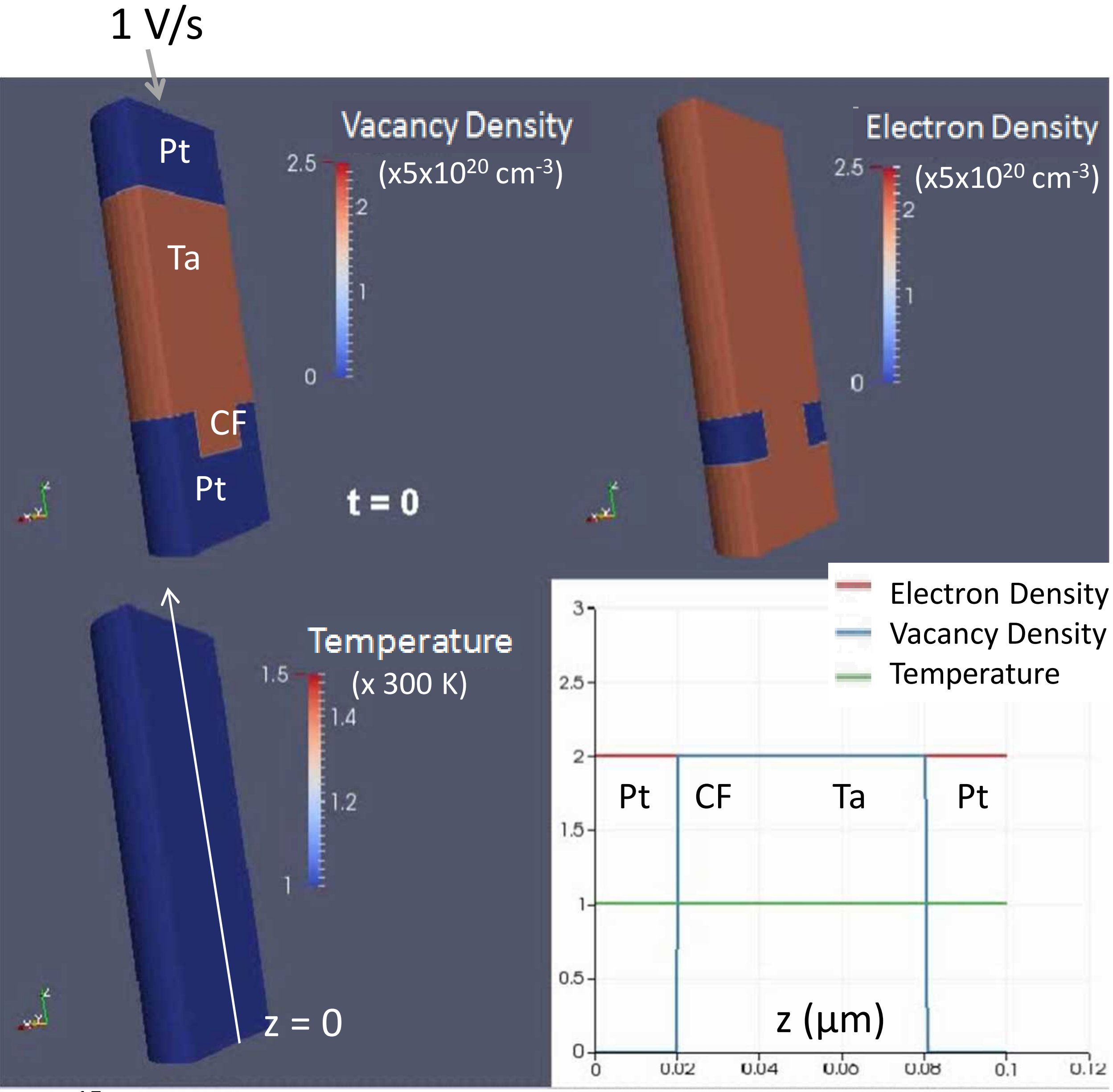


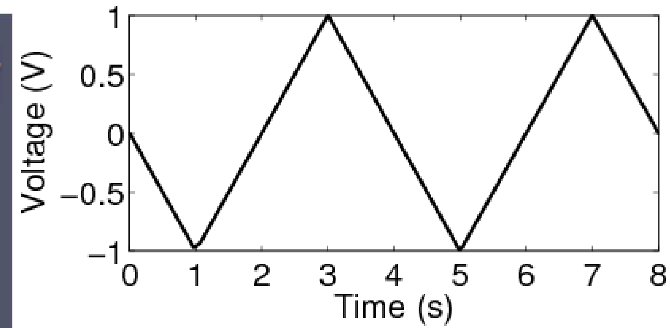


- Current-voltage hysteresis is NOT observed for the 1 V/s voltage ramping
- Current-voltage hysteresis is clearly observed for the 1.5 V/s and 2 V/s cases, and shows qualitative agreement with experimental result

[3] Patrick. R. Mickel et al., Adv. Mater. **26**, 4486-4490 (2014).

