Multiscale Modeling of Memristor Devices for Novel Memory and Logic Architectures

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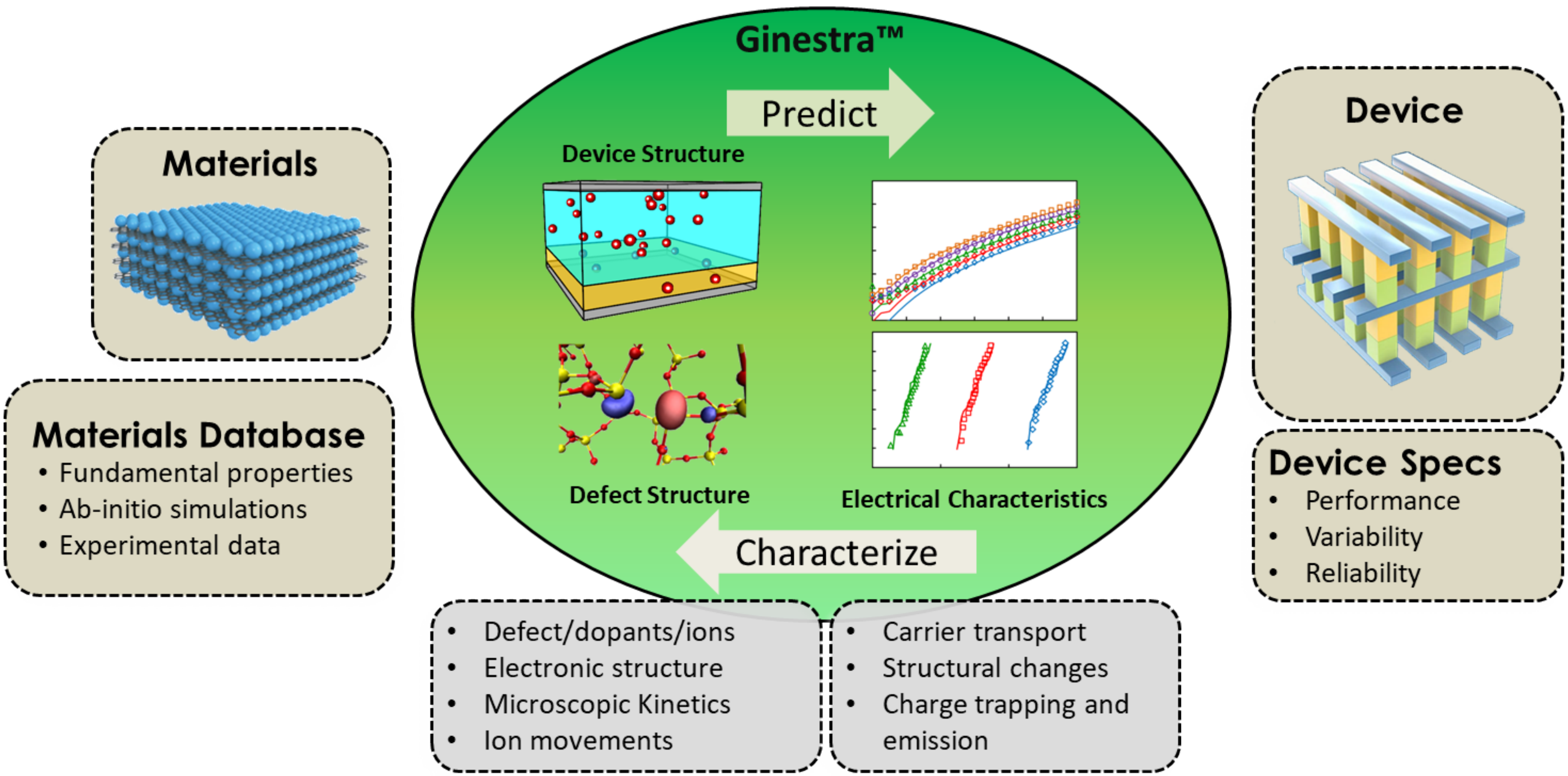
Outline

- Multiscale modeling platform
  - Physics
- Simulation results
  - HfO_x RRAM for memories
  - RRAM devices for neuromorphic
- Conclusions

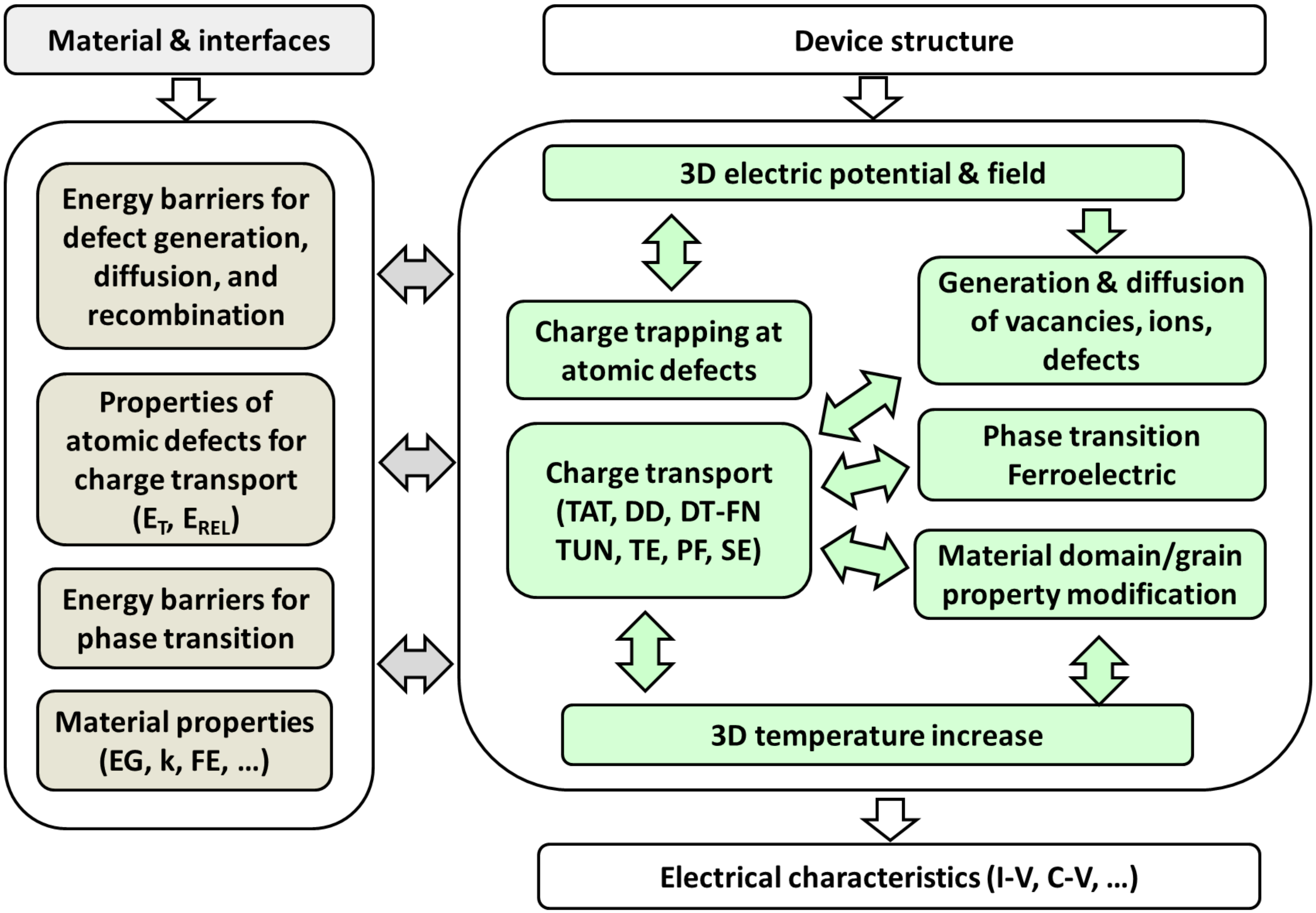
A multiscale modeling platform

- Connects atomic material properties to electrical device characteristics
- Focus on novel materials, charge and ion transport, and structural changes, consistently modeled in a friendly environment
- kMC description to account for variability and reliability



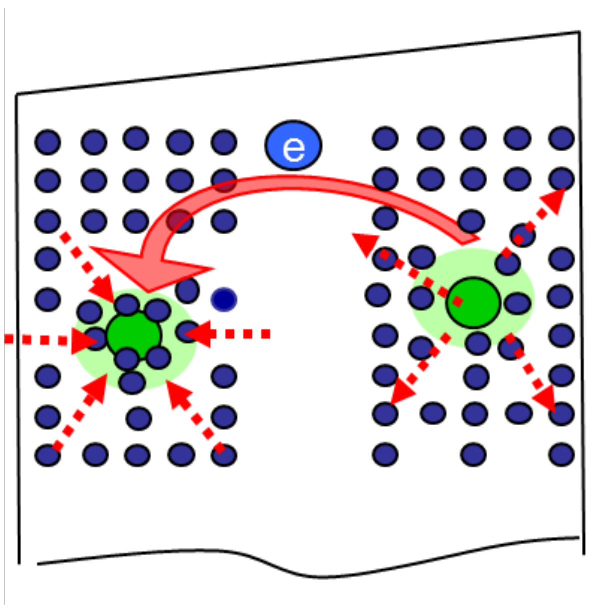
Ginestra™ Physics

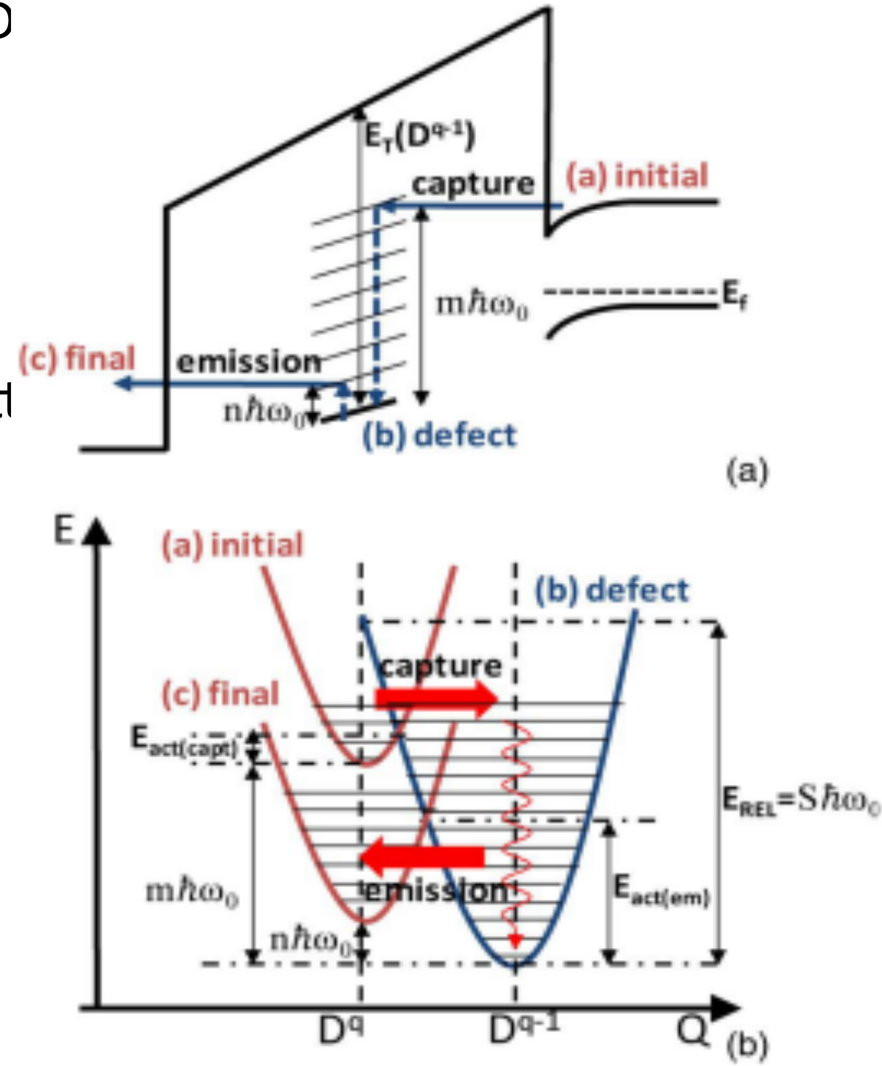
- Novel devices (e.g. memories, neuromorphic computing) need to account for structural material changes, ion/vacancy migration, individual species contribution, ferroelectric effect, phase change, …



