

Modeling of ReRAMs based on the Valence Change Mechanism: From Atomistic to Circuit-Level Models

S. Menzel¹

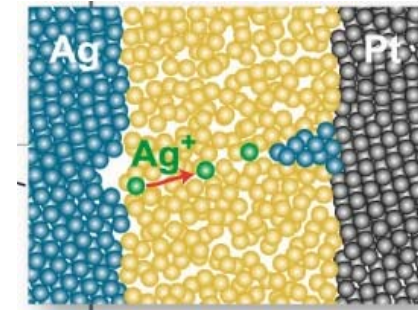
¹Peter Grünberg Institut (PGI-7), Forschungszentrum Jülich, Germany

*Resistive Switching,
Edited by D. Ielmini, R. Waser
Wiley-VCH 2016*

Redox-based Memristive Devices

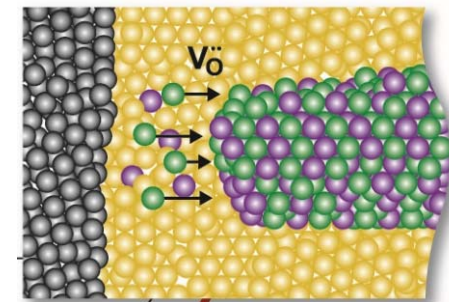
ElectroChemical Metallization Cells

- also called CBRAM or Atomic Switch
- bipolar
- filamentary



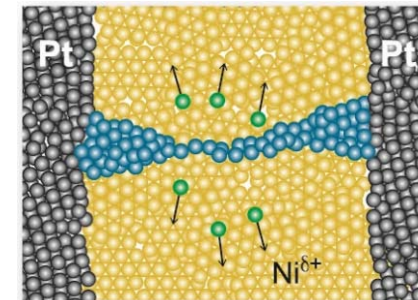
Valence Change Mechanism Cells

- also OxRAM or RRAM
- bipolar
- filamentary and non-filamentary

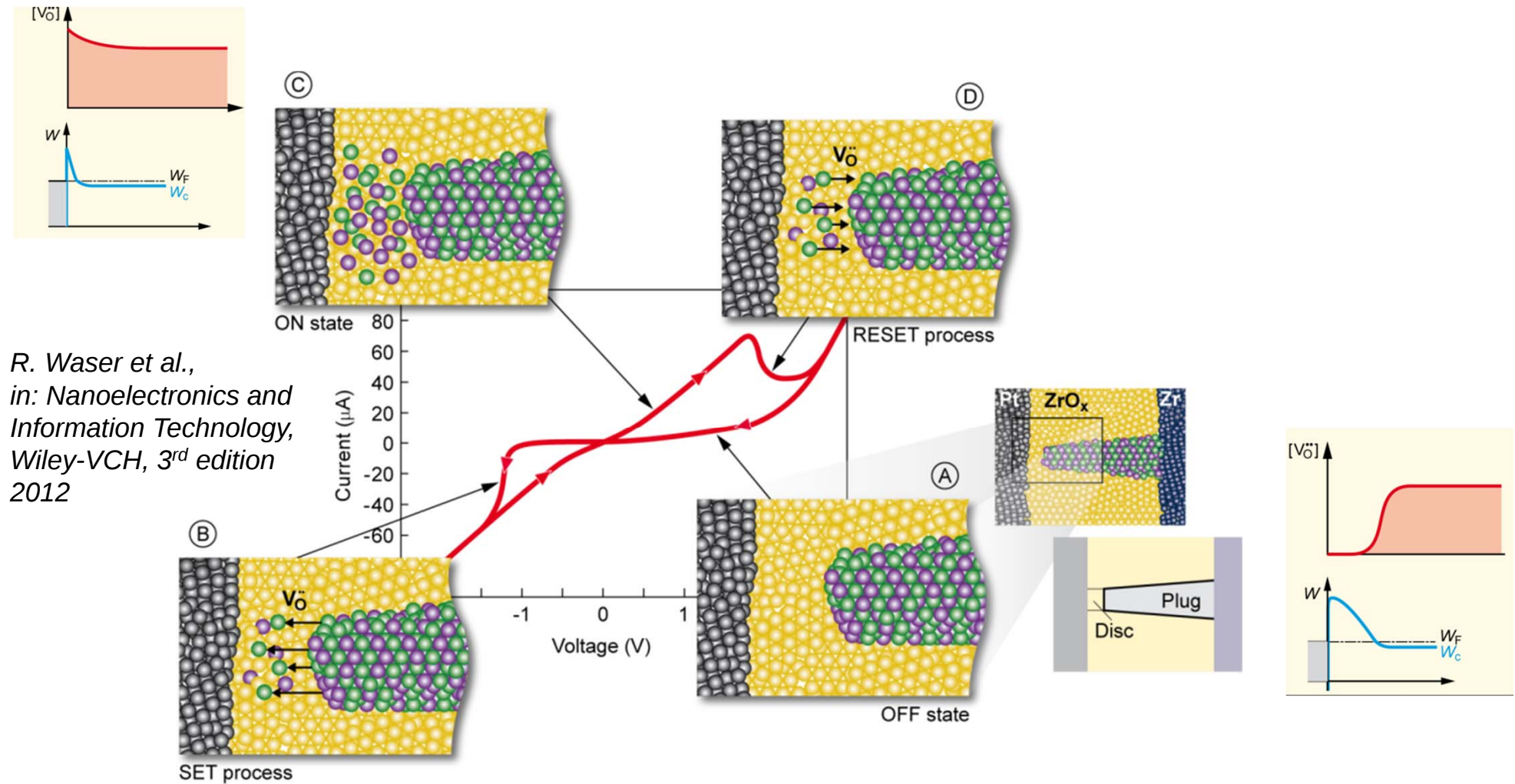


ThermoChemical Mechanism Cells

- unipolar
- low endurance
- only minor activities

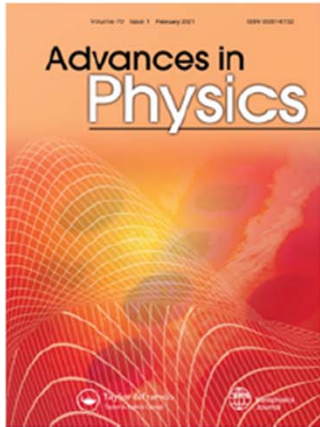


Filamentary VCM Cells: Switching Mechanism



→ Processes: ion motion, oxygen exchange, Joule heating

Comprehensive Review Article on VCM Cells



Advances in Physics



ISSN: (Print) (Online) Journal homepage: <https://www.tandfonline.com/loi/tadp20>

