Comparative Study of Transport Models for Bipolar Switching in Memristors

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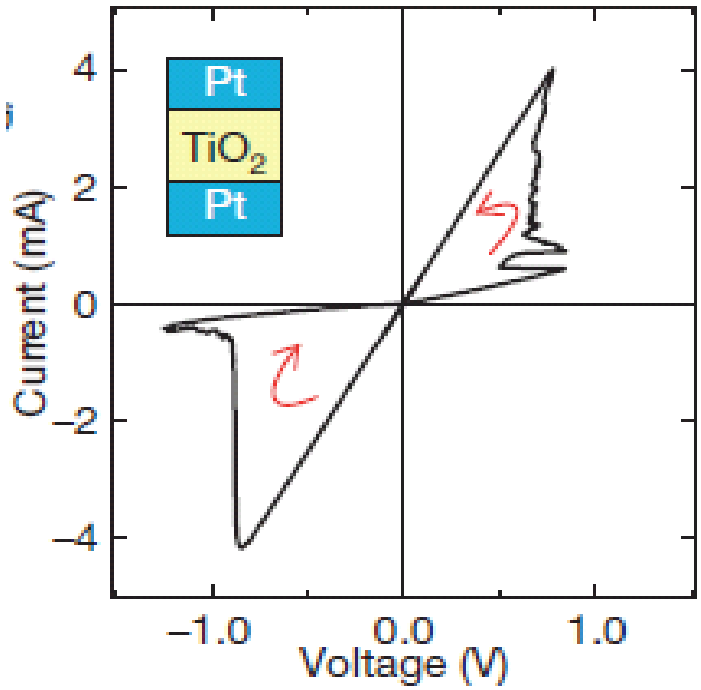
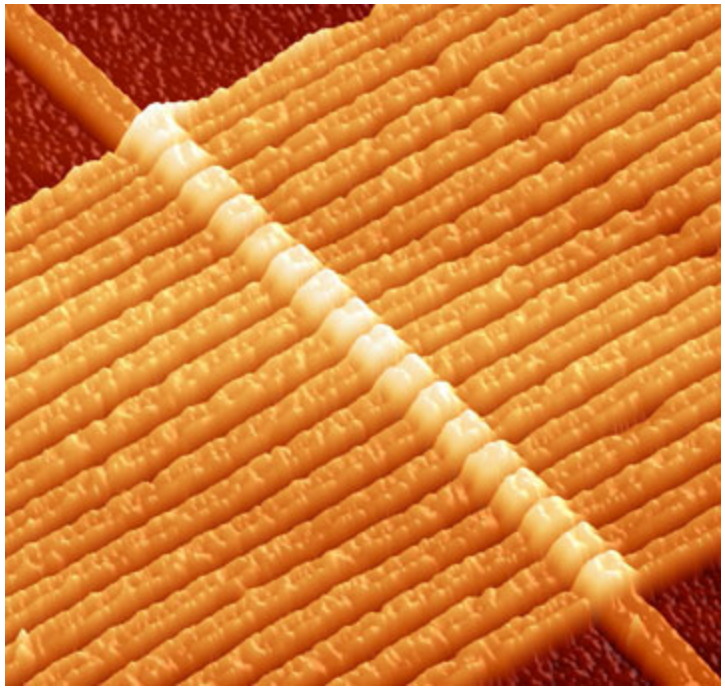
Memristors – Explosive Recent Interest

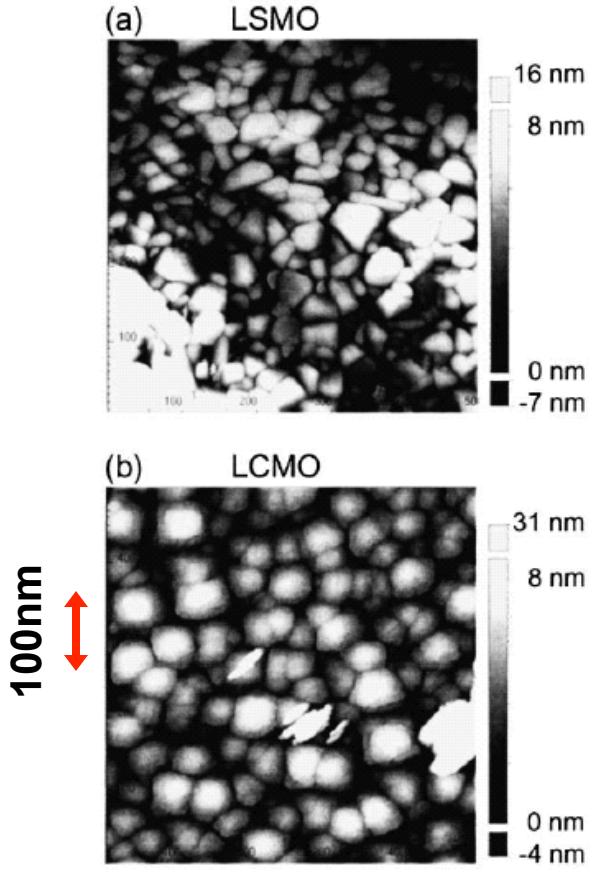
HP group of Stan Williams reported hysteretic switching behavior in Pt/TiO/Pt structures (Nature 2008)
As of midnight: 529 citations