Ginestra TAT charge transport models

- Mechanisms: DT and FN tunnel, D Poole-Frenkel, TE, hopping, Trap-Assisted Tunneling (TAT)
- Defects (oxygen vacancies) assist trap-assisted-tunneling (TAT)
- Electron-phonon coupling and lati relaxation included



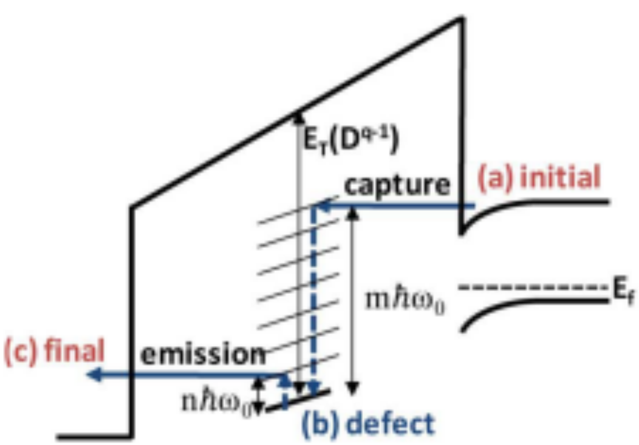


L. Vandelli et al., TED 58, 2011 - L. Larcher, TED 50, 2003

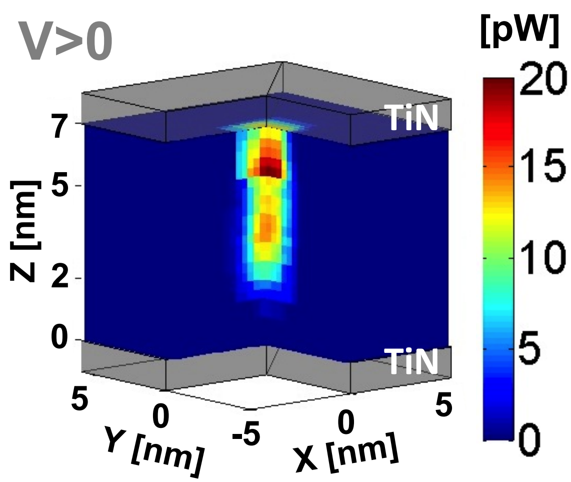
Power dissipation & temperature increase

- 3D power dissipation map calculated from the power released at every defects by TAT electrons and within the conduction/valence band
- 3D temperature map calculated by solving the heat Fourier equation with imposing appropriated boundary conditions

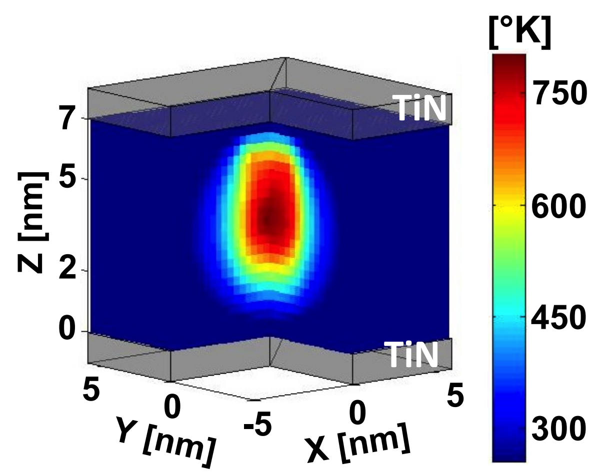
TAT & drift



Power dissipation



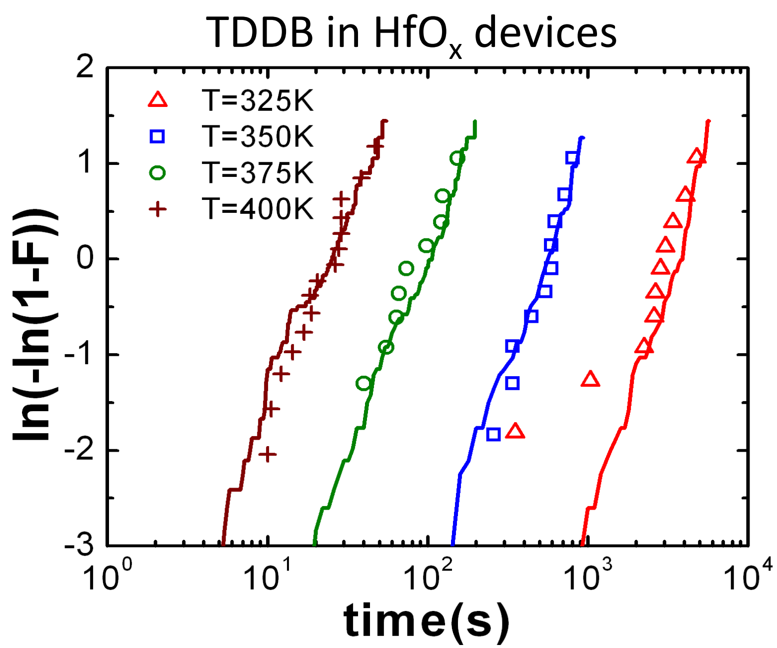
Temperature

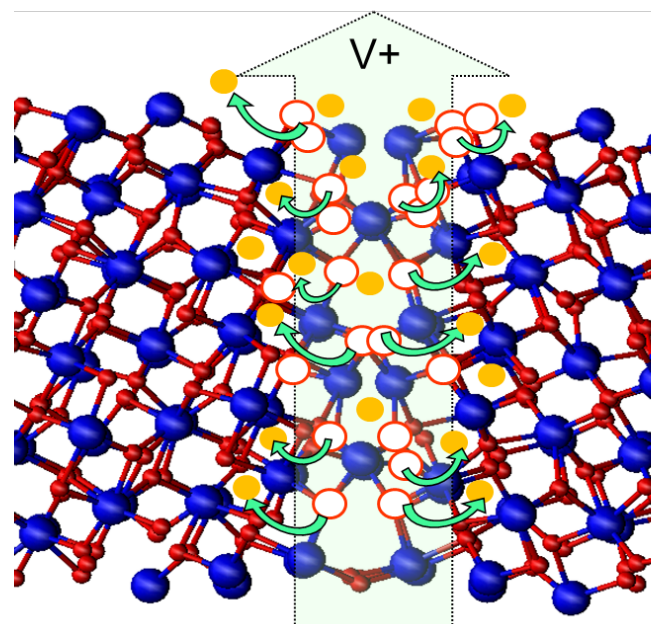


L. Vandelli *et al.*, IMW 2011 - L. Vandelli *et al.*, IEDM 2011 – L. Larcher et el., IEDM 2012

Stress-induced structural material changes

- Generation of vacancies (O) and interstitial ions (O, H, ..) due to atomic bond breakage induced by:
  - Temperature and field driven (thermochemical model)
  - Precursors and defect assisted defect generations
  - Electron injection and impact ionization
  - Material morphology (grain vs GBs)

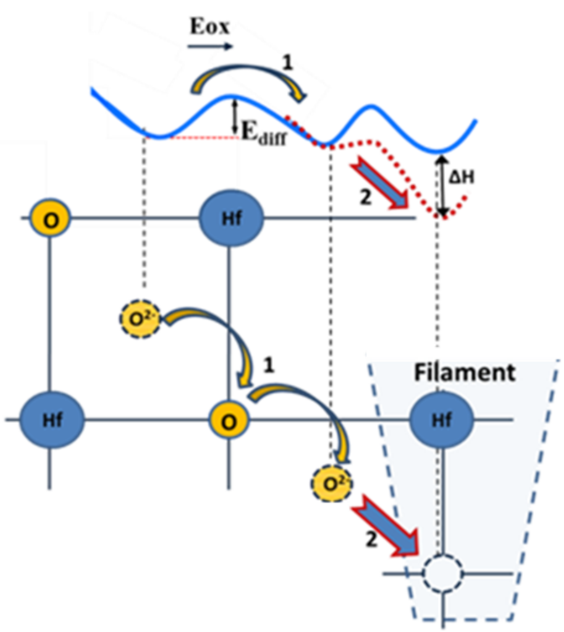


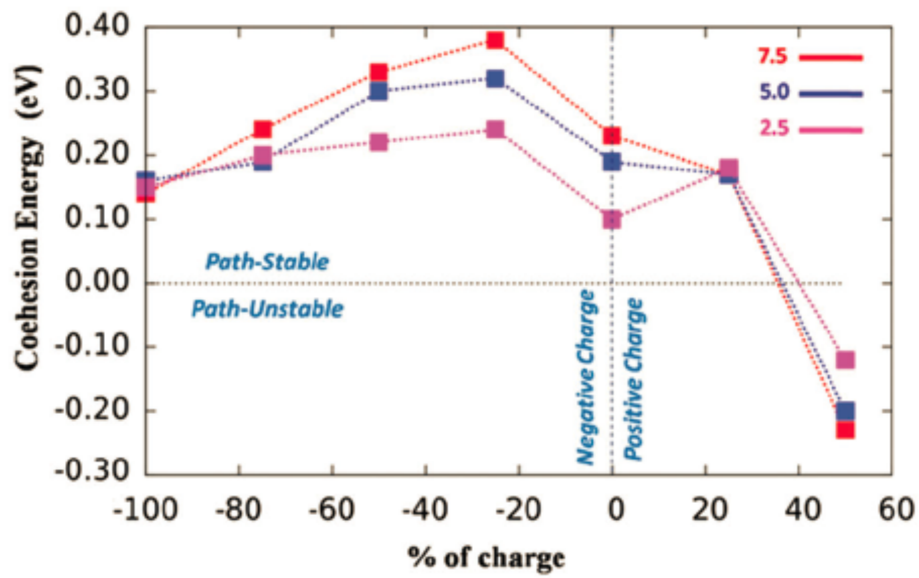


L. Vandelli et al., TED 2013

Stress-induced structural material changes

- Phase changes, including ferroelectric
- Morphology: e.g. GBs and grains
- Diffusion of O ions and vacancies
  - depends on field, temperature, morphology, stoichiometry, cohesion/isolation forces