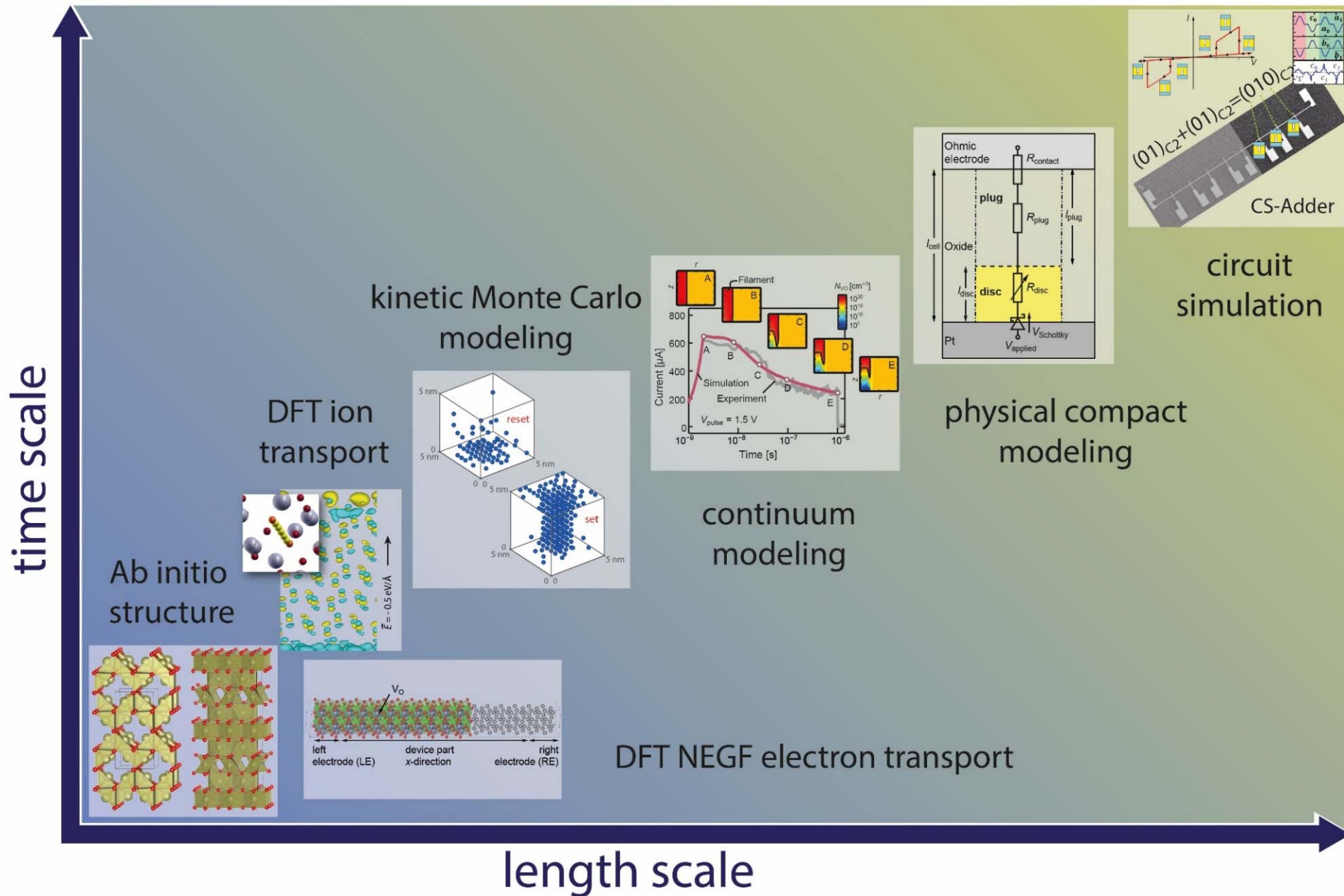
Nanoionic memristive phenomena in metal oxides: the valence change mechanism

Regina Dittmann, Stephan Menzel & Rainer Waser

To cite this article: Regina Dittmann, Stephan Menzel & Rainer Waser (2022): Nanoionic memristive phenomena in metal oxides: the valence change mechanism, *Advances in Physics*, DOI: [10.1080/00018732.2022.2084006](https://doi.org/10.1080/00018732.2022.2084006)

To link to this article: <https://doi.org/10.1080/00018732.2022.2084006>

Multiscale Modeling



Outline



Motivation



**Electronic Transport in VCM Cells:
A DFT-NEGF study**



Switching Variability of VCM Cells:
Kinetic Monte Carlo Modeling



Switching Dynamics of VCM Cells:
Continuum Modeling



Towards Circuit Simulations:
VCM Compact Models (JART)