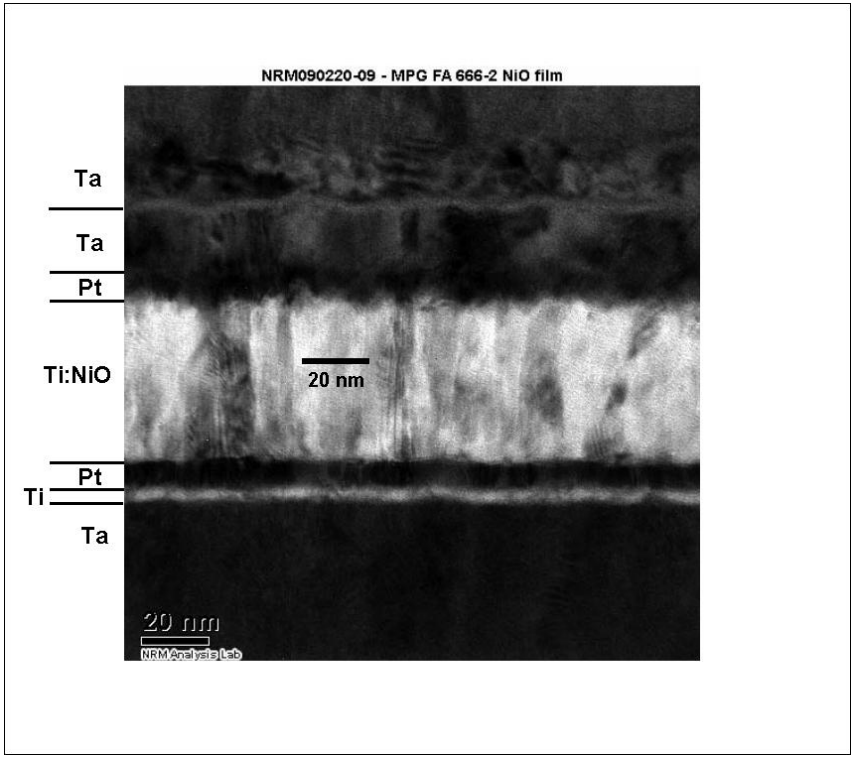


Switching by Channel Formation

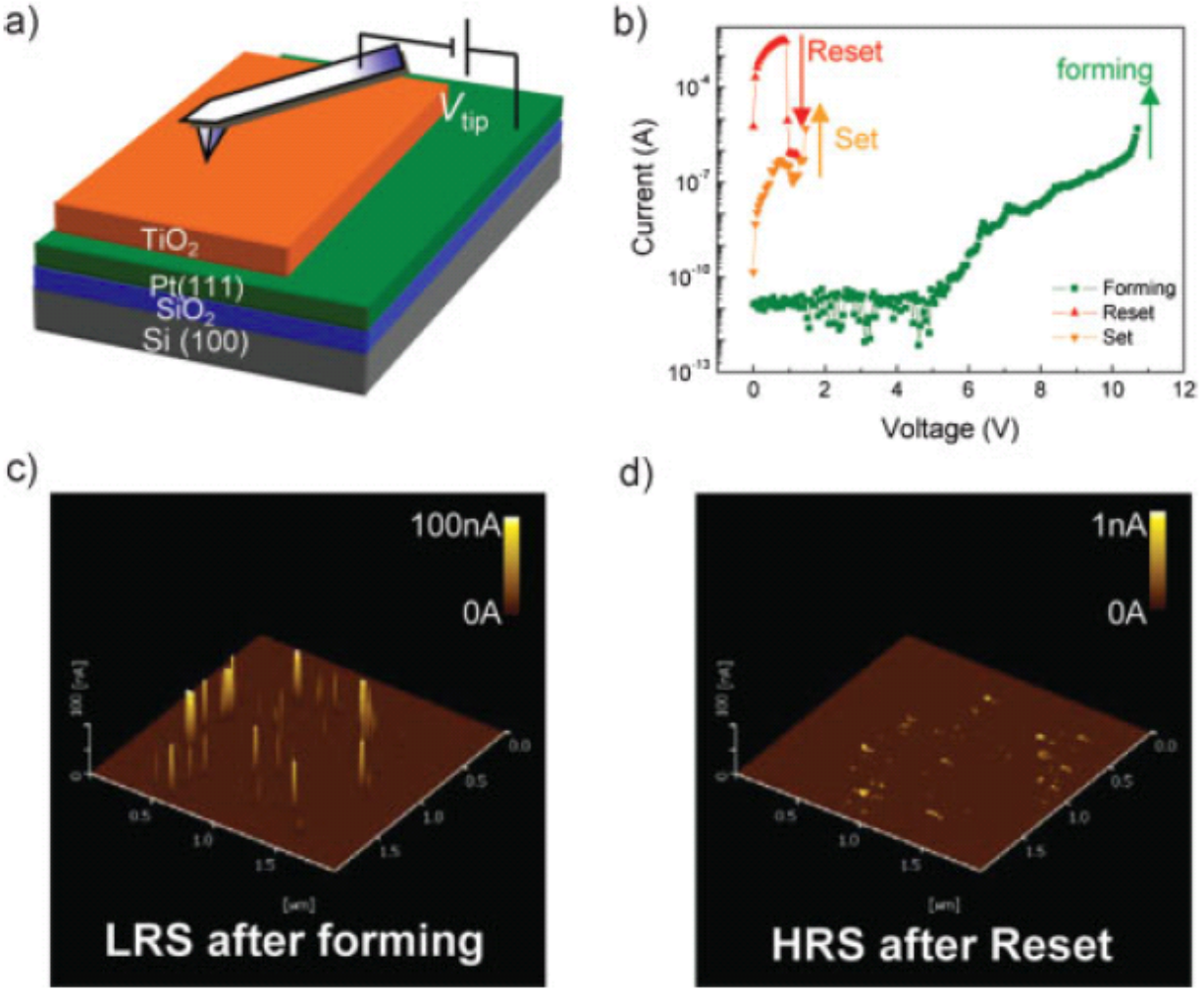
- TMO systems are inherently inhomogeneous
- Switching mechanism: channel formation by oxygen vacancy migration