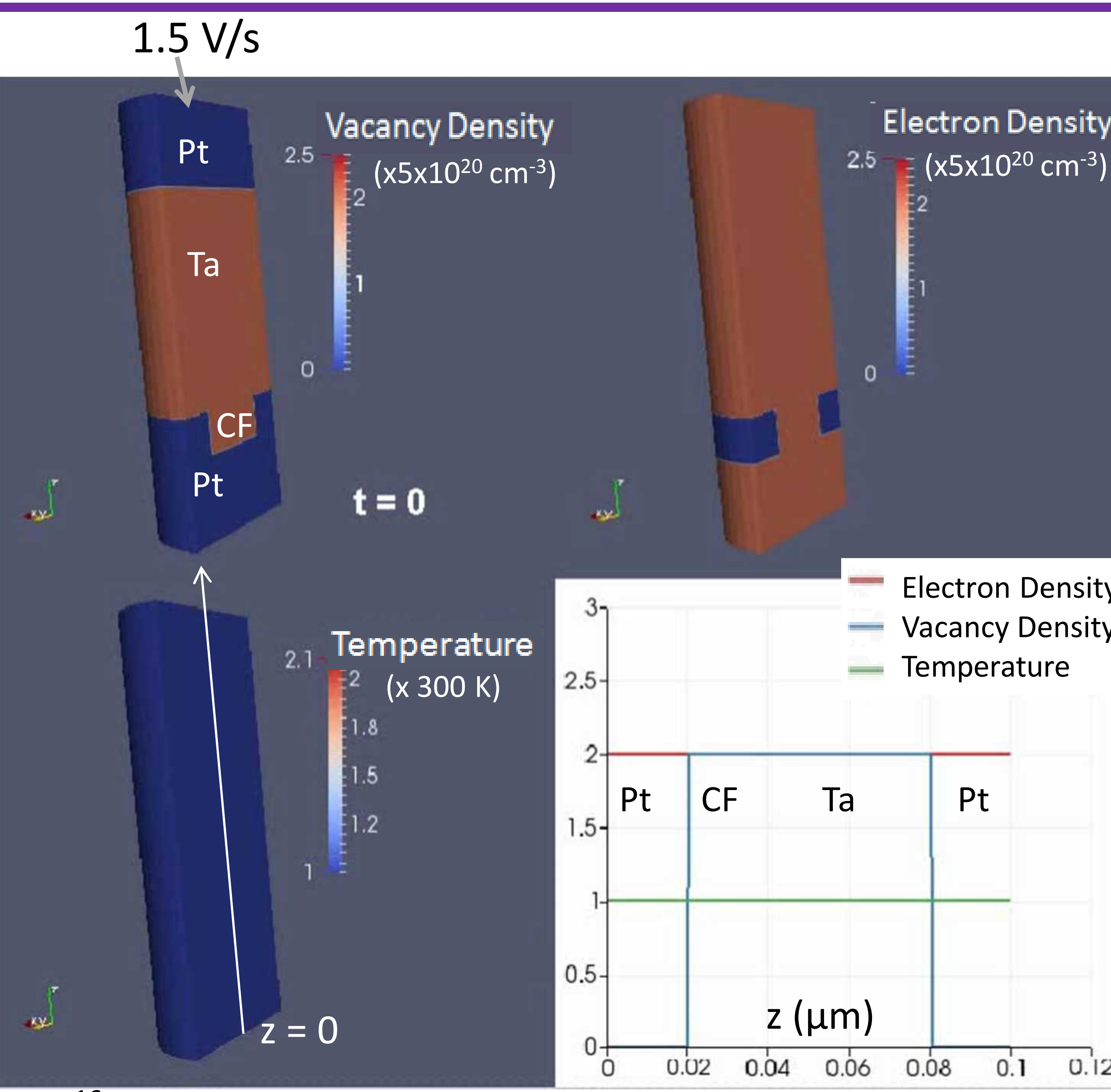
What Happens During Voltage Sweep

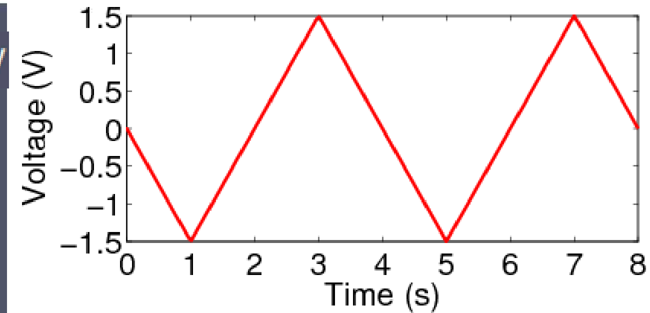




- Given the 1 V/s triangular voltage, device never turned off during negative voltage, due to insufficient heating

What Happens During Voltage Sweep





- Given the 1.5 V/s triangular voltage, device fully turned off during negative voltage, and was able to turn on during positive voltage

Conclusion

Developed a fully-coupled electrical and thermal model

$$\nabla \bullet \varepsilon \nabla(\phi) = -q(p - n + C + z_V N_V)$$

$$q\frac{\partial n}{\partial t} = \nabla \bullet \vec{J}_n - qR_{net}$$

$$q\frac{\partial p}{\partial t} = -\nabla \bullet \vec{J}_p - qR_{net}$$

$$q\frac{\partial N_V}{\partial t} = -\nabla \bullet \vec{J}_V$$

$$\frac{\partial}{\partial t}(c_L T) - \nabla \bullet (\kappa_L \nabla T) = H$$

Capture all important processes in memristor

Applied the model to simulate a TaOx memristor

- OFF-resistance increases with time and voltage
- ON-resistance decreases with time and voltage
- Current-voltage hysteresis

- Qualitative agreement with experiment
- Both field and thermal are important

Calibration and quantitative comparison with experimental data are a work in progress