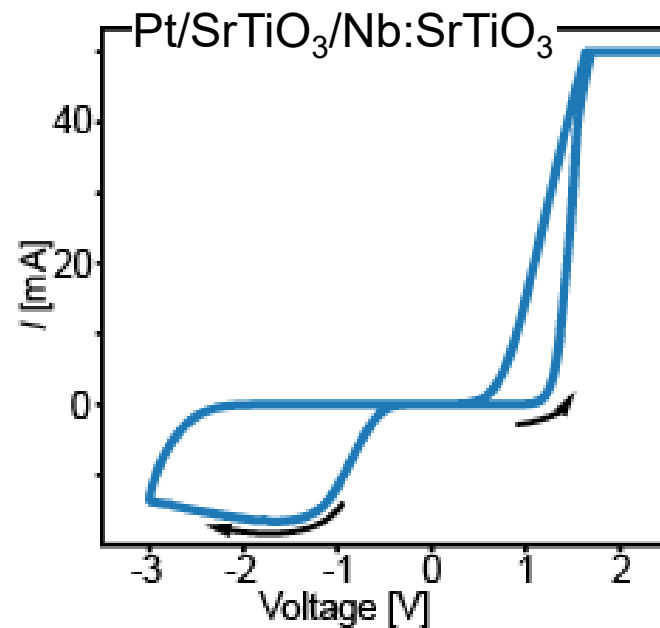
Array Level Modeling



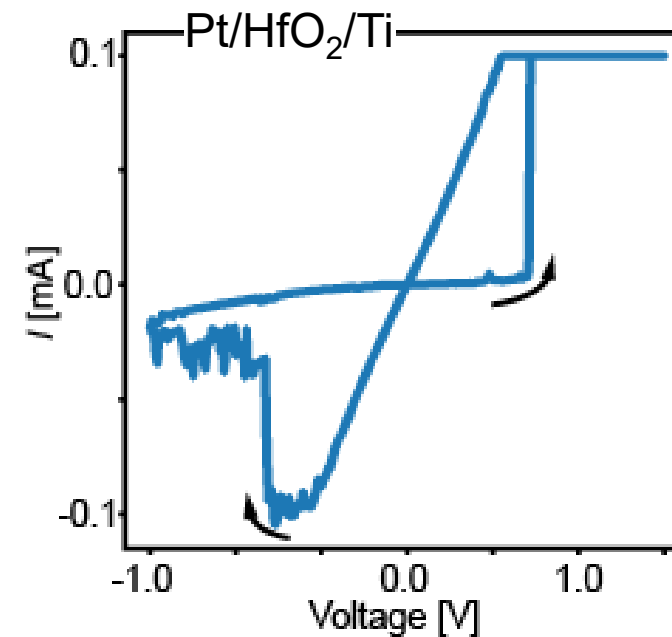
Summary & Conclusion

Typical I - V Characteristics of VCM Cells

Type I Conduction



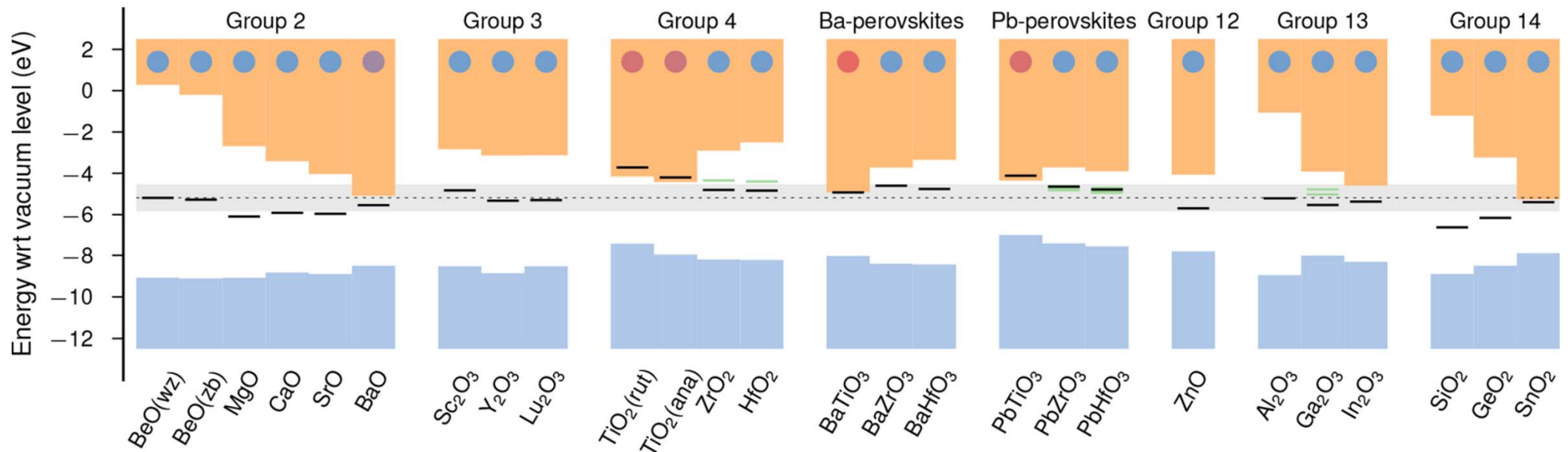
Type II Conduction



→ How do these materials differ?