Becker et al PRL '02

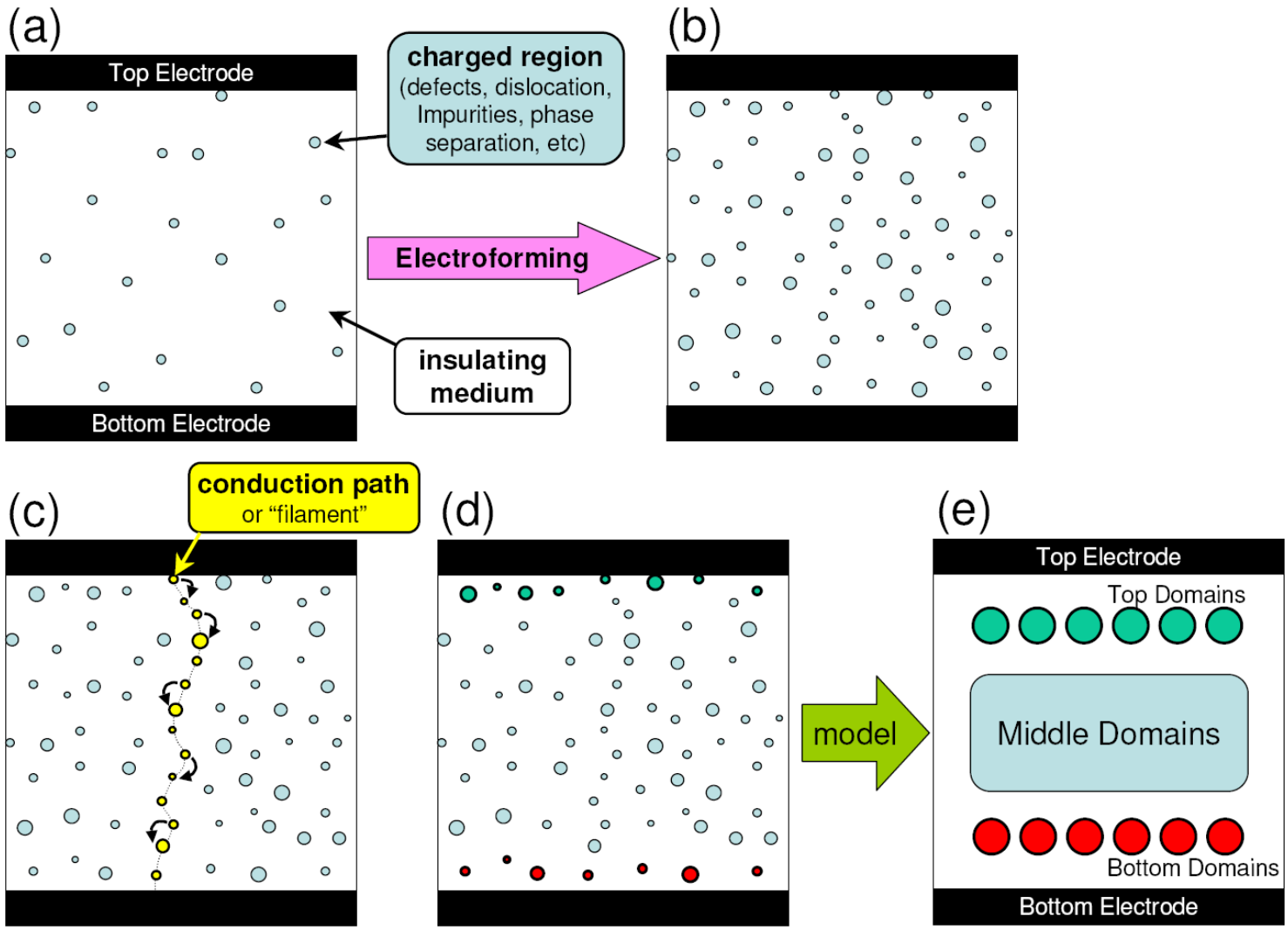


TM transport evidence for channel formation

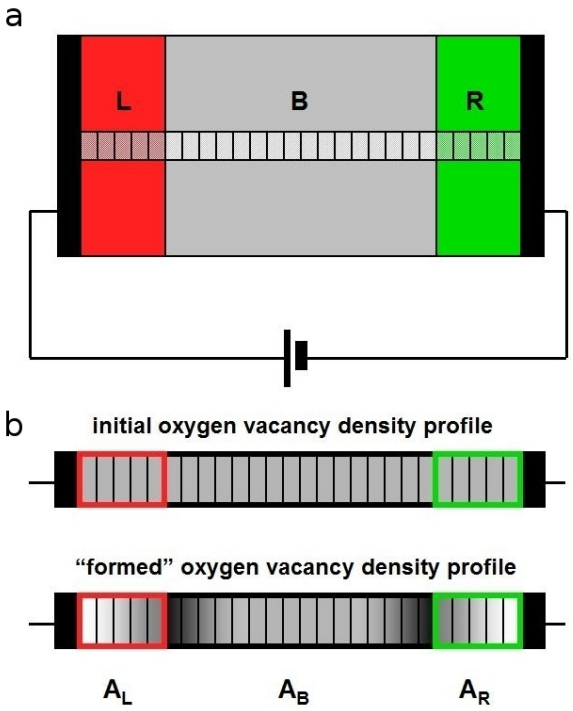


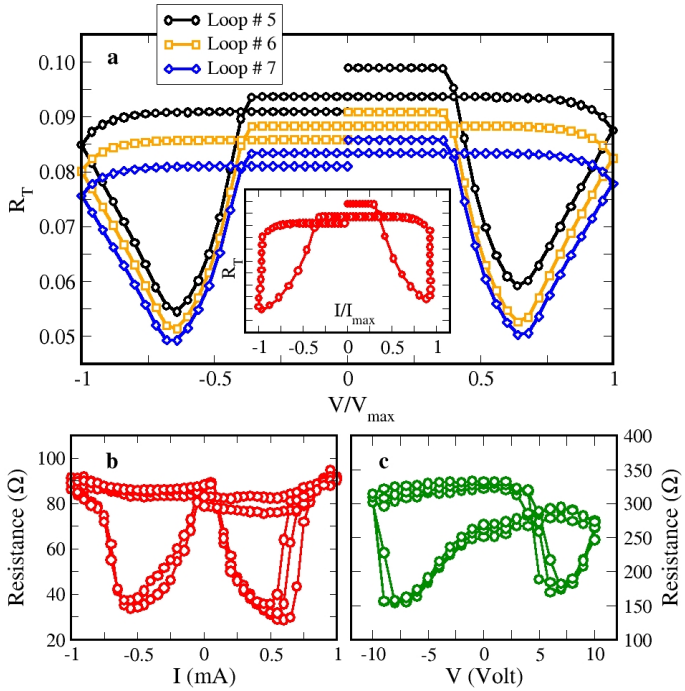
Chae (2008)

Electronic Channel Formation model

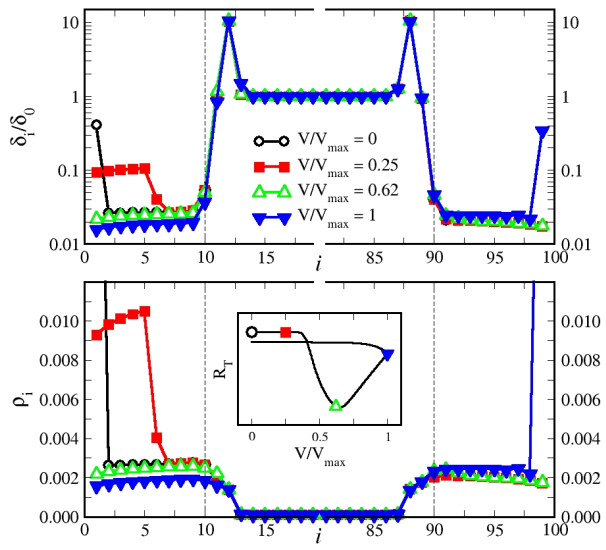


Channel Model of
Rozenberg, Sanchez, Levy et al





Channel Model of Rozenberg, Sanchez, Levy et al

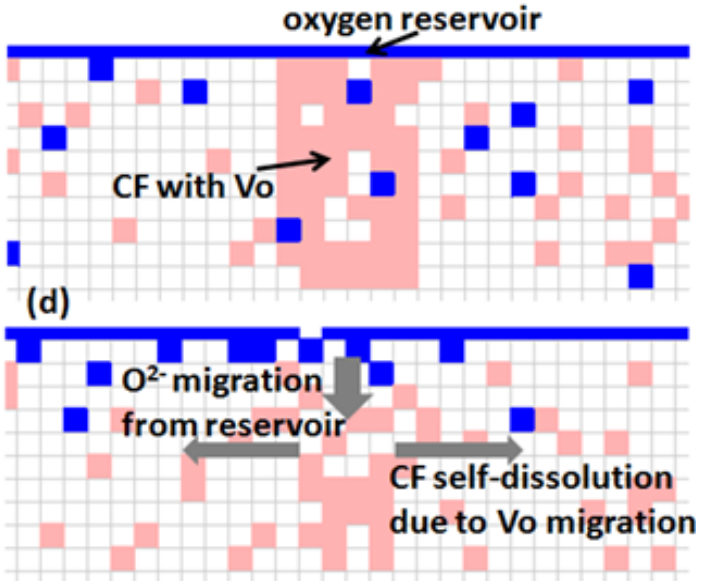


	Rozenberg et al (2010)
Vacancies	increase resistance
Boundary layer (“A”)	present
Electron dynamics	implicit
Pile-up next to interface	vacancies
Cause of switching	vacancy bump inside interface moves from next to electrode into bulk

Metallic conduction: not intended for binary oxide systems

Channel lateral dynamics model of Kittl group

HfO system

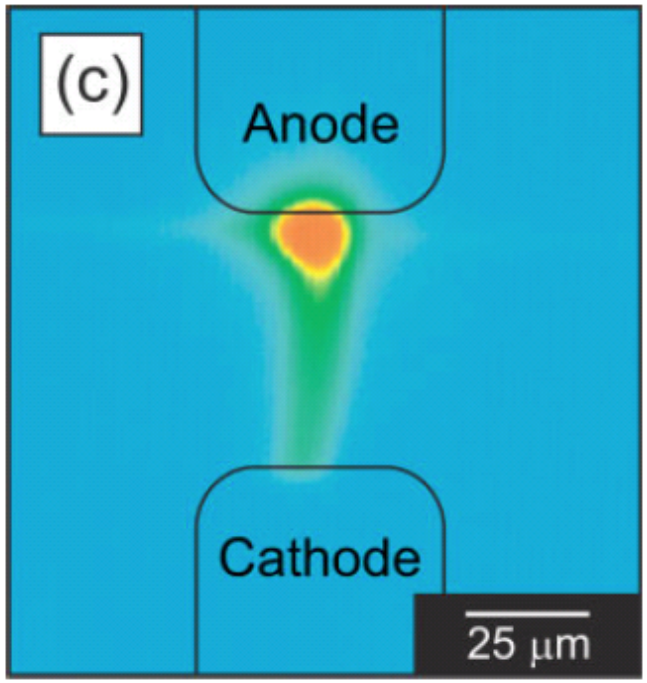


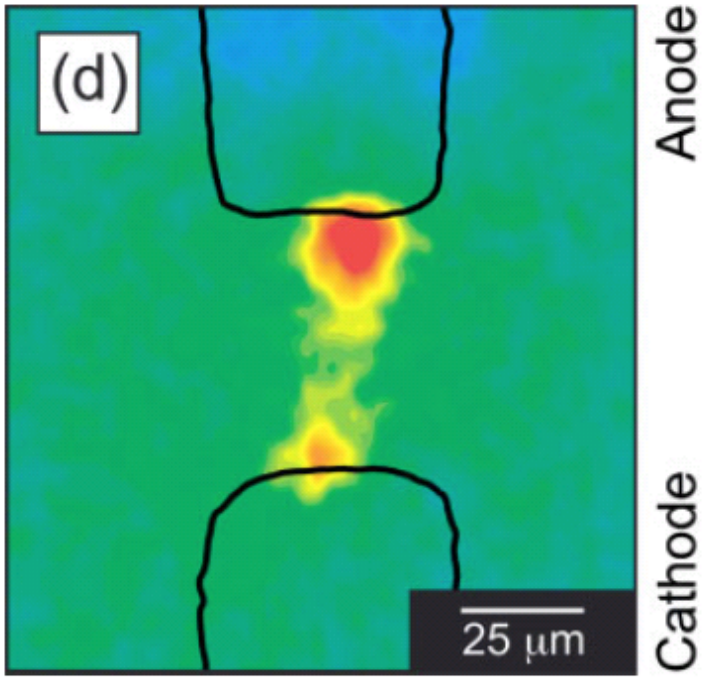
	Kittl et al (2012)
Vacancies	increase conductance TAT
Boundary layer (“A”)	absent
Electron dynamics	TAT network, no feedback to vacancies
Pile-up next to interface	none
Cause of switching	conducting channel disintegrates/reassembles