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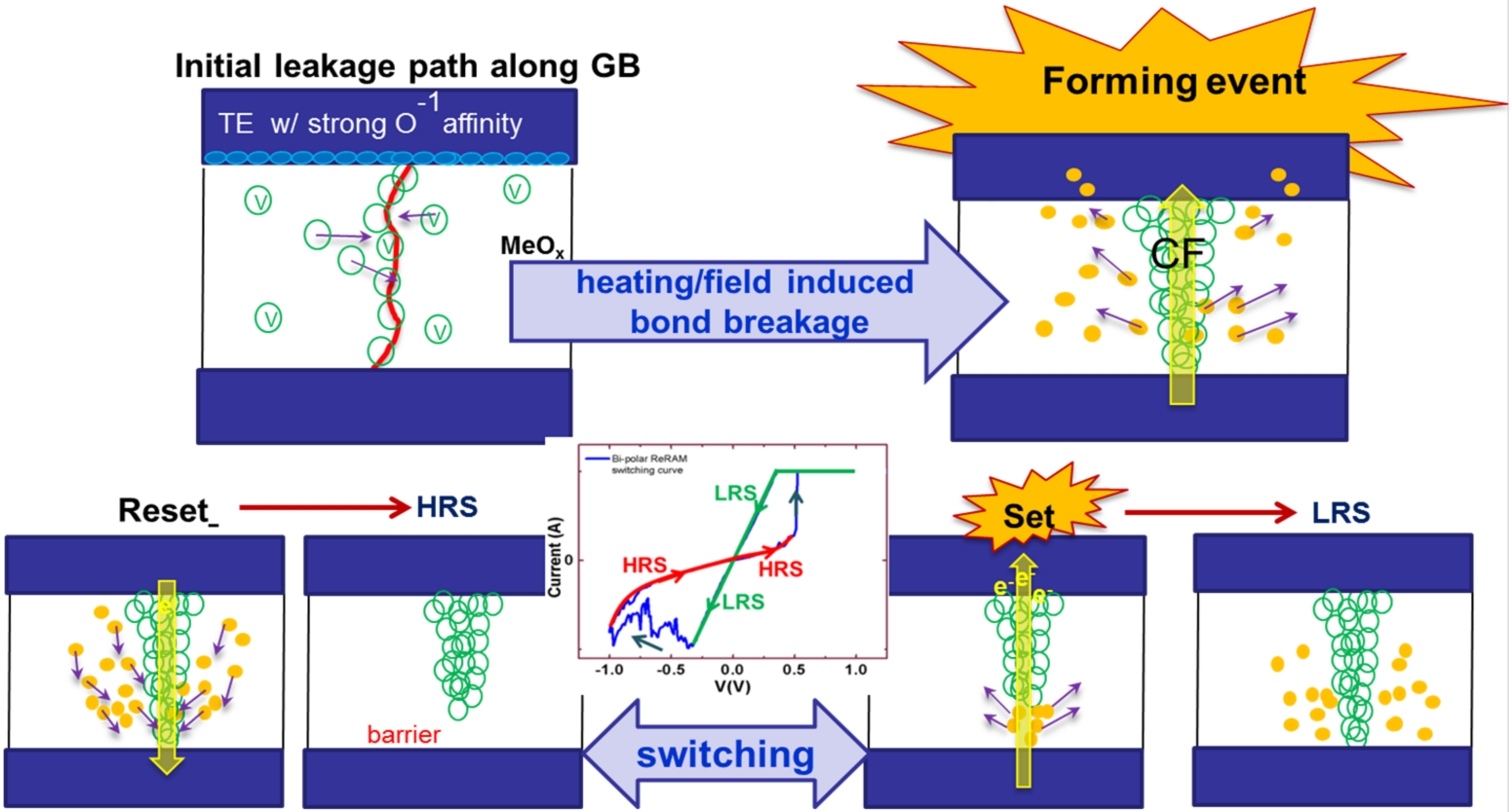
RRAM modeling purposes

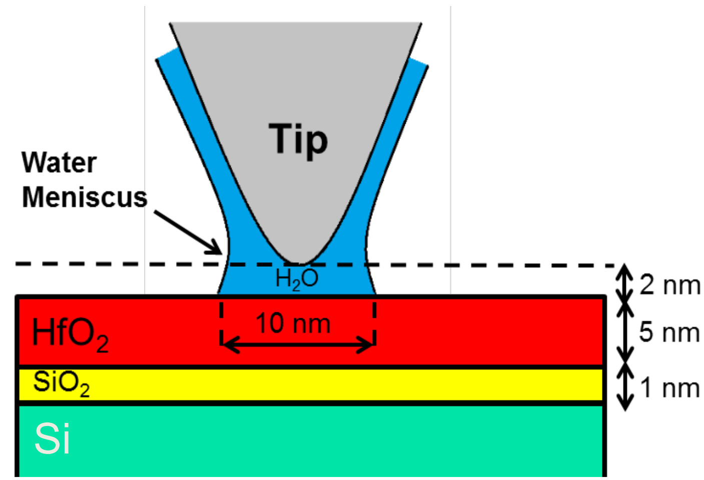
- Goal: connect material properties to the electrical device operations: from **charge transport, to forming, switching and reliability**



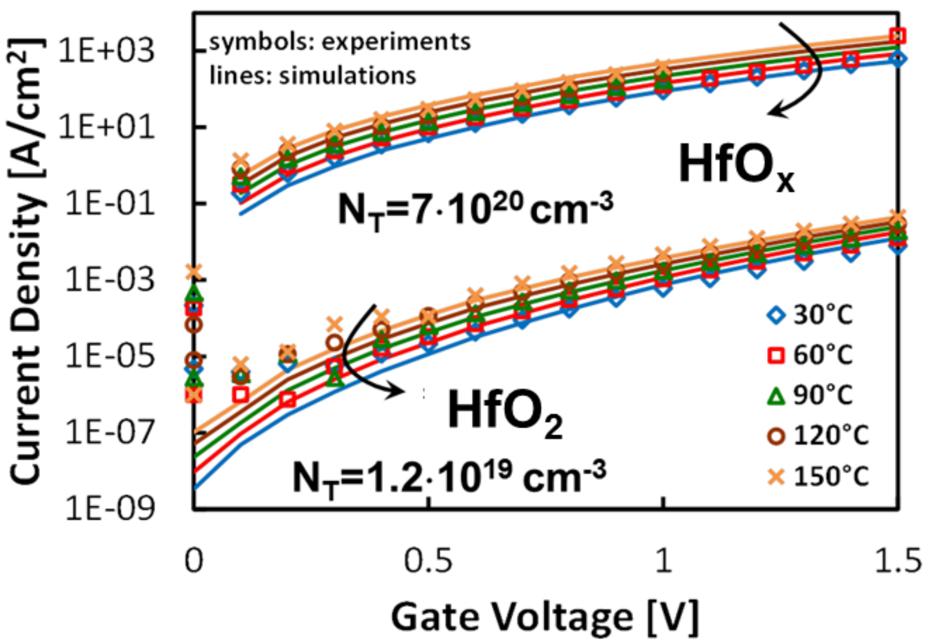
G.Bersuker et al, JAP 2011 – L. Larcher et al., IEDM 2012

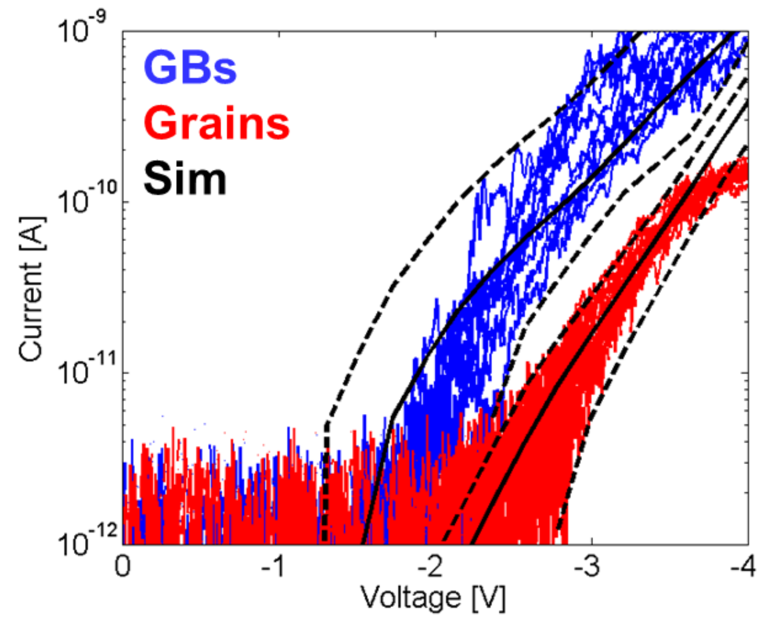
Preforming current simulations - HfO_x

- **TAT current** assisted by O vacancies on grains and (mostly) GBs - CAFM
- T & V dependence across large area MIM cap with different stoichiometry



TiN/Ti/ 5nm HfO_x/TiN

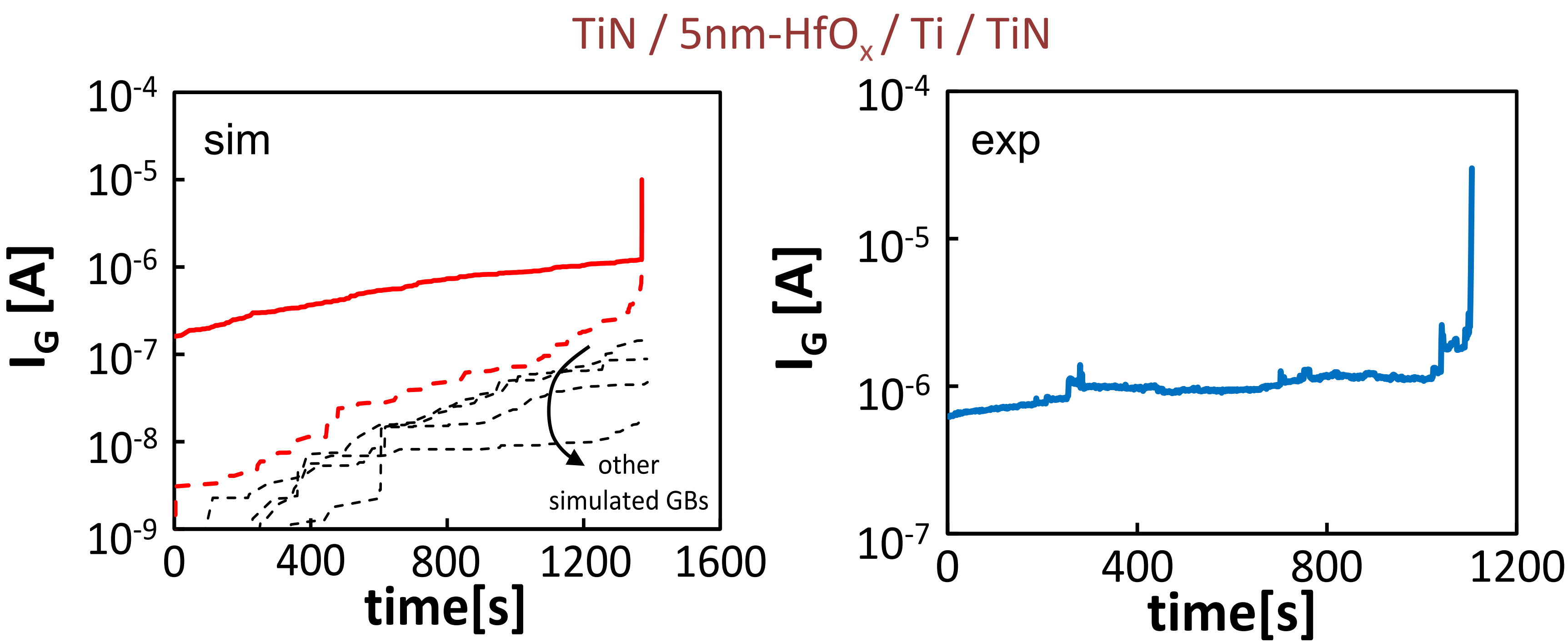




O. Pirrotta et al., JAP 2013 – A. Padovani et a., EDL 2013

HfO_x RRAM forming simulations

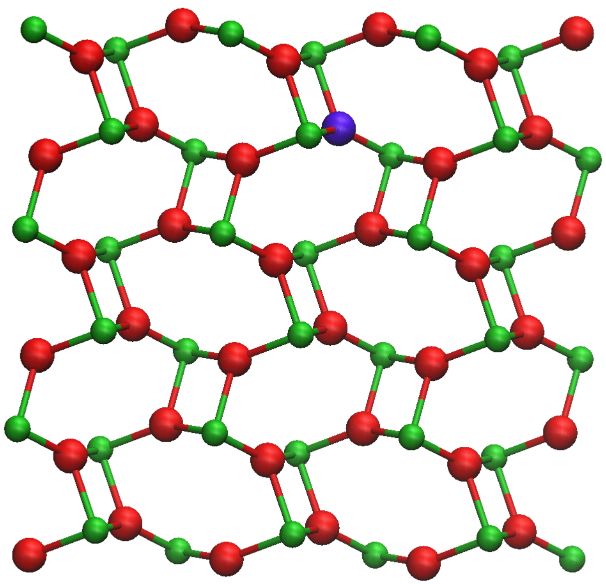
- Multiple grains and GB spots included: abrupt current increase due to a single spot that gets converted into the CF
- Forming involves breakage of Hf-O bonds, and out-diffusion of released O ions: dominant mechanism assisted by electron injection and preexisting vacancies