Oxygen Vacancy Defects in Oxides

C. Linderälv, P. Erhart et al.,
J. Phys. Chem. Lett., vol. 9, no. 1, 222-228

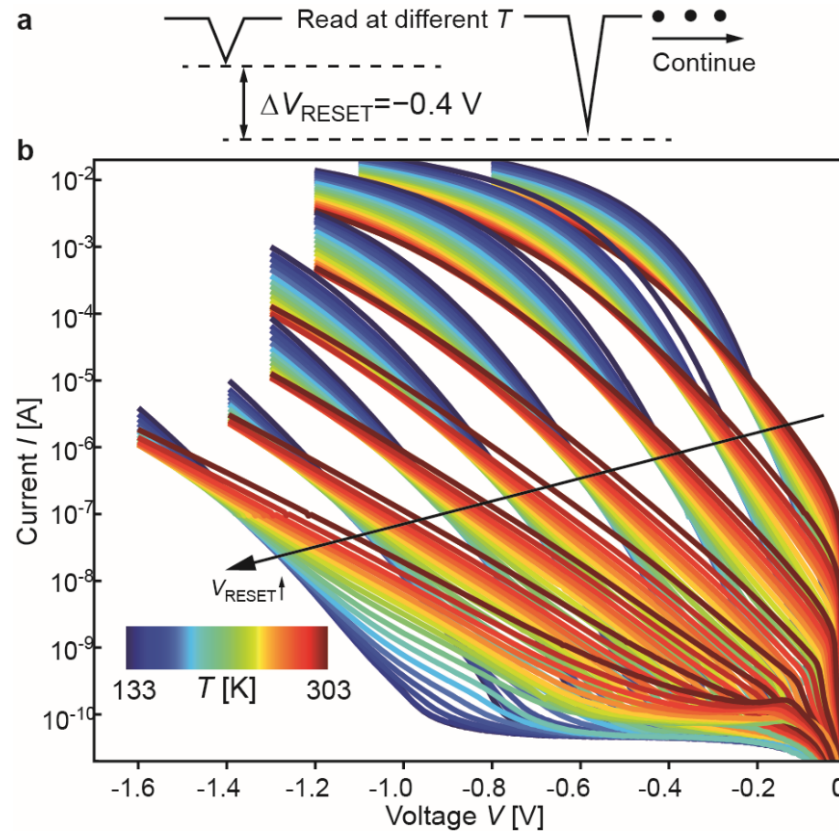


→ Type 1: shallow defect states and delocalized electrons

→ Type 2: deep defect states and localized electrons

Experimental Data Pt/SrTiO₃

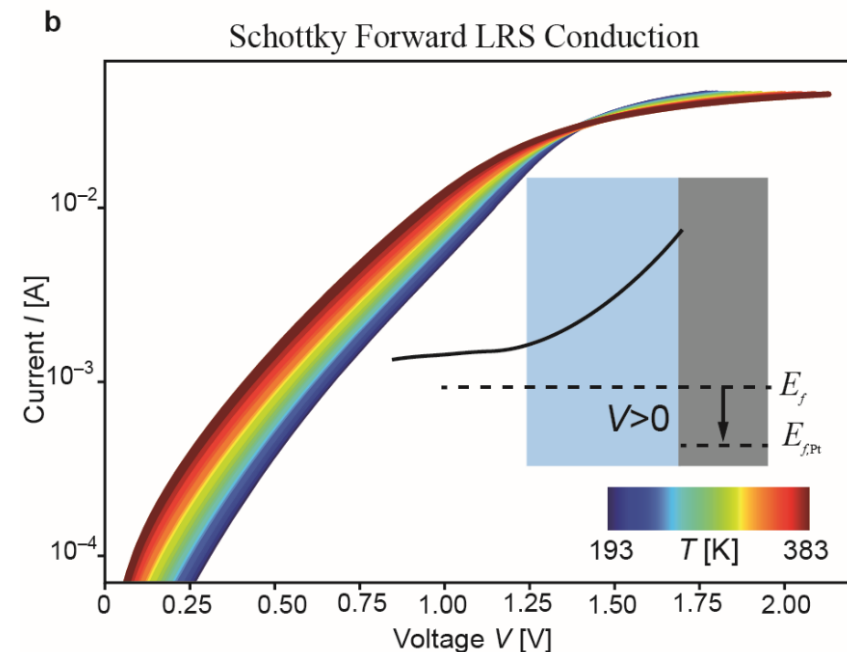
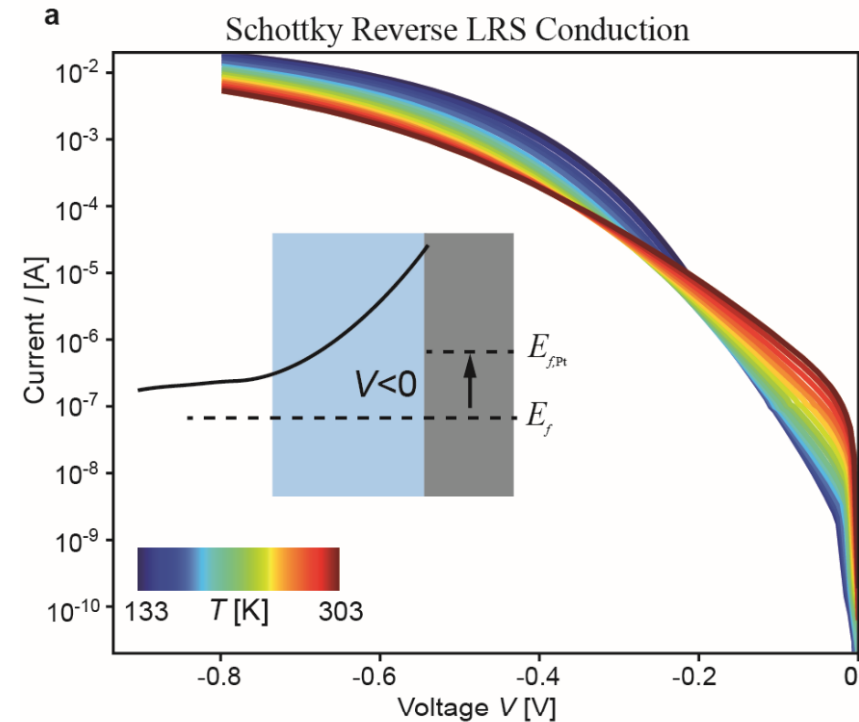
I - V - T of multilevel states



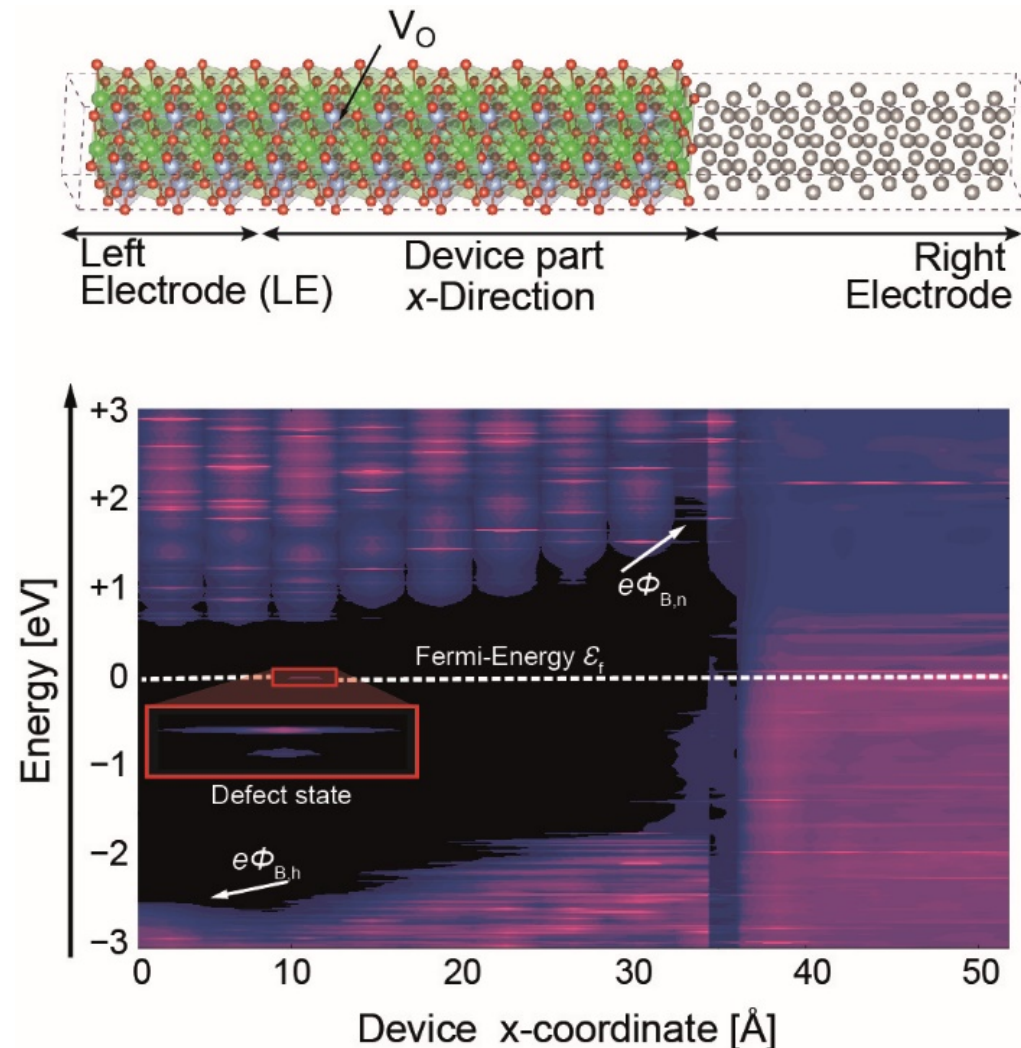
→ Change of T -dependence

C. Funck, S. Menzel et al.,
Phys. Rev. B, vol. 102, 035307, (2020)

I - V - T of LRS state



DFT-Nonequilibrium Green's Function (NEGF) Formalism



2×2×9 [100] SrTiO₃ supercell
2×2×4 [100] Pt supercell



DFT PBE-GGA

Local density of states (LDOS)

DFT calculation details:

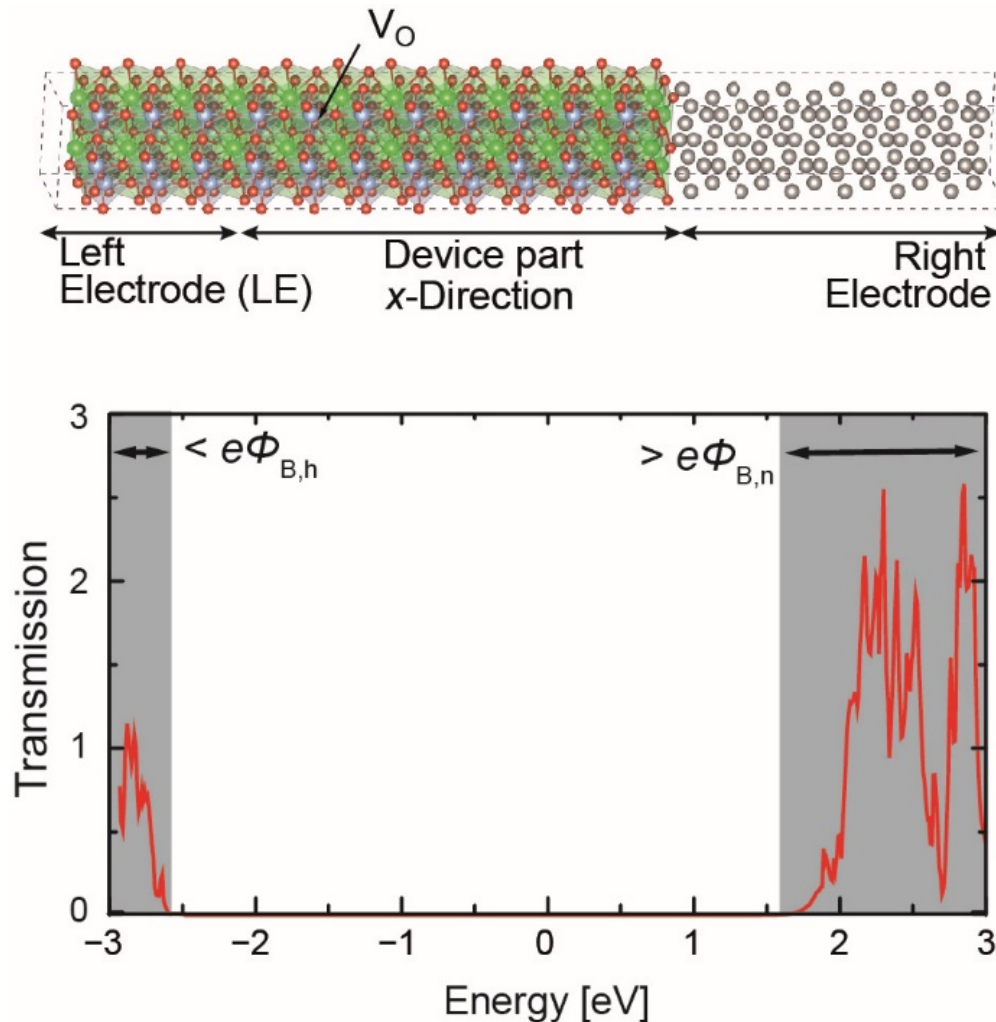
Code: ATK 2015

Exchange correlation: PBE

k-point Sampling for electrodes
(3×3×100)

Local atomic basis set.

DFT-Nonequilibrium Green's Function (NEGF) Formalism



2×2×9 [100] SrTiO₃ supercell
2×2×4 [100] Pt supercell

DFT PBE-GGA

Local density of states (LDOS)

NEGF

Transmission spectrum

Different T

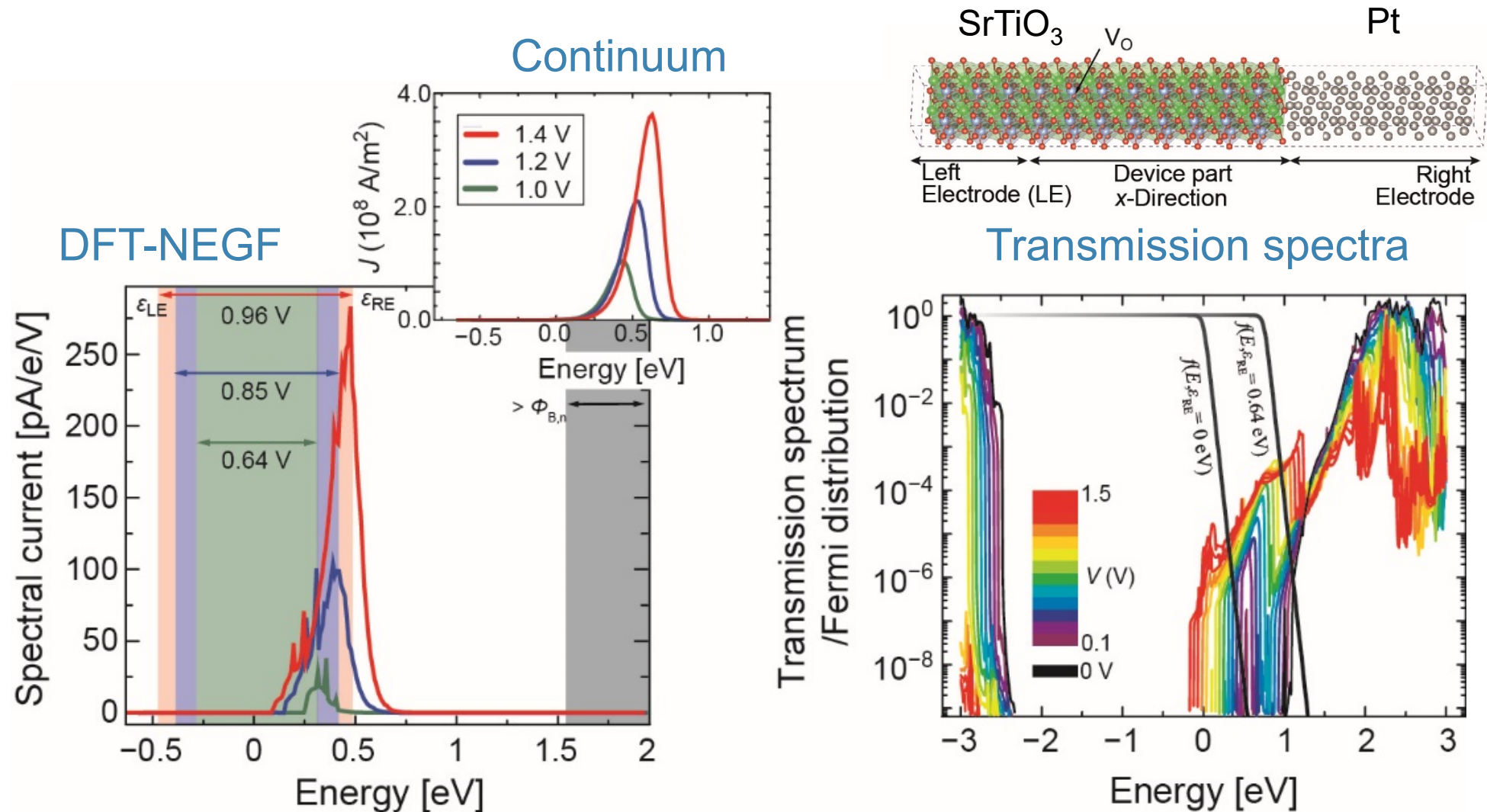
No phonon scattering

Current characteristics

C. Funck, S. Menzel et al., *Adv. Electron. Mater.*,
vol. 4, no. 7, 1800062, (2018)

$$I = \frac{e}{h} \int_{-\infty}^{\infty} T_R(E, \varepsilon_{LE}, \varepsilon_{RE}) [f(E - \varepsilon_{LE}, T) - f(E - \varepsilon_{RE}, T)] dE,$$