Limited utility:

- for narrow devices
- in light of direct imaging

Switching by Front Dynamics





Thermal image

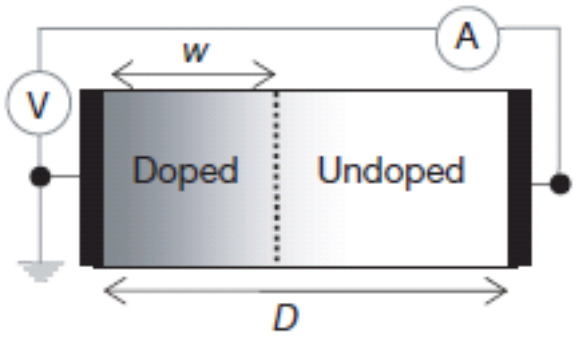
O vacancy density from
X-ray fluorescence

Switching may involve
sample-wide front/wall moving

Janousch et al, (2006)

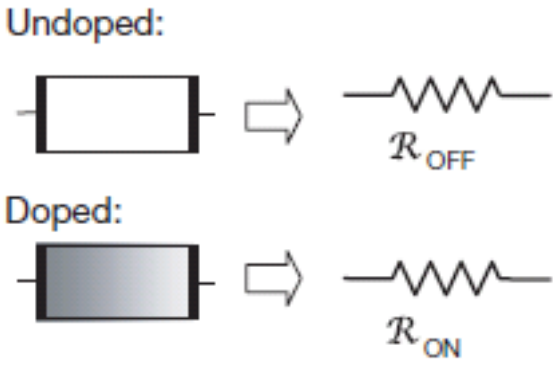
HP Modeling: Pickett et al.

Switching = Movement of wall of O vacancy-rich region



Phenomenology: variable w, domain wall location between high R and low R region moves

Double exponential dynamics is introduced to reproduce data, lacking clear motivation:



$$\dot{w} = f_{\text{off}} \sinh\left(\frac{i}{i_{\text{off}}}\right) \exp\left[-\exp\left(\frac{w - a_{\text{off}}}{w_c} - \frac{|i|}{b}\right) - \frac{w}{w_c}\right]$$

Experimental evidence for Front model

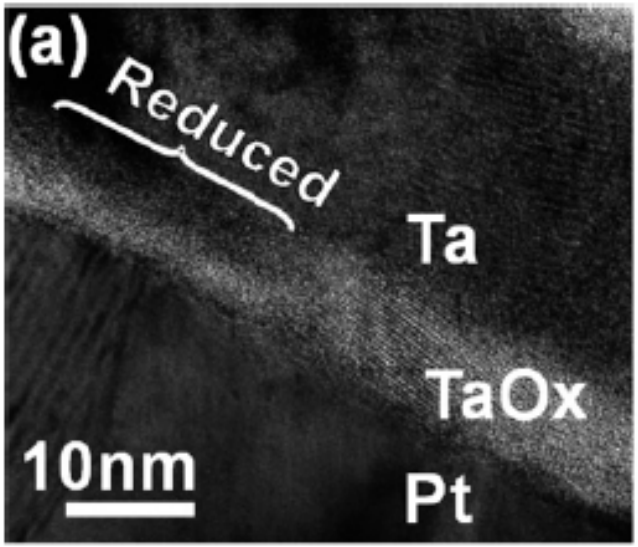
1. Direct imaging

Shows dynamics of front explicitly

2. HP group analyzed scaling of I-V with lateral width of contact: front/channel in TiO: x~50-100nm

3. In devices of decreasing size: do front and channel pictures converge? Device lateral size can get in the same range of ~30-50nm

However, in small devices the channels can get smaller as well, only few nm, still distinct from front of size, comparable to system size



HP Modeling: Strukov et al.

Vacancies and electrons couple
only through Coulomb interaction:

1. Both of them are sources of the potential ϕ

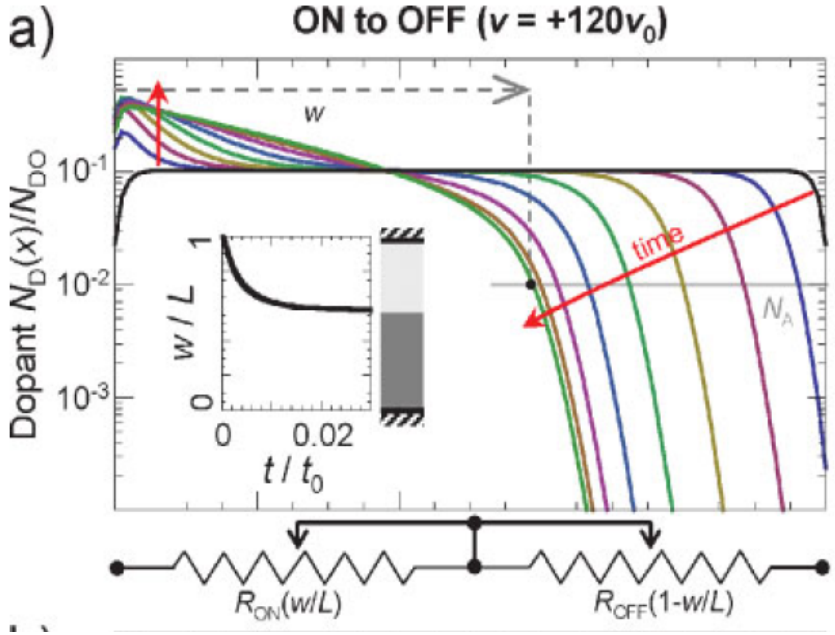
$$-\varepsilon\varepsilon_0\Delta\varphi(x) = e(p(x) - n(x) + f_{\mathrm{D}}(x)N_{\mathrm{D}}(x) - f_{\mathrm{A}}(x)N_{\mathrm{A}})$$

2. The dynamics of both of them is driven by ϕ

$$J_{\mathrm{ION}}(x) = -eD_{\mathrm{i}}\nabla N_{\mathrm{D}}(x) - eN_{\mathrm{D}}(x)u_{\mathrm{i}}\nabla\varphi(x)$$