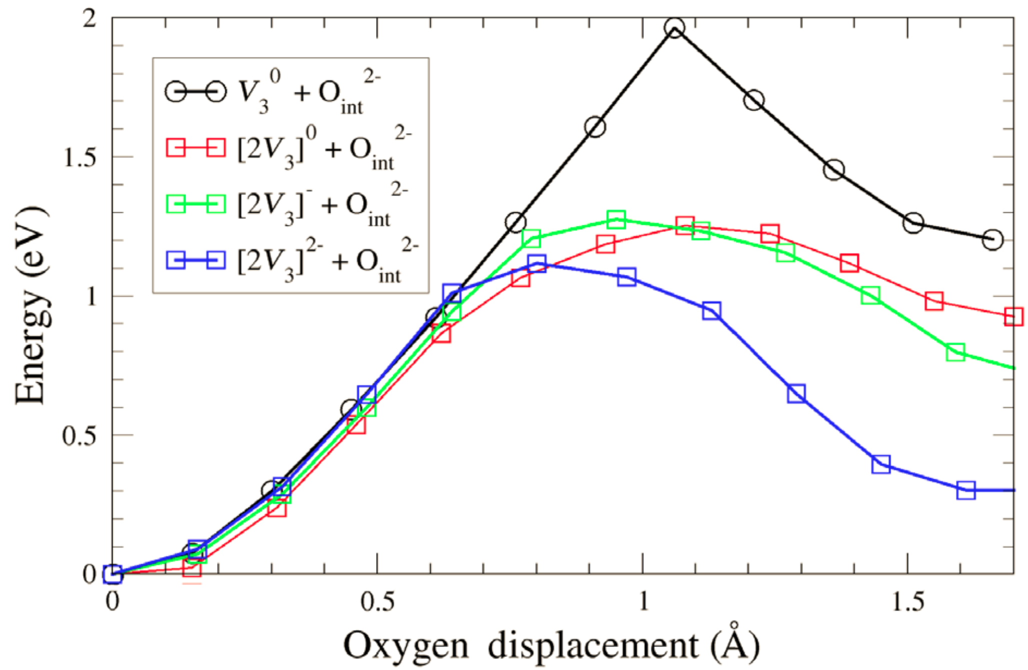
L. Vandelli et al., IEEE-IMW, 2011 - L. Larcher et. al., Journ. on Comp. El., 2013

Generation of O vacancies & ions in HfO_2

- Electron injection & preexisting O vacancies reduce the activation energy for defect creation in their proximity



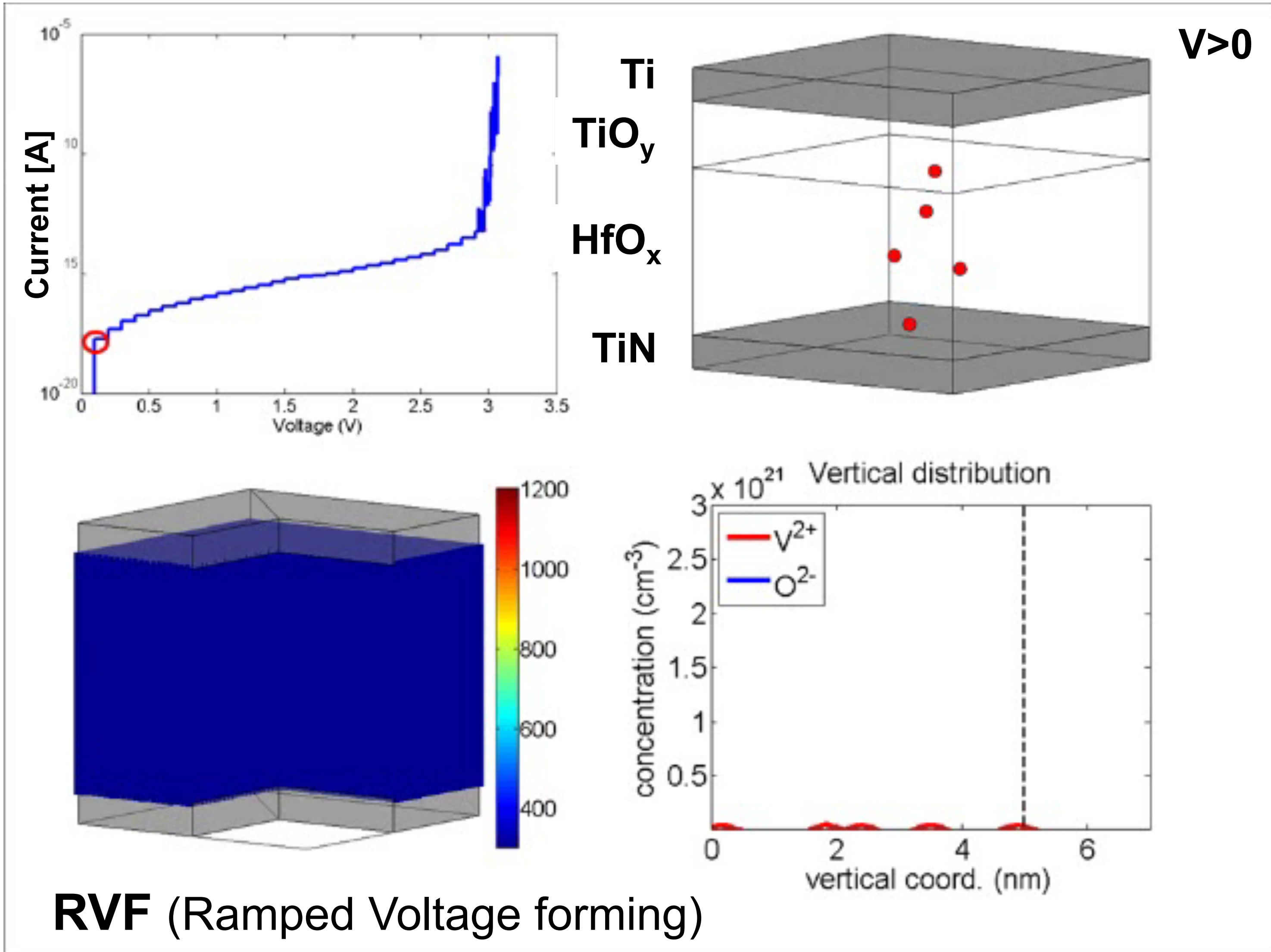
$O_{vac}^{0} + O_{int}^{2-}$ Barrier = 1.96 eV



n_{elec}	Frenkel pair formation energy
0	Unstable (O_{int} and O_{vac} recombine)
1	Unstable (O_{int} and O_{vac} recombine)
2	1.19 eV (O_{int}^{2-}, O_{vac}^{0})

D. Gao et al., PRB 20015; S. R. Bradley et al., Physical Review Applied 4, 064008 (2015)

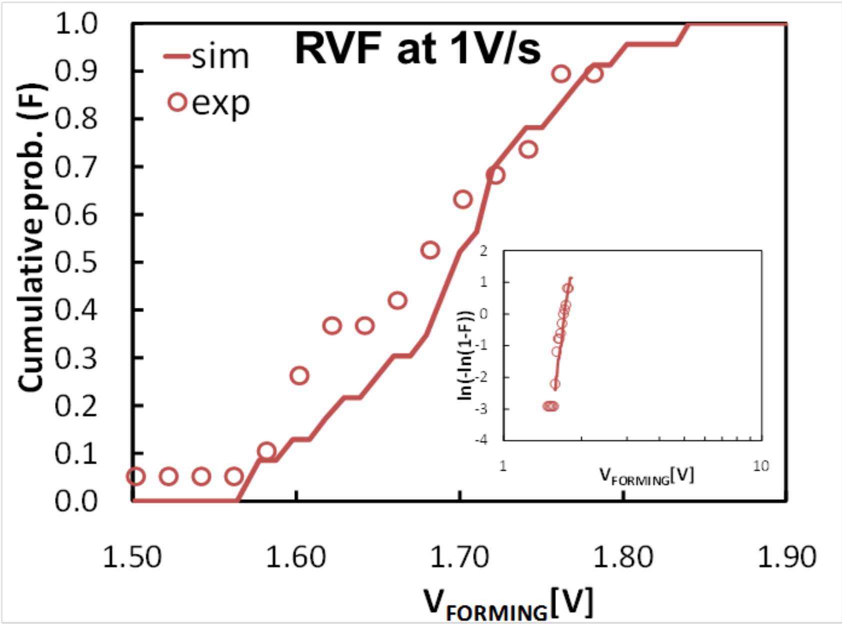
HfO$_x$ RRAM forming kinetics simulations

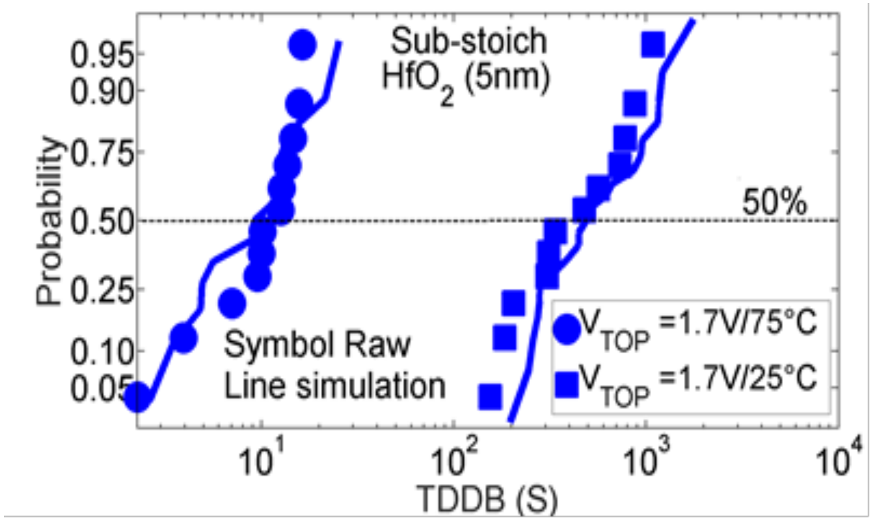


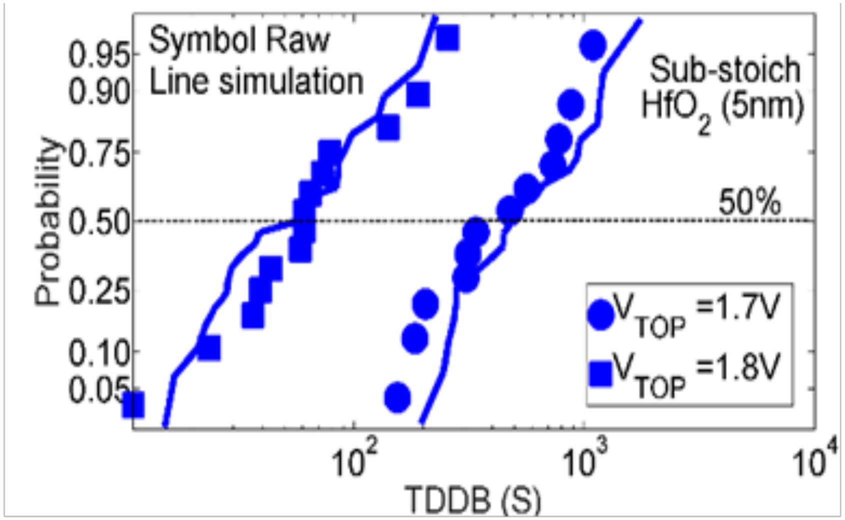
L. Vandelli et al., IEEE-IMW, 2011

HfO_x RRAM forming simulations

- Accurate simulation of forming voltage V_F and TDDB distributions
- Temperature and voltage dependences correctly reproduced