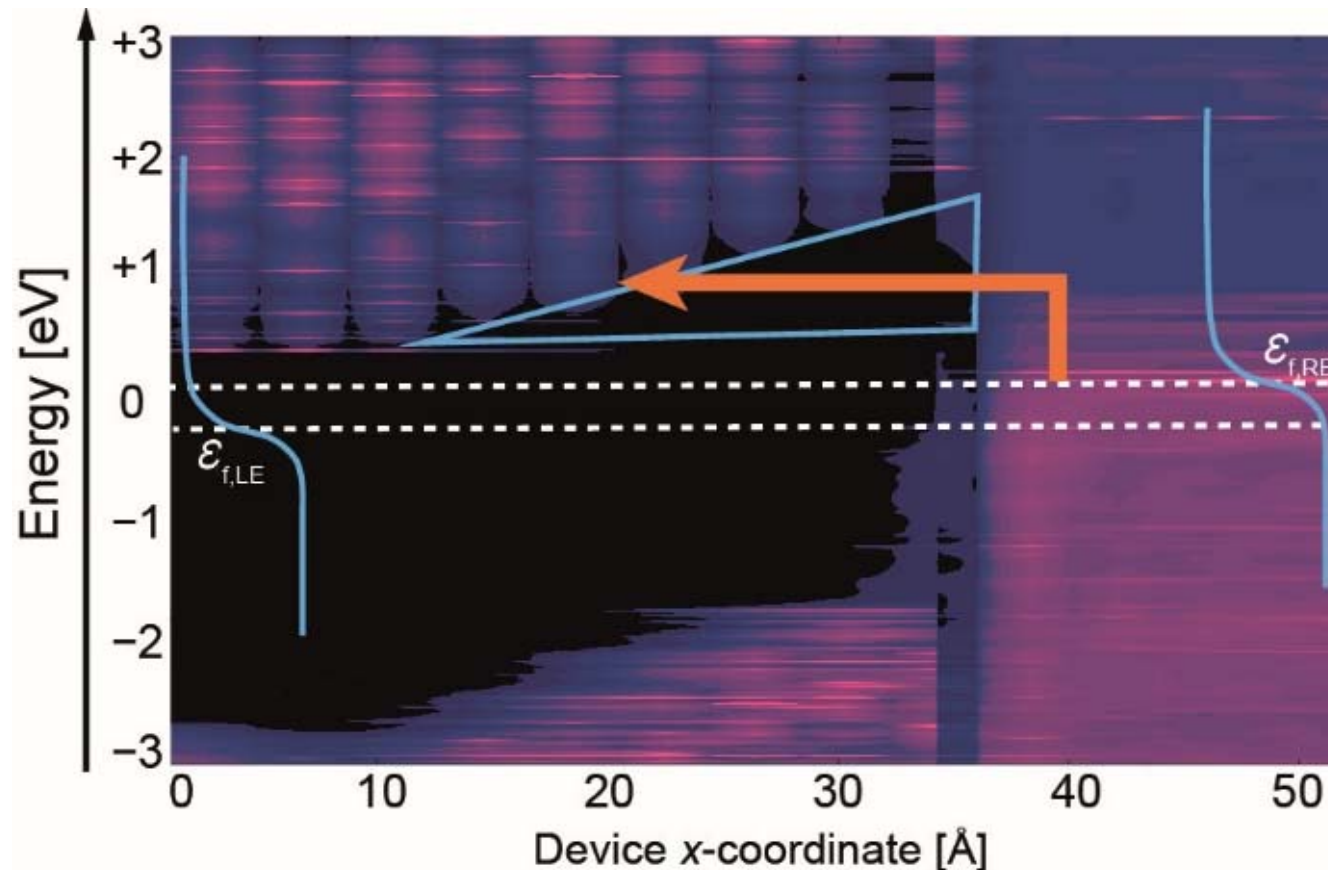
Spectral Current Analysis in Reverse Direction