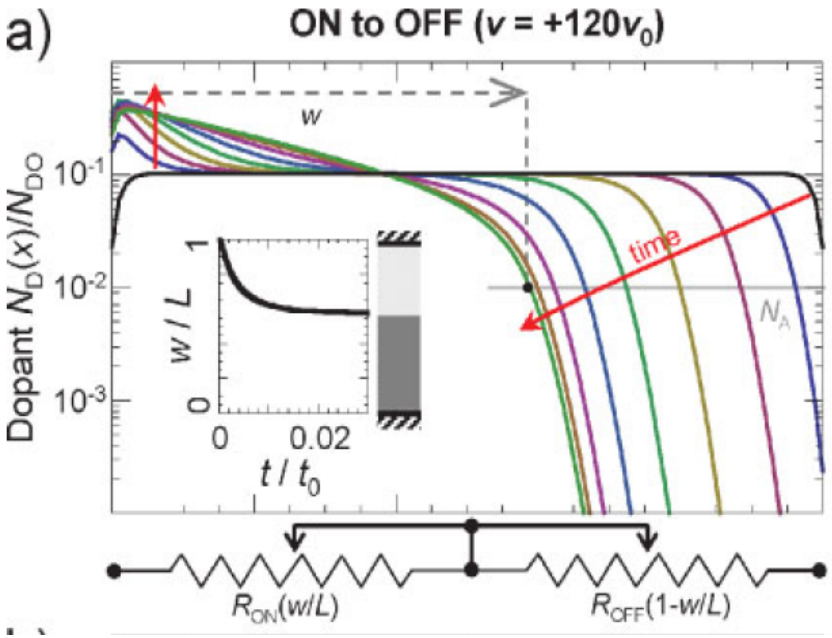
$$\nabla\cdot(-en(x)\mu_{\mathrm{n}}\nabla\varphi_{\mathrm{n}}(x)) = 0$$

3. Electron mobility is not effected by vacancies

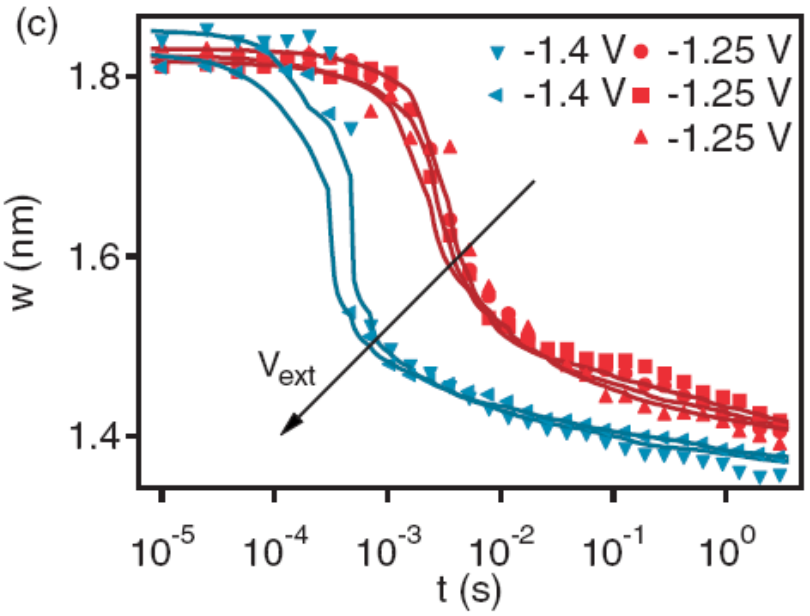


HP Modeling: Strukov et al.

HP simulations



HP measurement of ON/OFF width



4. Simulation: w(ON)=0
Self arrest: NO

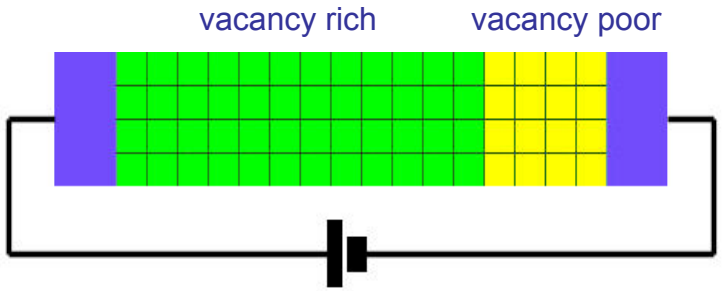
Expt: w(ON)=1.4nm
YES

So, we decided to check out the vacancies

by checking in the Bates Motel

What could possibly go wrong?

Our Simulations



Motivated by $TiO_2/TiO_{(2-x)}$ layered binary oxide structures

Pre-formed system, no additional formation is needed: the front separating high and low vacancy density regions is prepared

Can be equally appropriate for a formed channel

Thickness of insulating TiO_2 layer is about 2nm or less

(1) calculate the full energy of the electron system, driven by an applied voltage

(2) move the electrons with Monte-Carlo dynamics until a steady current state is established (1-100 million MC steps)

(3) move the vacancies according to a Monte-Carlo dynamics using the electron configuration related to steady current

(4) recalculate the electronic current

(5) repeat the vacancy & electron updates until both reach steady state, then record the current, corresponding to the applied voltage

(6) change the voltage incrementally and repeat steps (1)-(5)

Energetics

Electron energy

$$E_i = C^s\left(n_i - N_{\text{avg}}\right)^2 + \frac{C^c}{2}\sum_{k\neq i}\frac{(n_k - N_{\text{avg}})(n_i - N_{\text{avg}})}{d_{ik}} + C^p V_i n_i + C^{\text{d}} L_{\text{i}} n_{\text{i}}$$

grain charging energy

Coulomb interaction

potential due to external voltage

disordered grain energy

Electrodes

Electron reservoirs, separated from bulk with a work function W

Dynamics

Electron dynamics

$\delta_j < \delta_0$: tunneling, in boundary layer

$p(i \rightarrow j) = p_0 \exp(-(V_0 + \Delta E_{ij} - const.\delta_j))\ \Theta(-\Delta E_{ij})$

Tunneling barrier lowered by energy gradient and vacancy density

$\delta_j > \delta_0$: metallic, in bulk

$p(i \rightarrow j) = p_0\ \Theta(-\Delta E_{ij})$

Vacancy dynamics

$\delta\rho(i \rightarrow j) = \mu \exp(-(V_{00} - \Delta V_{ij})/E_0)$

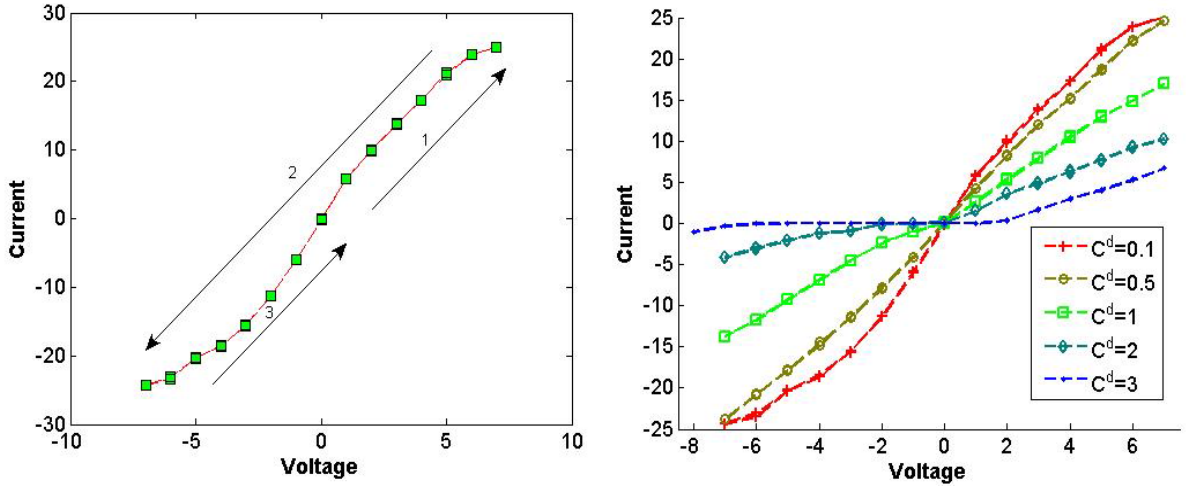
Mott-Guerney type

Results: No mobile vacancies

Onset/switching could have been observed without vacancy dynamics:

(a) Anderson localization
(b) Interacting localization (Coulomb Glass)
(c) Some kind of depinning
(d) Mott transition