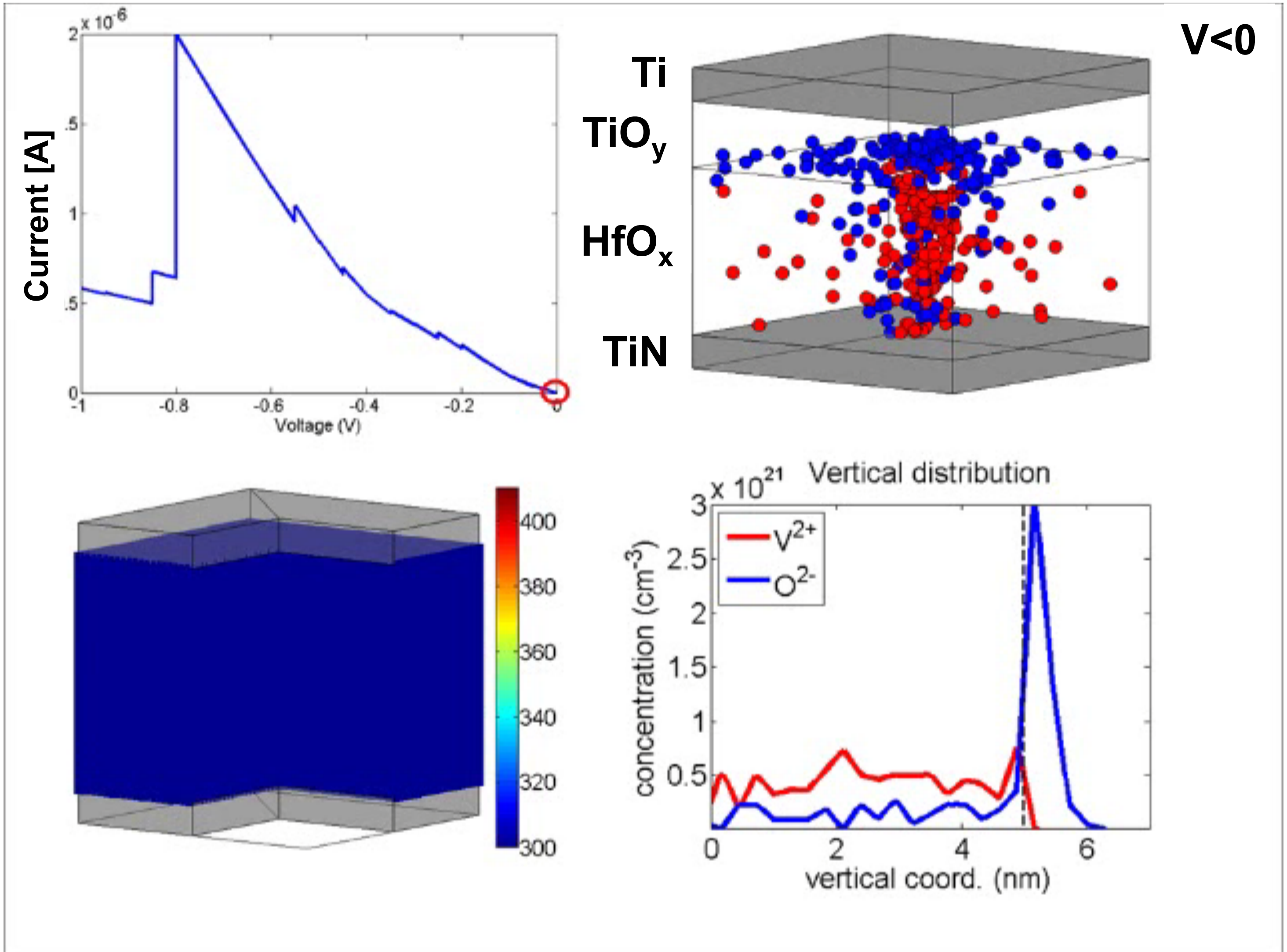






B. Butcher et al., A. Padovani et al., IMW 2012 - A. Kalatarian et. al., IRPS 2012

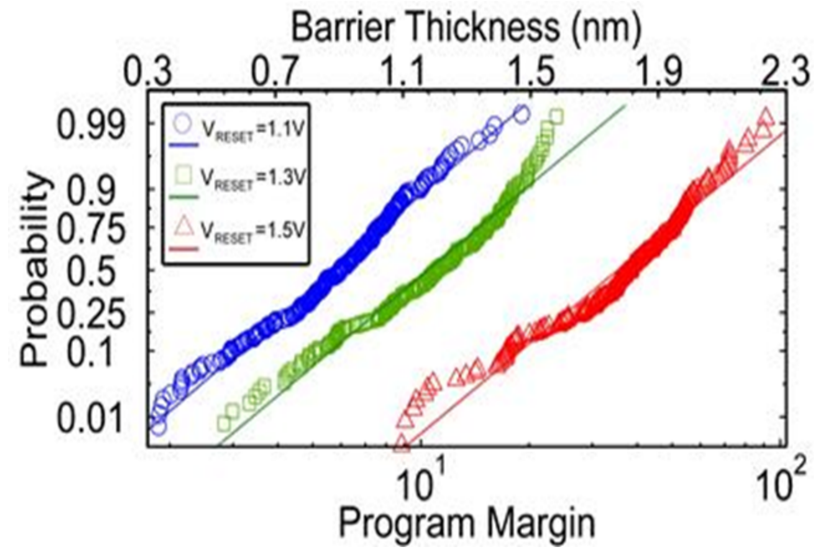
HfO_x RRAM reset simulations

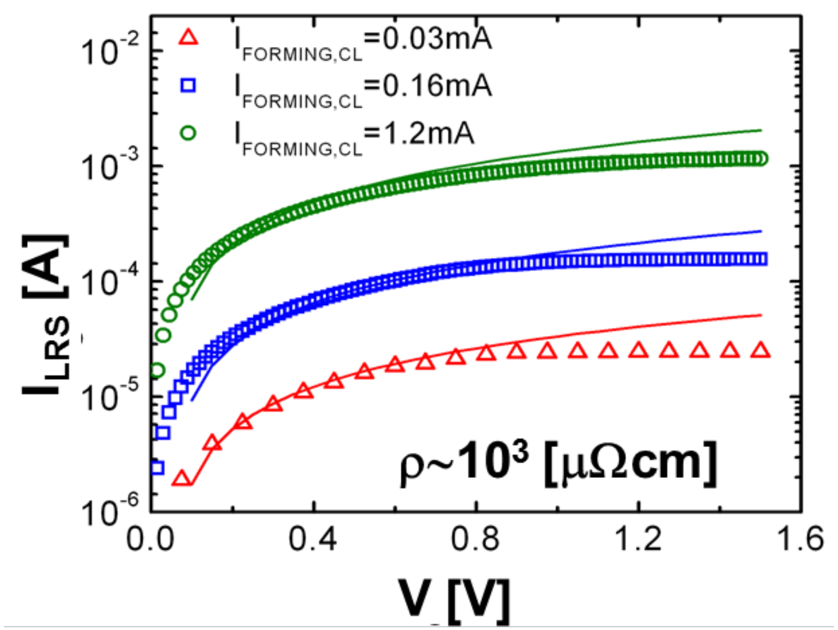


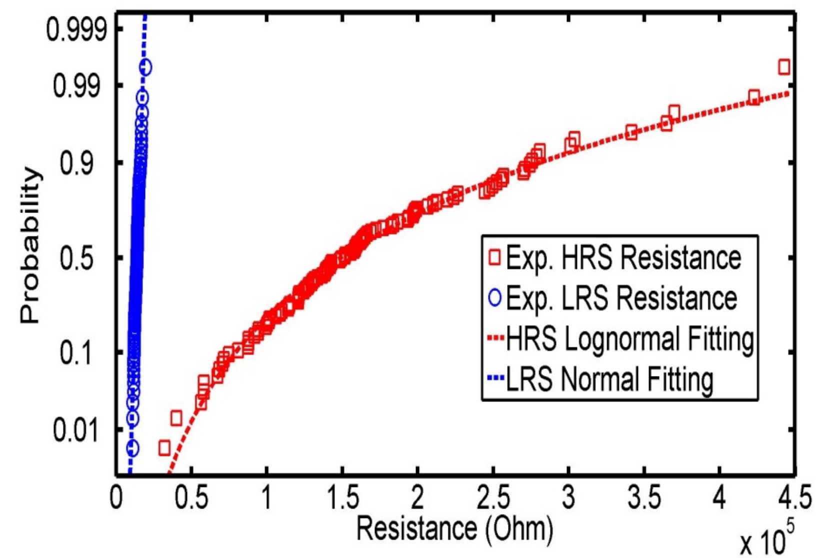
L. Vandelli et al., IEEE-IMW, 2011

LRS - HRS current distribution - HfO_x

- I_{LRS} due to electron drift through O vacancy sub-band
- Lognormal I_{HRS} distribution due to a ~1-2nm barrier thickness depending on V_{reset}