→ Spectral current reveals strong tunneling contribution

Analysis of the Voltage Dependence

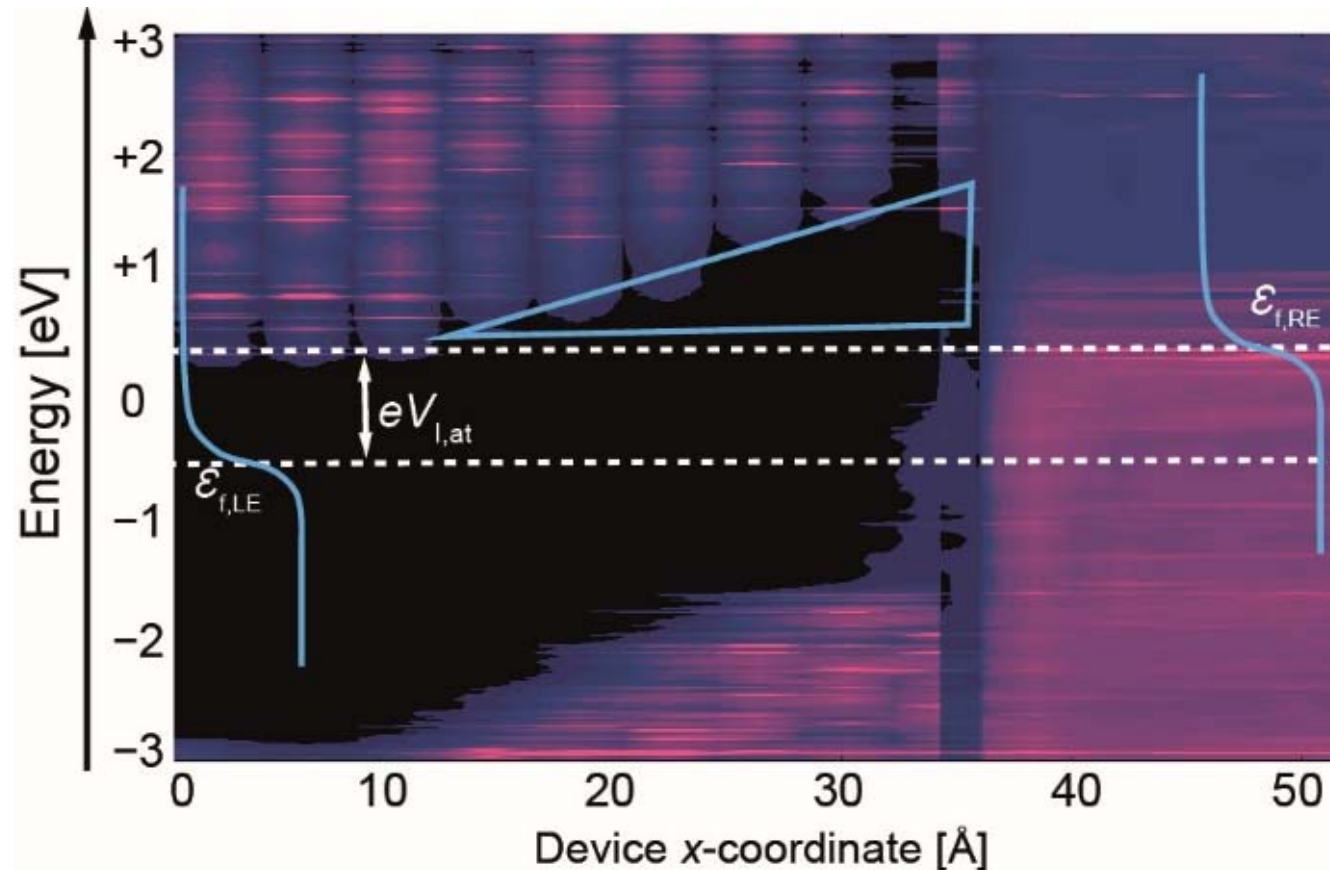
Low voltage regime



- Only thermally excited electrons can tunnel (Boltzmann approximation valid)
- Current increases with T

Analysis of the Voltage Dependence

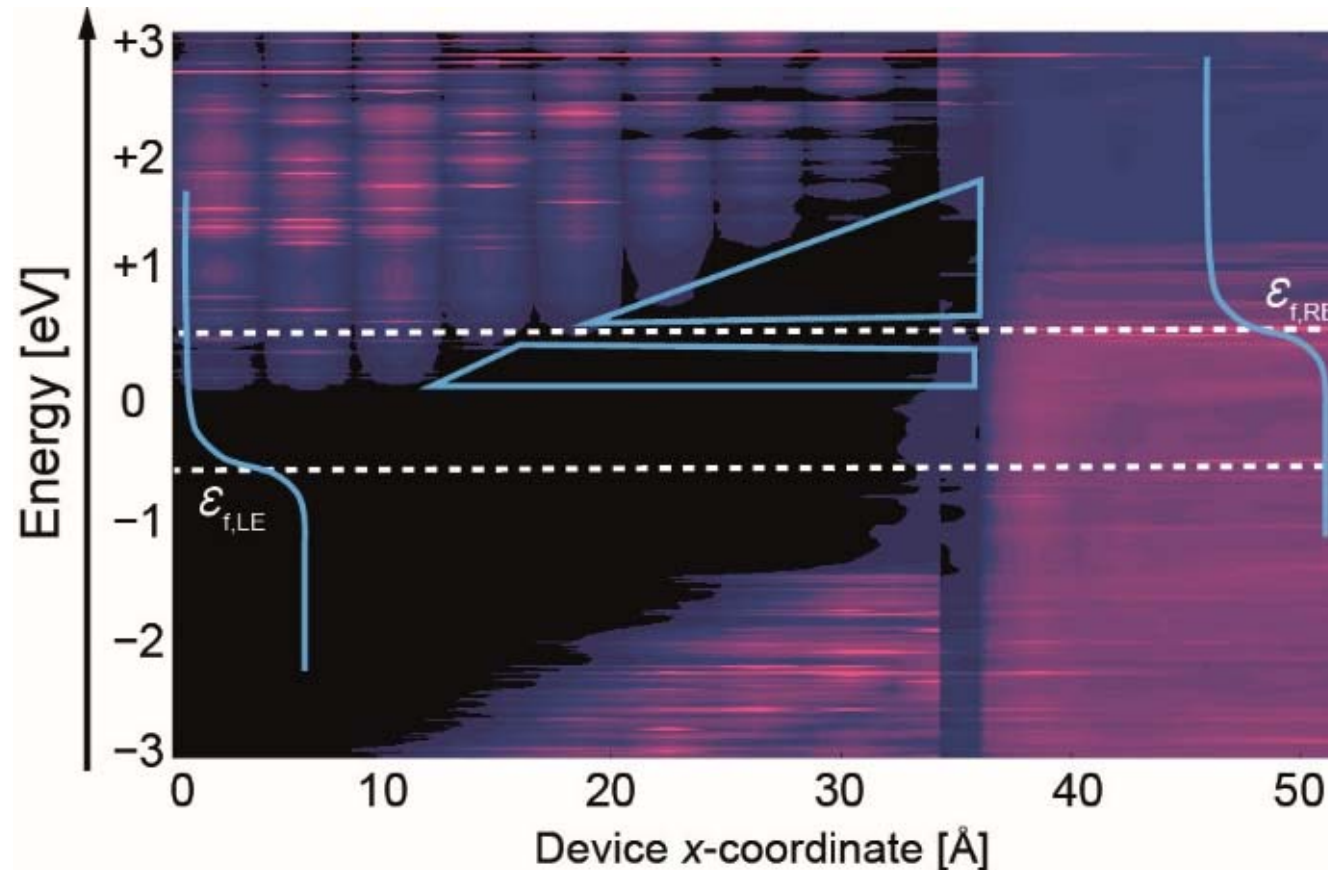
Intersection voltage V_i



- RE Fermi level and maximum of spectral current coincide
- Boltzmann approximation invalid