Instead: no hysteresis, no switching



Mobile vacancies are essential for switching phenomena

Results: Mobile vacancies

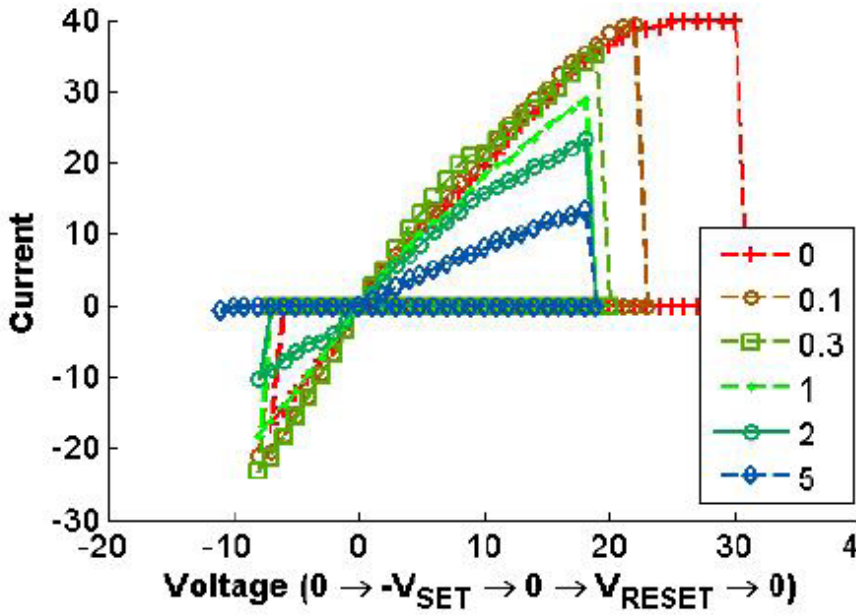
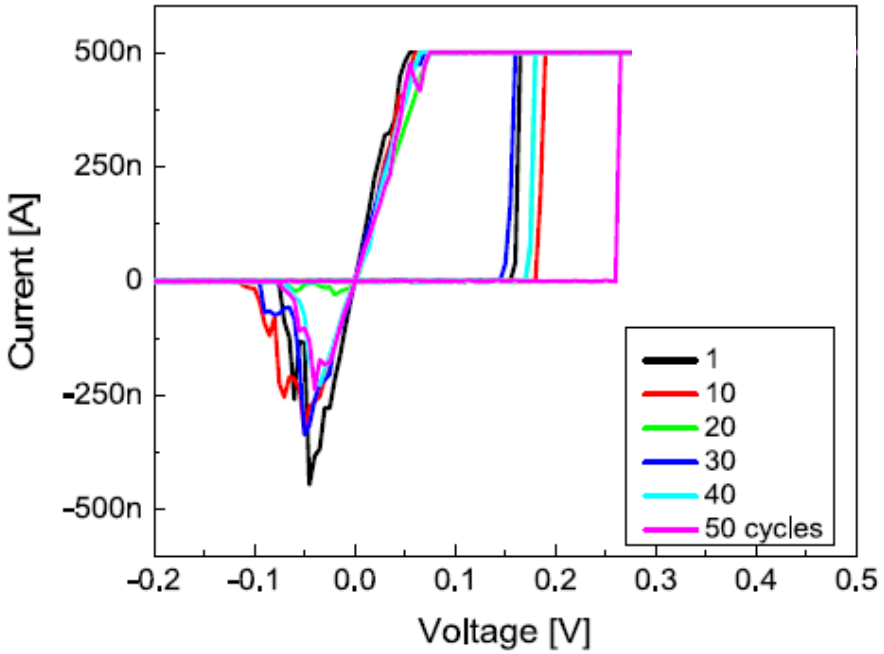


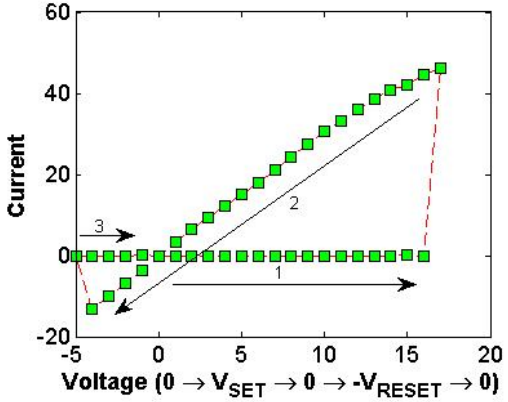
FIG. 6. IV curves with varying disorders