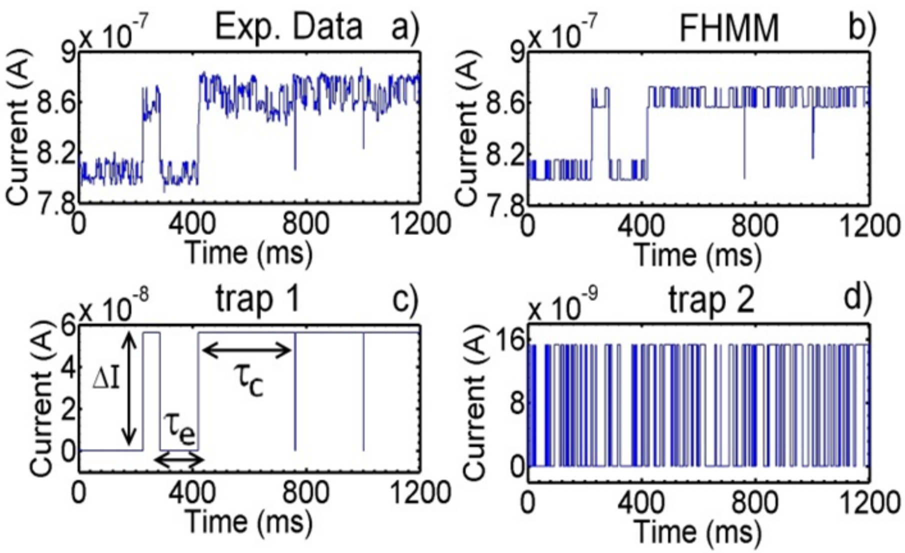




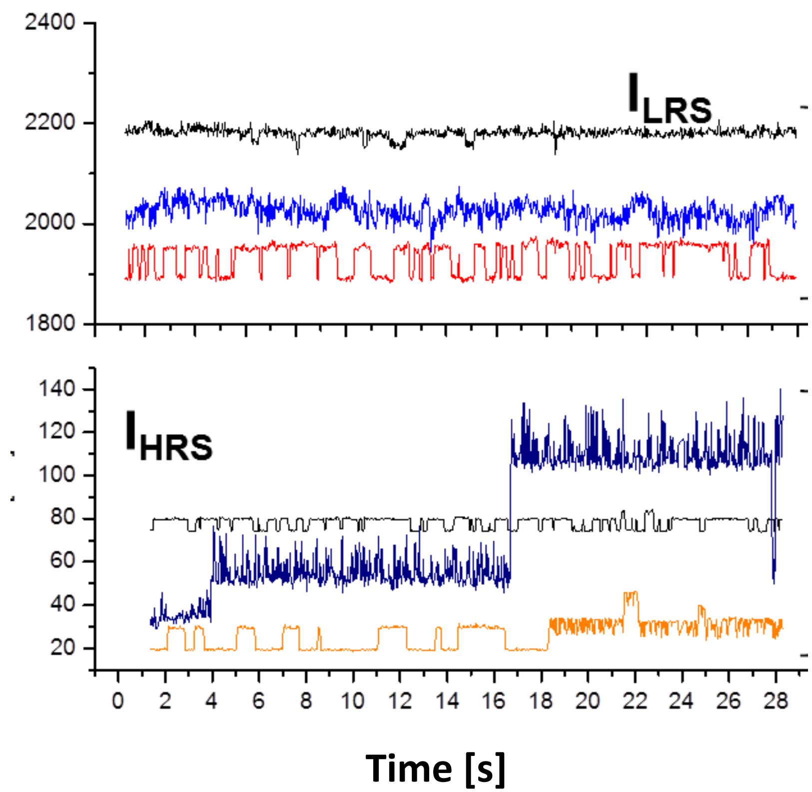
F. Puglisi et al., ICICDT 2013 - L. Larcher et al., 2014, TED - G. Bersuker et al., JAP 2011

Current fluctuations: RTN

- Multi-level RTN signal decomposed into two-level signals through FHMM
- Relative current fluctuations higher in HRS compared to LRS
- RTN in HRS due to the activation/deactivation of defects supporting TAT

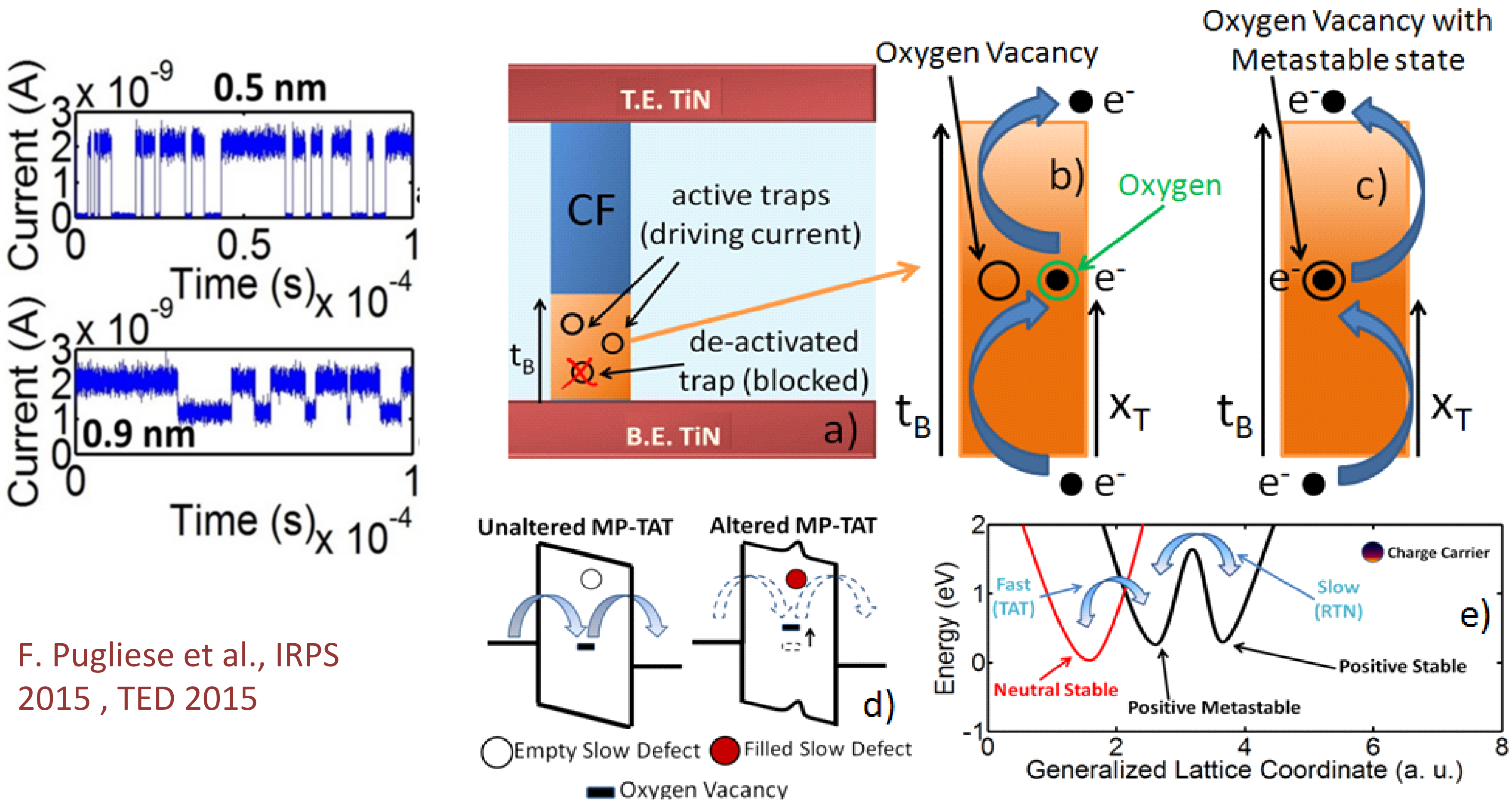


D. Veksler et al., IEDM 2012
F. Puglisi et al., ESSDERC 2012, IRPS 2014, IRPS2015



HRS RTN physical mechanisms

- Trap activation/deactivation due to 2 different mechanisms
  - Coulomb blockade due to trapping in adjacent slower traps (O ions)
  - Metastable states of O vacancies



F. Pugliese et al., IRPS 2015 , TED 2015

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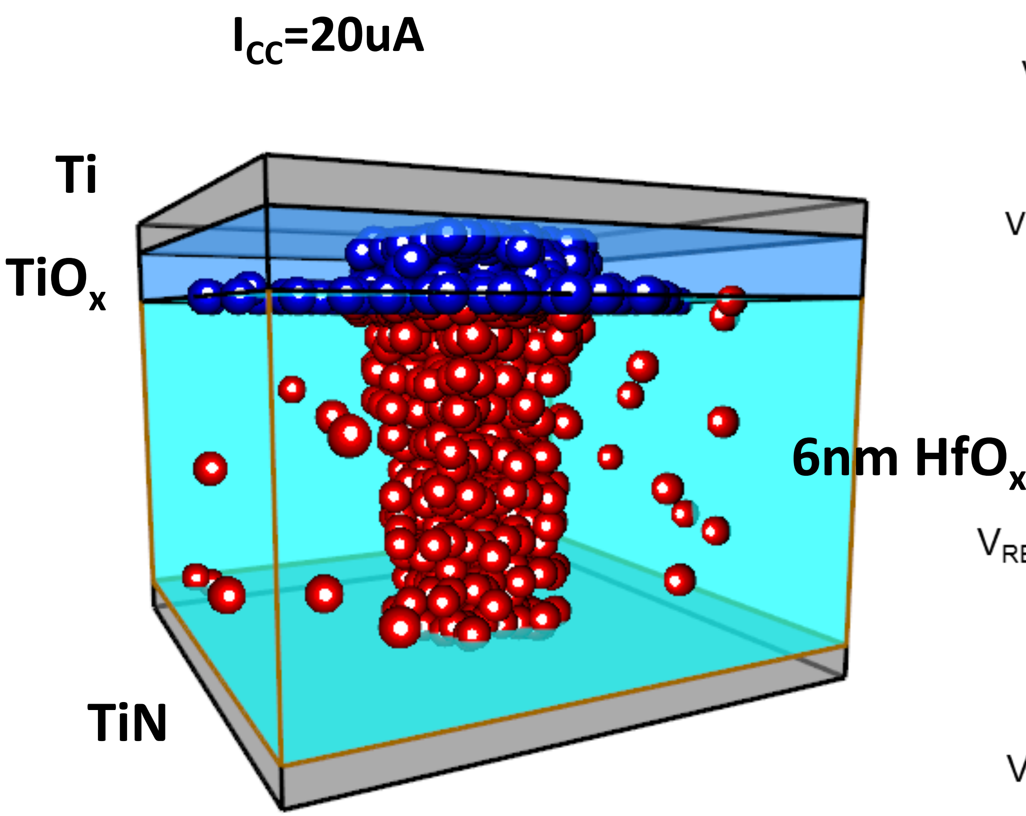
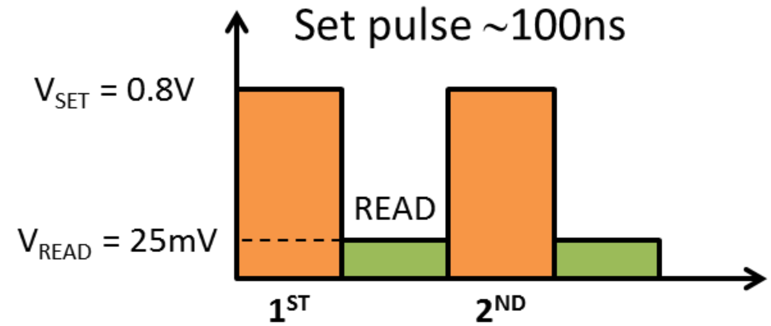
HfOx RRAM under pulse switching regime

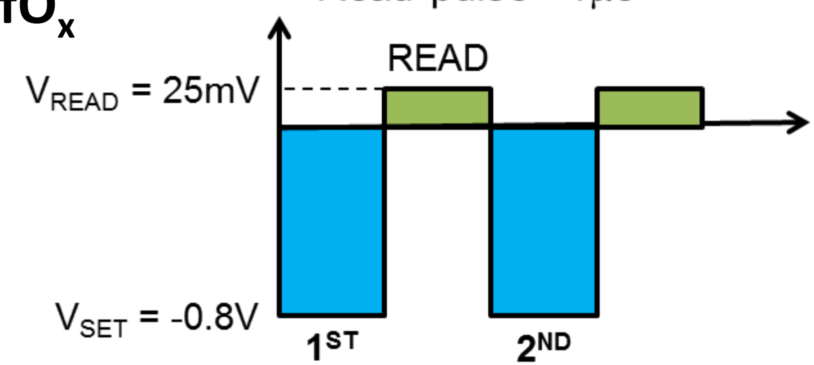
- Pulse regime proposed for a more gradual change of CF/interface properties for analog conductance modulation
- Forming simulations to determine initial O/Vo distributions