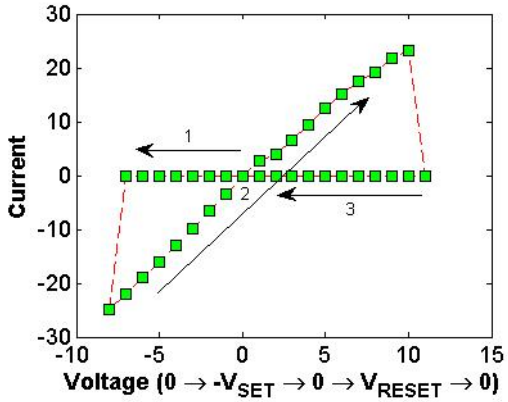


Simulation

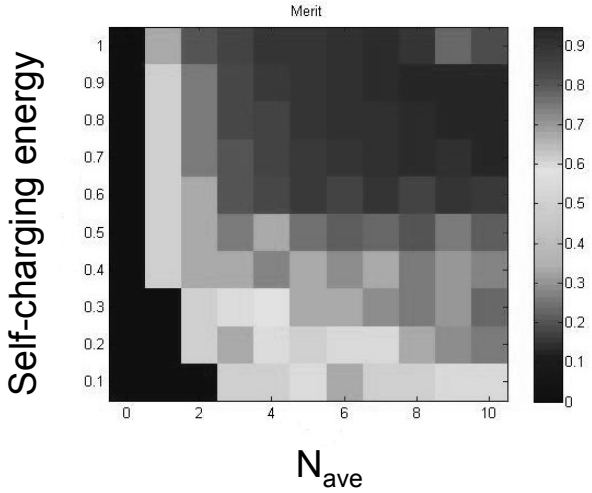
WO3/PT cell

Results: Parameter space exploration



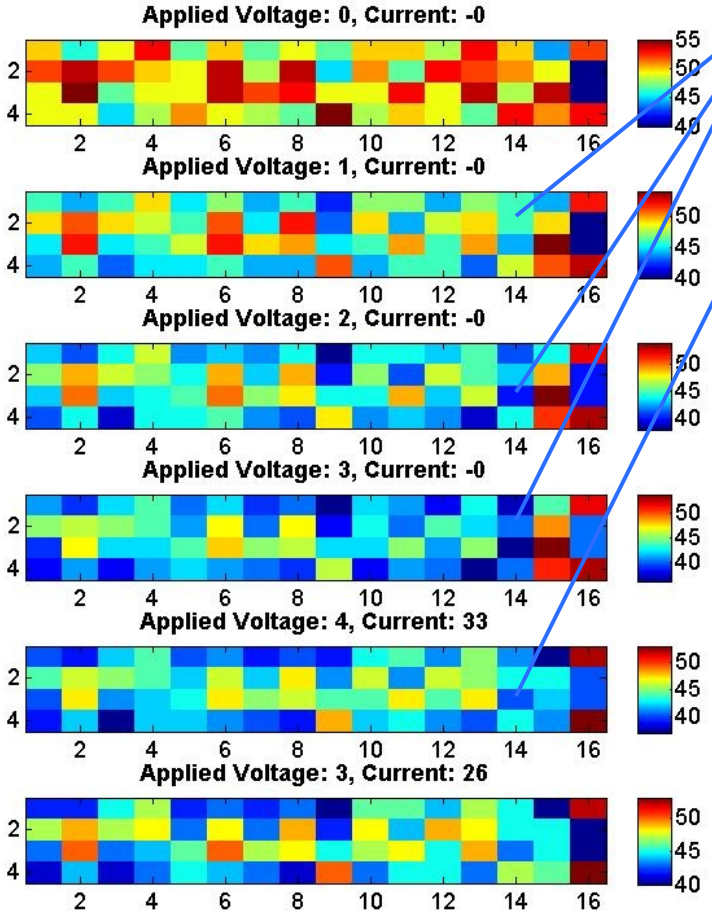


Different types of I-V curves



R_{on}/R_{off} ratio as a function of parameters

Switching Mechanism

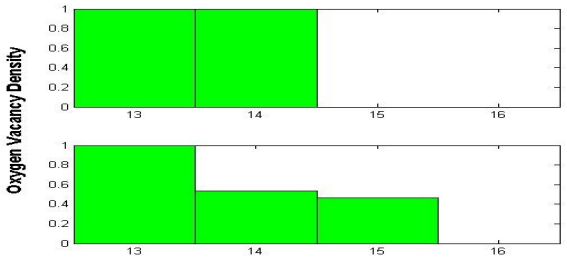


1. Electron depletion layer forms next to front, enhances total electric field felt by front

2. Total field depins front towards electrode

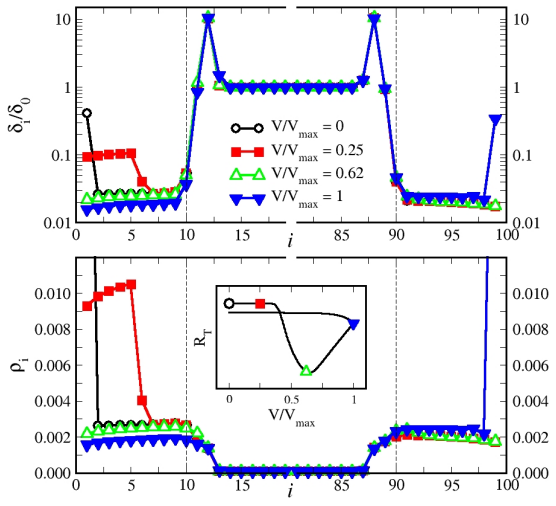
3. Insulating layer gets thinner: electron conduction switches ON, flushing out electron depletion layer

4. This reduces field, arrests further front motion



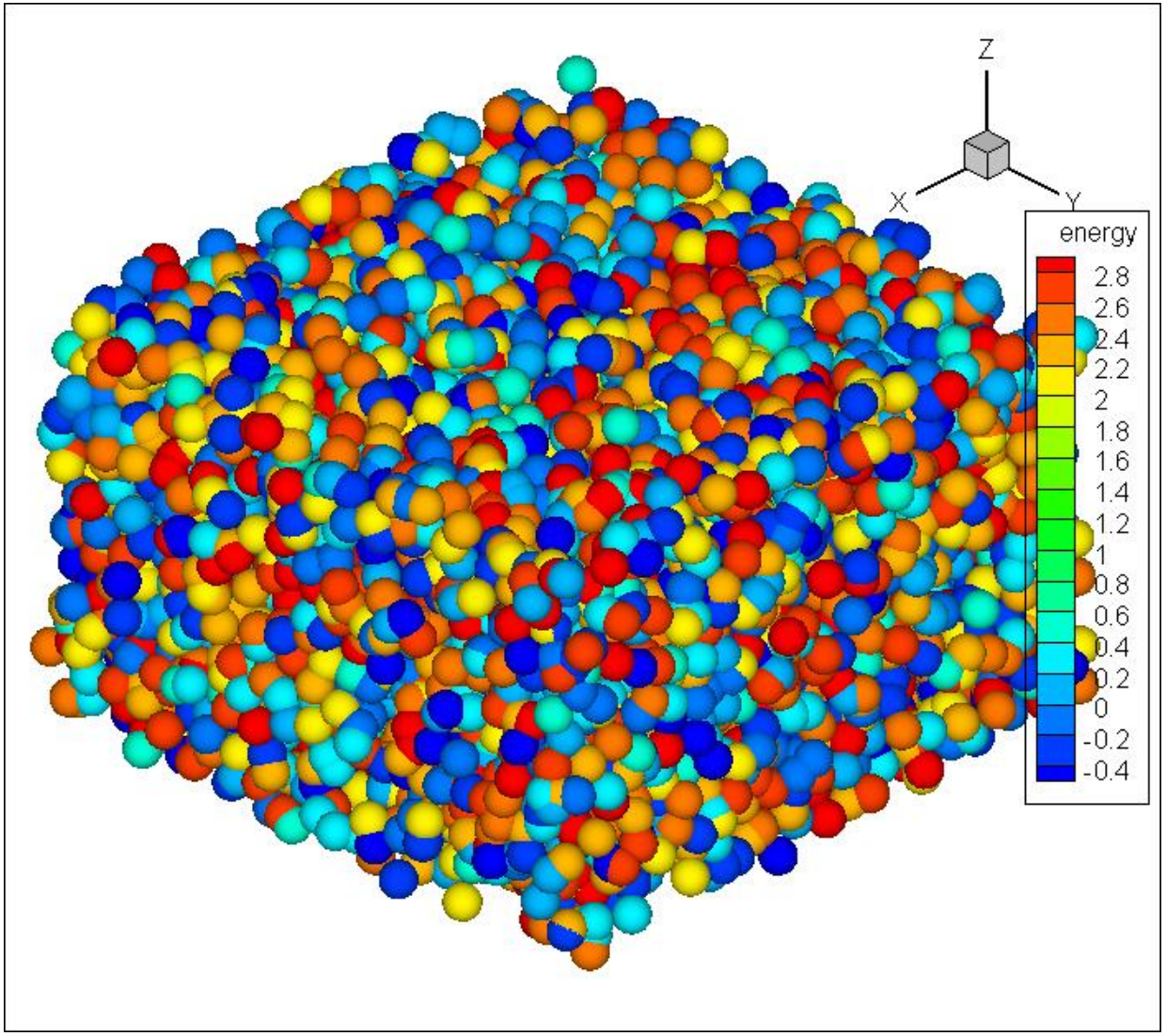
Comparison to other work

Rozenberg, Sanchez, Levy et al



	Rozenberg et al	Our work
Vacancies	increase resistance	increase conductance
Boundary layer (“A”)	present	defined by low vacancy concentration: dynamic
Electron dynamics	implicit	explicit
Pile-up next to interface	vacancies	electrons/holes
Cause of switching	vacancy bump inside interface moves from next to electrode into bulk	wall of high vacancy concentration moves driven by field with contribution from hole build-up

Our Model – Next Generation



- 3000 atoms
- Random energies
- Coulomb interaction (100,000 grid point)
- Electrons jump by master eq.

Summary

1. Reviewed some existing simulations, their applicability and limits

2. We studied the “coupled mobile electrons-mobile vacancies” model with explicit electron dynamics, having long range interactions and mobile vacancies

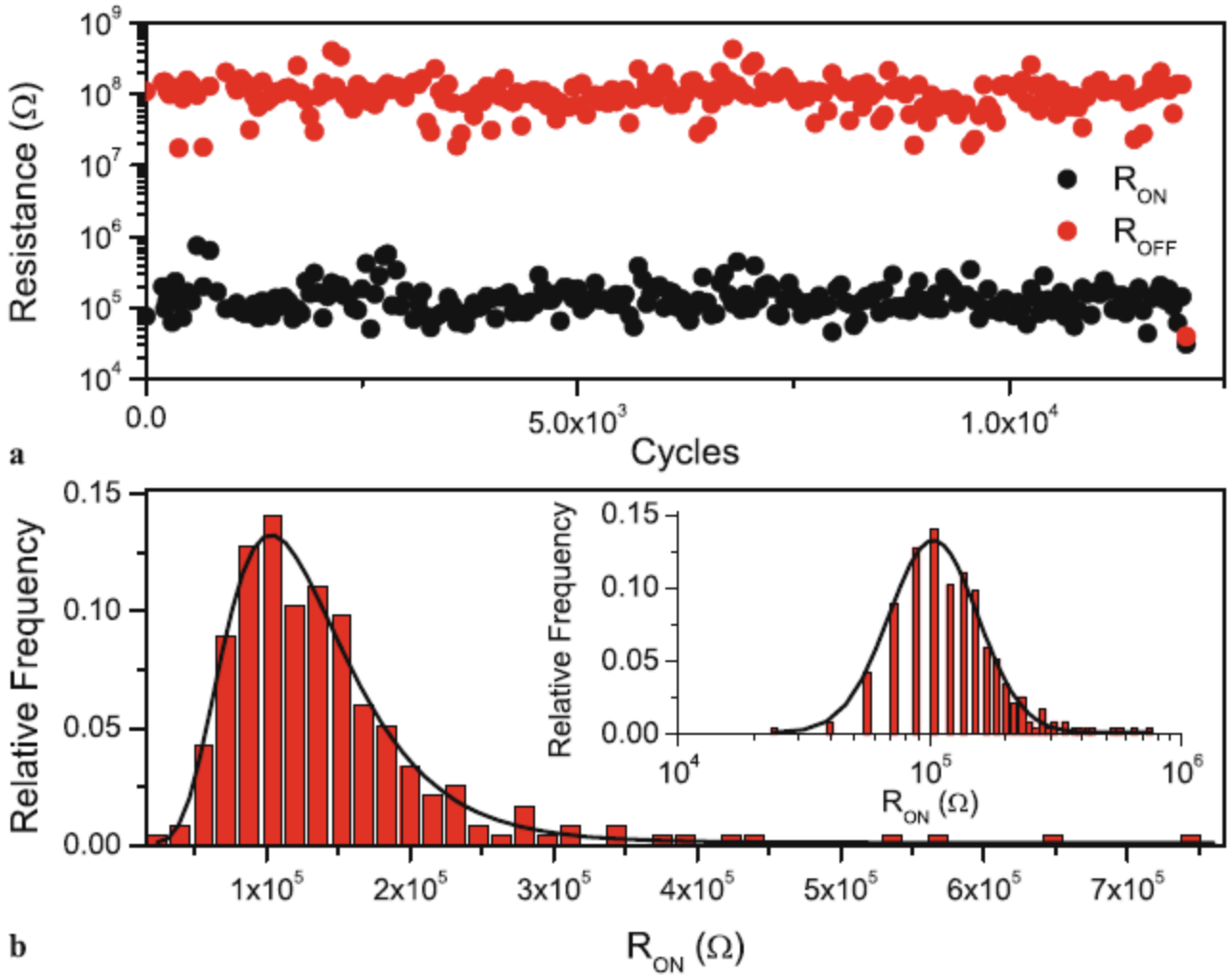
3. Switching requires mobility of vacancies

4. With mobile vacancies model reproduces experiments promisingly

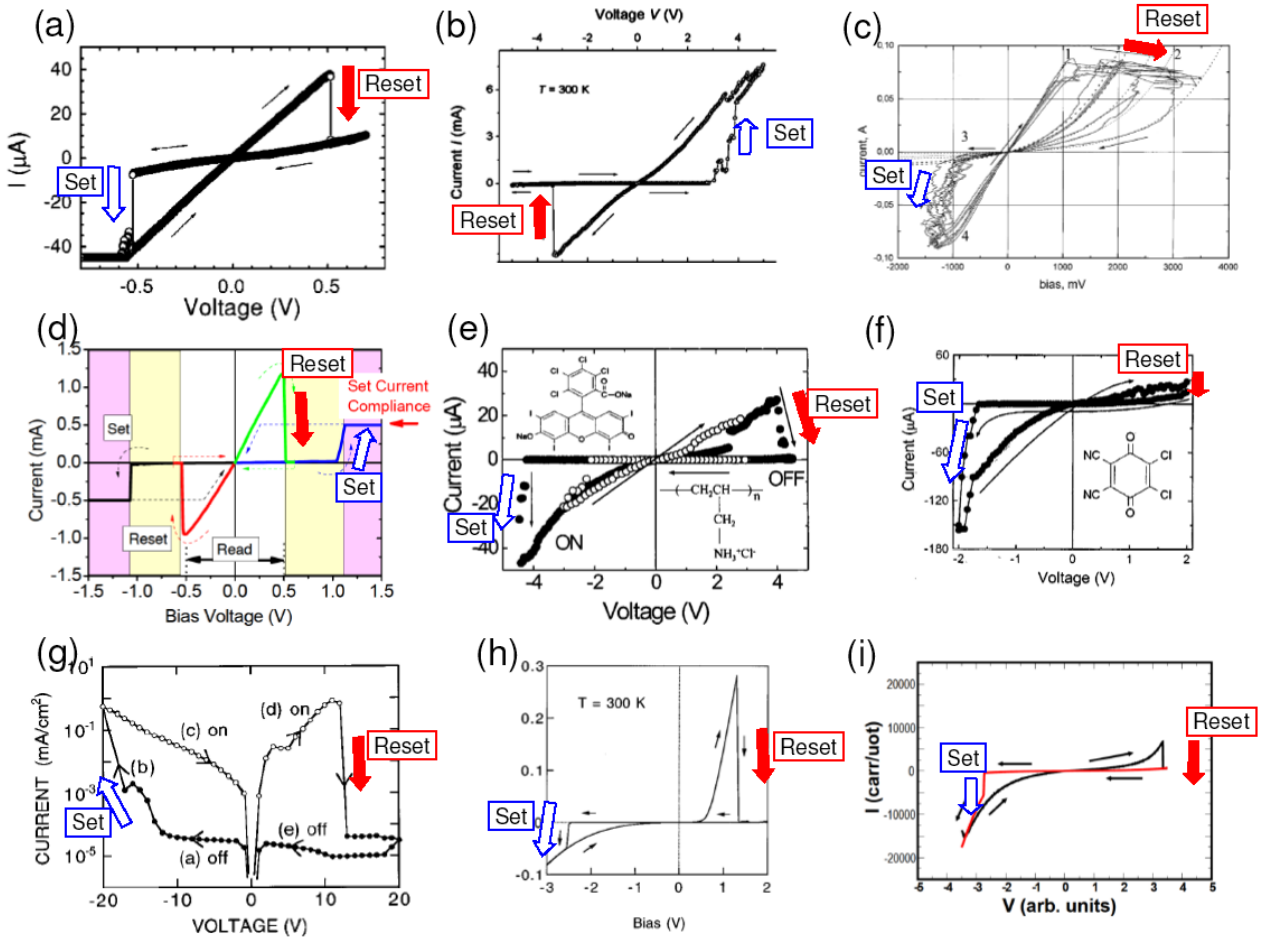
5. Switching is driven by hole pile-up, flushed out with ON switching

6. Switching is - self-arresting
   - sharp onset without assumption of double exponential w(i)
   - boundary layer is self-defined

Broad Distribution of Switching Parameters



Memristors everywhere



(a) Au/Ti/SrZr0.998Cr0.002O3/SrRuO3; (b) Ag/CeO2/La0.67Ca0.33MnO3;
(c) Ag/Bi2Sr2CaCu2O8+y heterojunction; (d) Pt/NiO/Pt; (e) Al/“Rose Bengal”/ITO;
(f) Al/DDQ/ITO; (g) Au/porus Si/p-type Si; (h) Double barrier AlAs/GaAs heterostructure.

Hysteretic/switching resistors: Bednorz strikes gold again

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Reproducible switching effect in thin oxide films for memory applications

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$SrTiO_3$, $SrZrO_3$