Pulse SET sequence
Set pulse ~100ns



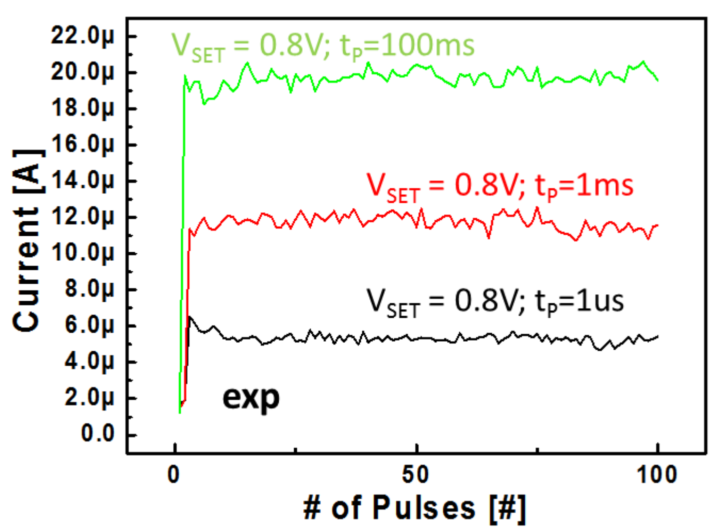
Pulse RESET sequence
Read pulse ~1µs

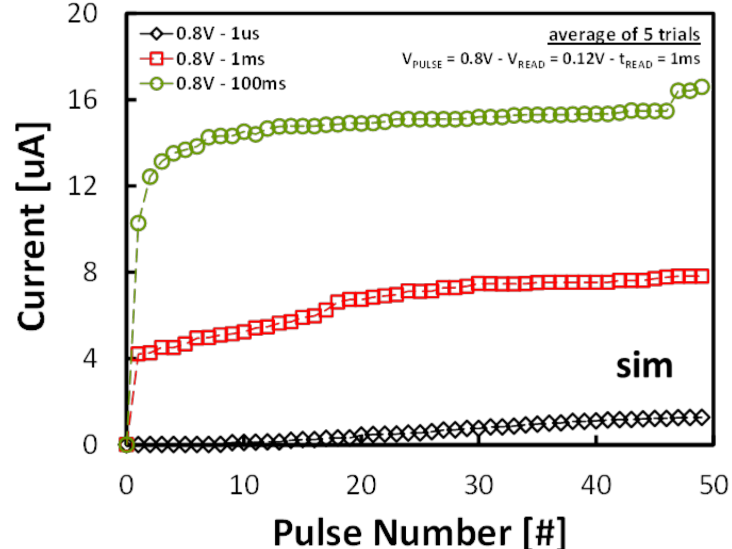


Pulsed SET simulations in HfO_x RRAM

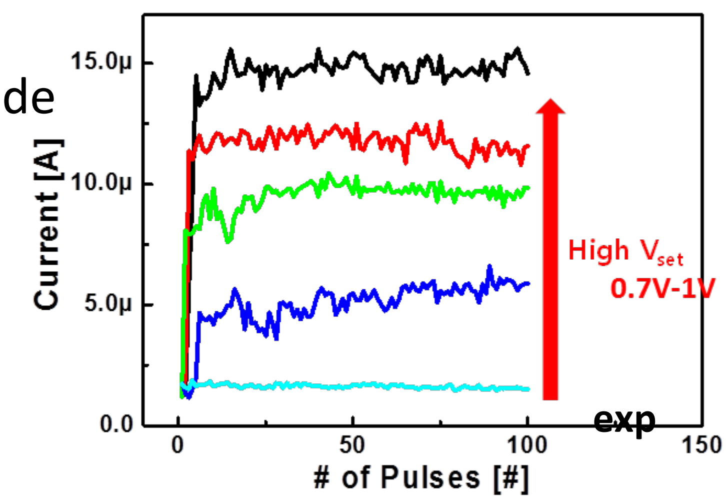
- Simulations explain current trend vs pulse set voltage and time

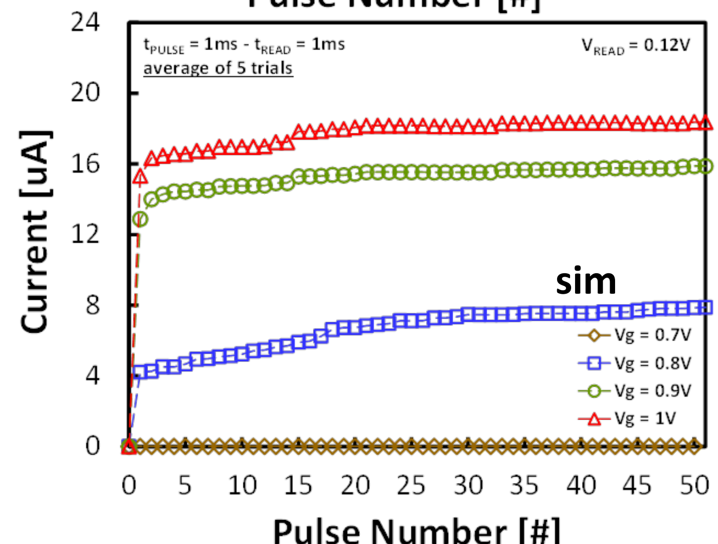
pulse voltage width





pulse voltage amplitude

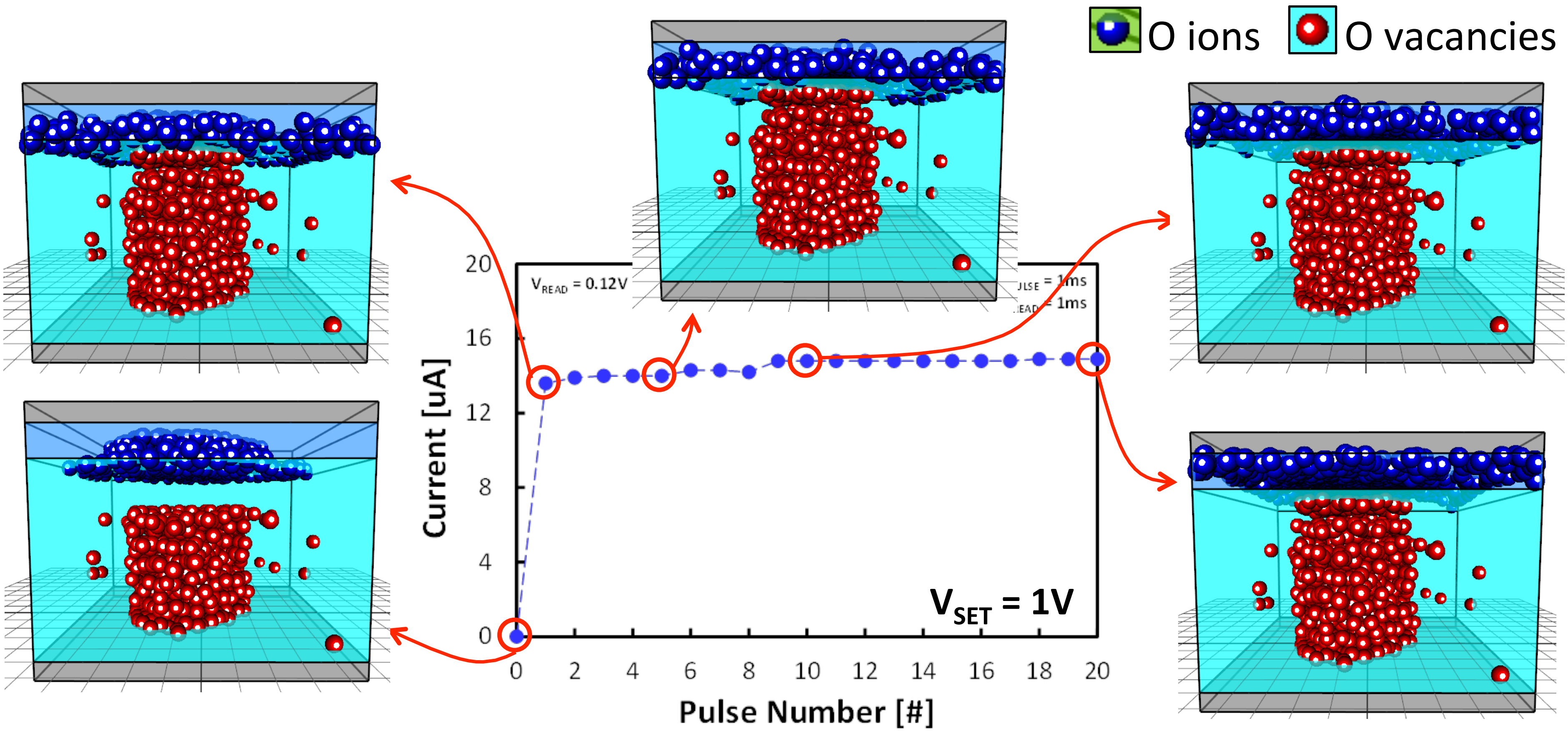




EDL data – collaboration with Prof. Hwang's group, Postech

Pulsed SET simulations in HfO_x RRAM

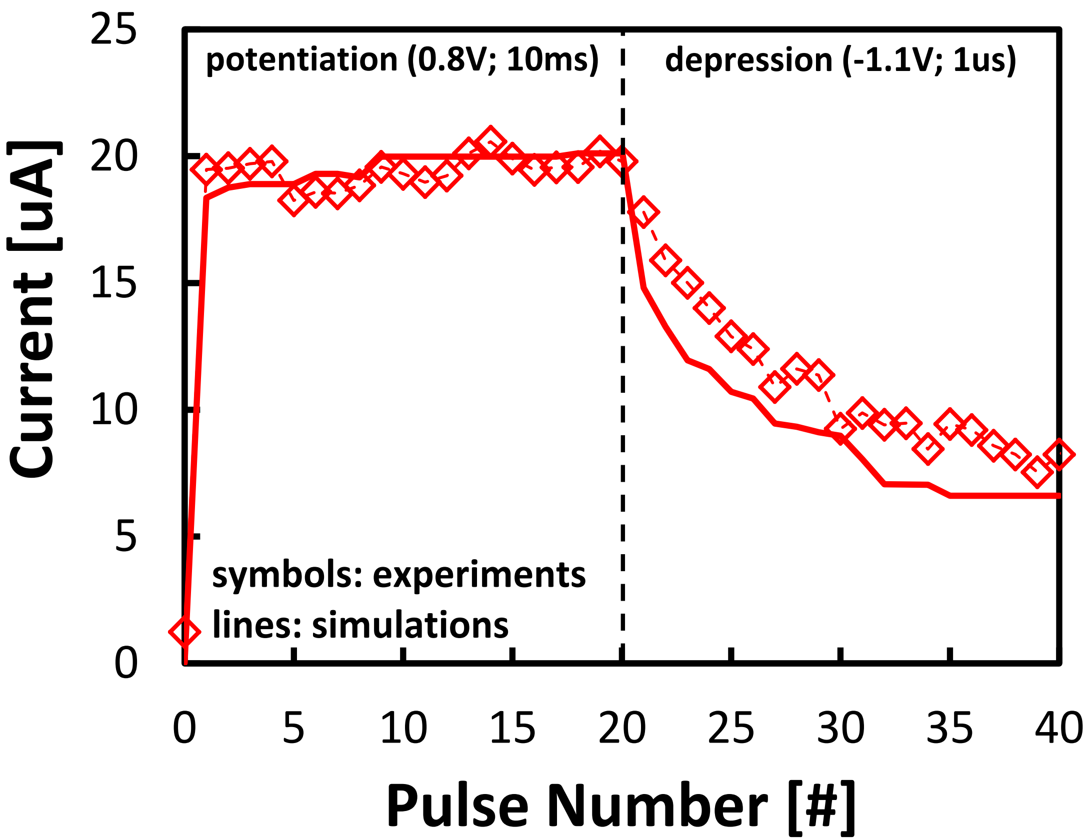
- The first voltage pulse creates Vo-O pairs due to the high field: the most of the CF is reconstructed after the first pulse, explaining the abrupt current increase
- Subsequent pulses do not affect significantly the CF



Unpublished data – collaboration with Prof. Hwang's group, Postech

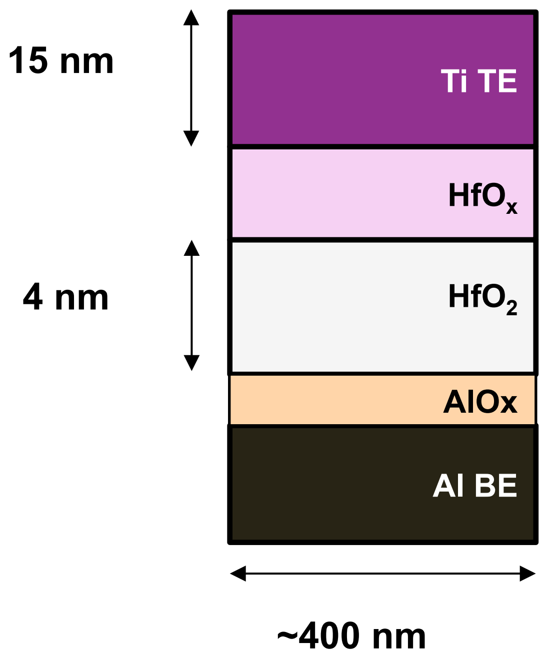
Pulsed RESET simulations in HfO_x RRAM

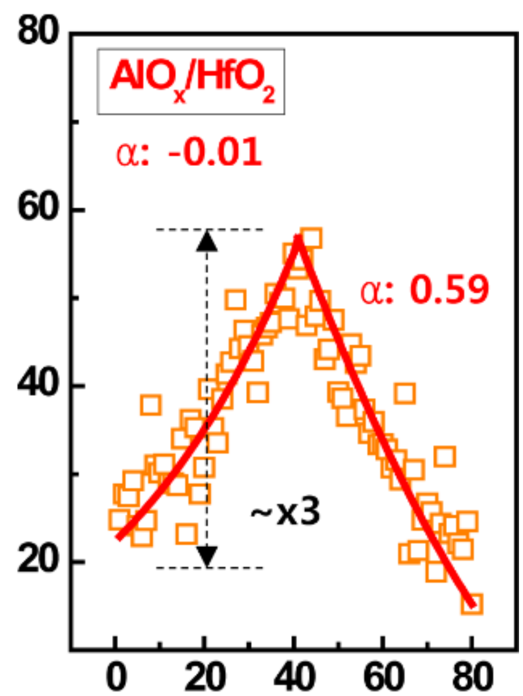
- Reset is much more gradual than set due to O ion diffusion
- The CF rupture/oxidation is controlled by the O ion supply – it more gradual compared to bond breakage (no field/temperature feedback)



AlO_x-HfO_x RRAM for analog switching

- AlO_x-HfO_x stacks show a linear current increases with subsequent pulses, more suitable for neuromorphic devices
- Field redistribution across two layers (one has to be very thin) allows to better control O ion supply, enabling a more gradual modulation of CF conductance

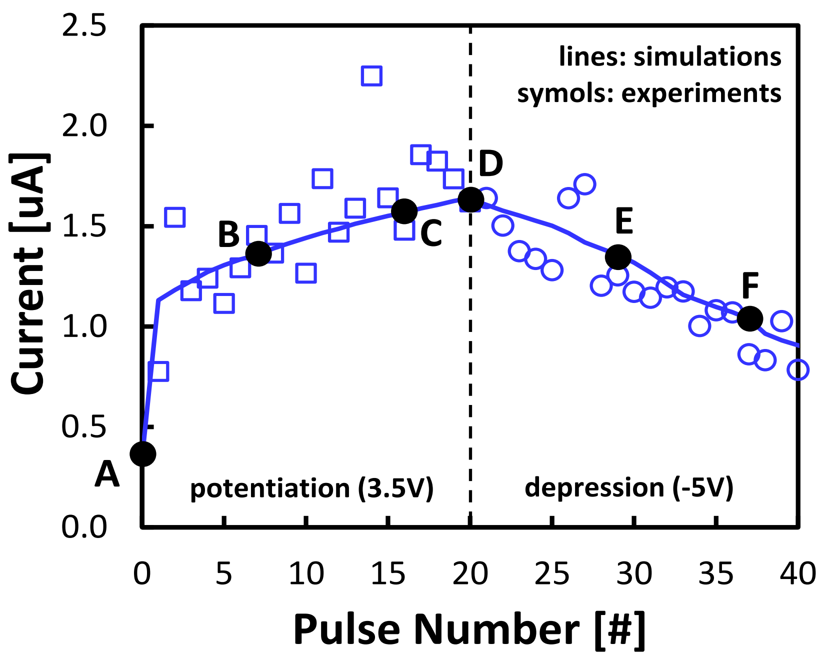


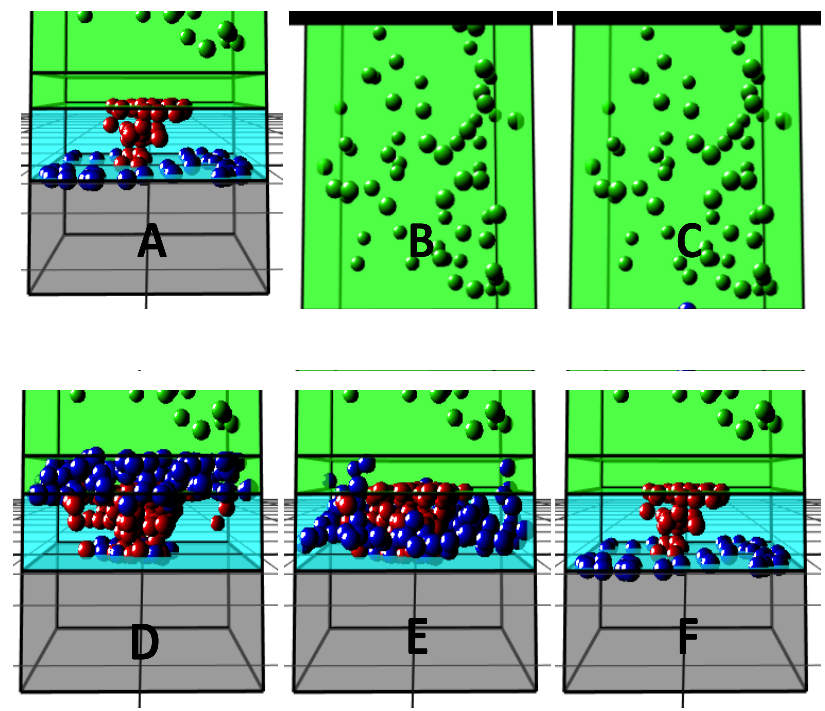


H. Hwang et al, EDL, 2016

Analog switching in TiO_x/TaO_y RRAM

- Simulation of Ti/35nmTiO_x/2nmTaO_y/TiN RRAM shows that the quasi-linear resistance changes during potentiation and depression are due to the higher control on the O ion supply, i.e. diffusion into switching and/or O reservoir layers





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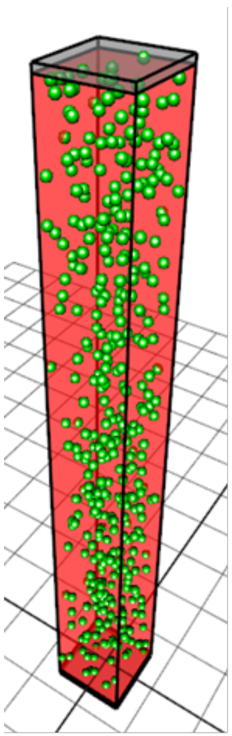
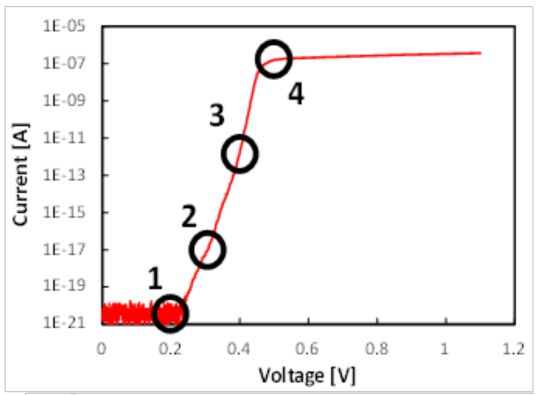
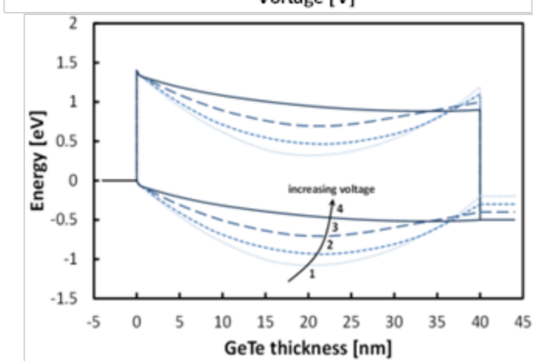
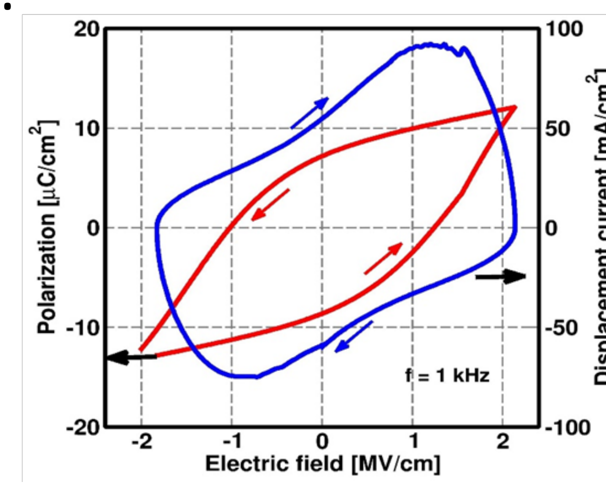
Conclusions

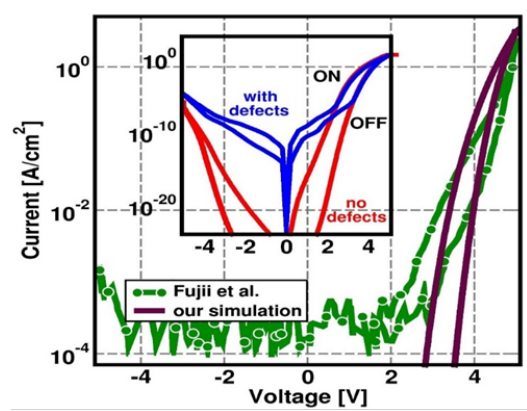
- Dynamic simulation platform connecting material properties to electrical device performances essential to engineer novel memories and neuromorphic computing devices
- Same approach allows targeting **selectors** (OTS, tunneling barriers), **ferroelectric memories, PCM,** …











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RRAM technology issues

- **Selector for cross-bar and 3D integration**
- **Analog switching for neuromorphic**
- **Variability & RTN**
- **Full understanding missing**
  - $V_{RESET} > V_{SET}$
  - O ion reservoir
  - High endurance