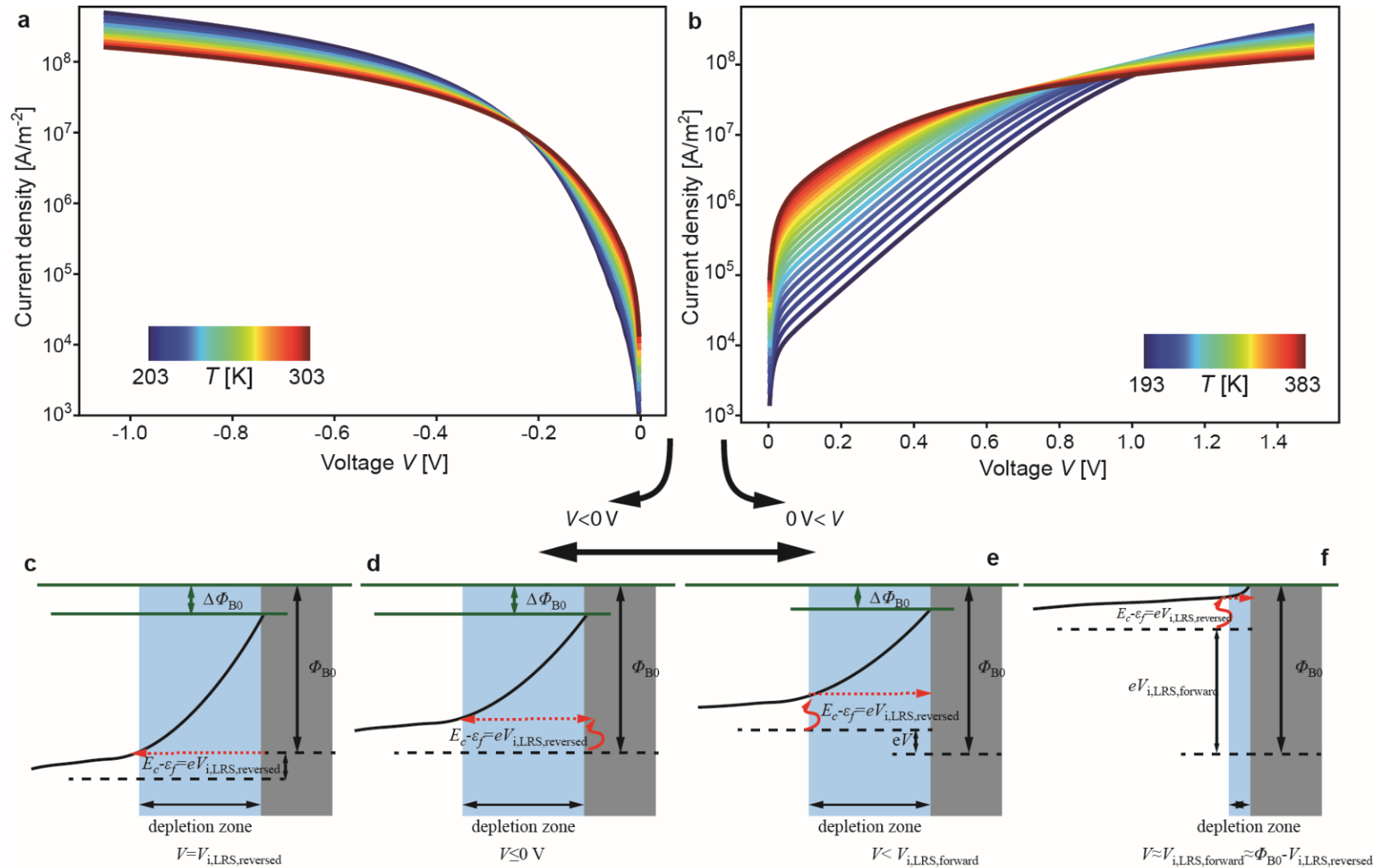
Analysis of the Voltage Dependence

High voltage regime



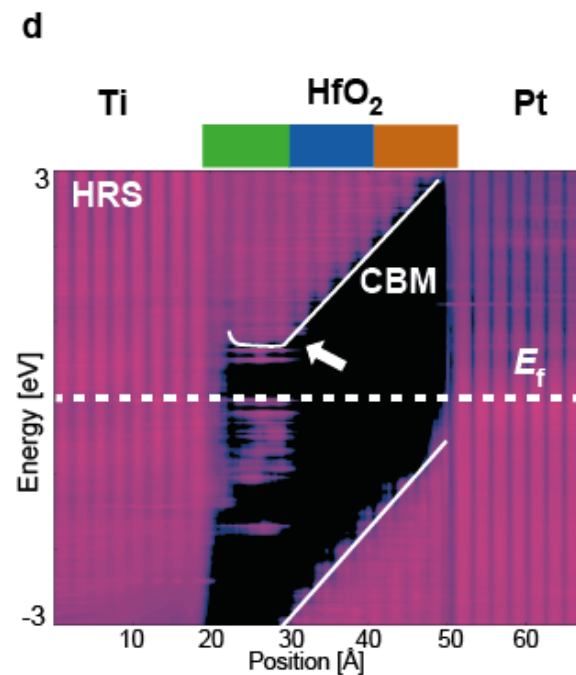
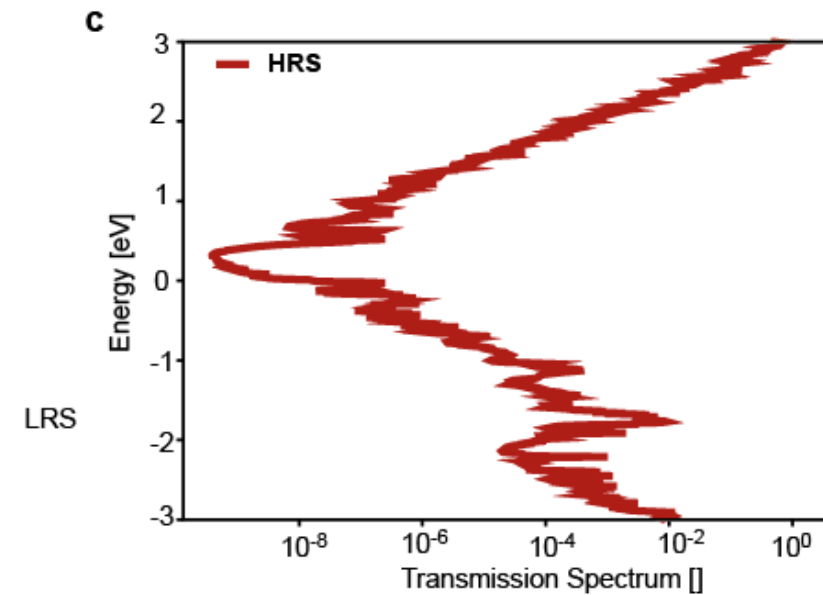
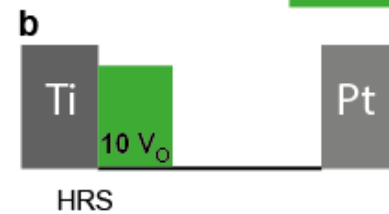
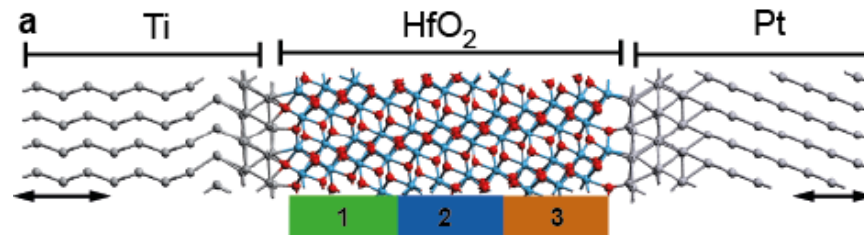
- All electrons tunnel (no T -dep by tunneling)
- T -dependence due to phonon scattering

Summary of Type I Conduction



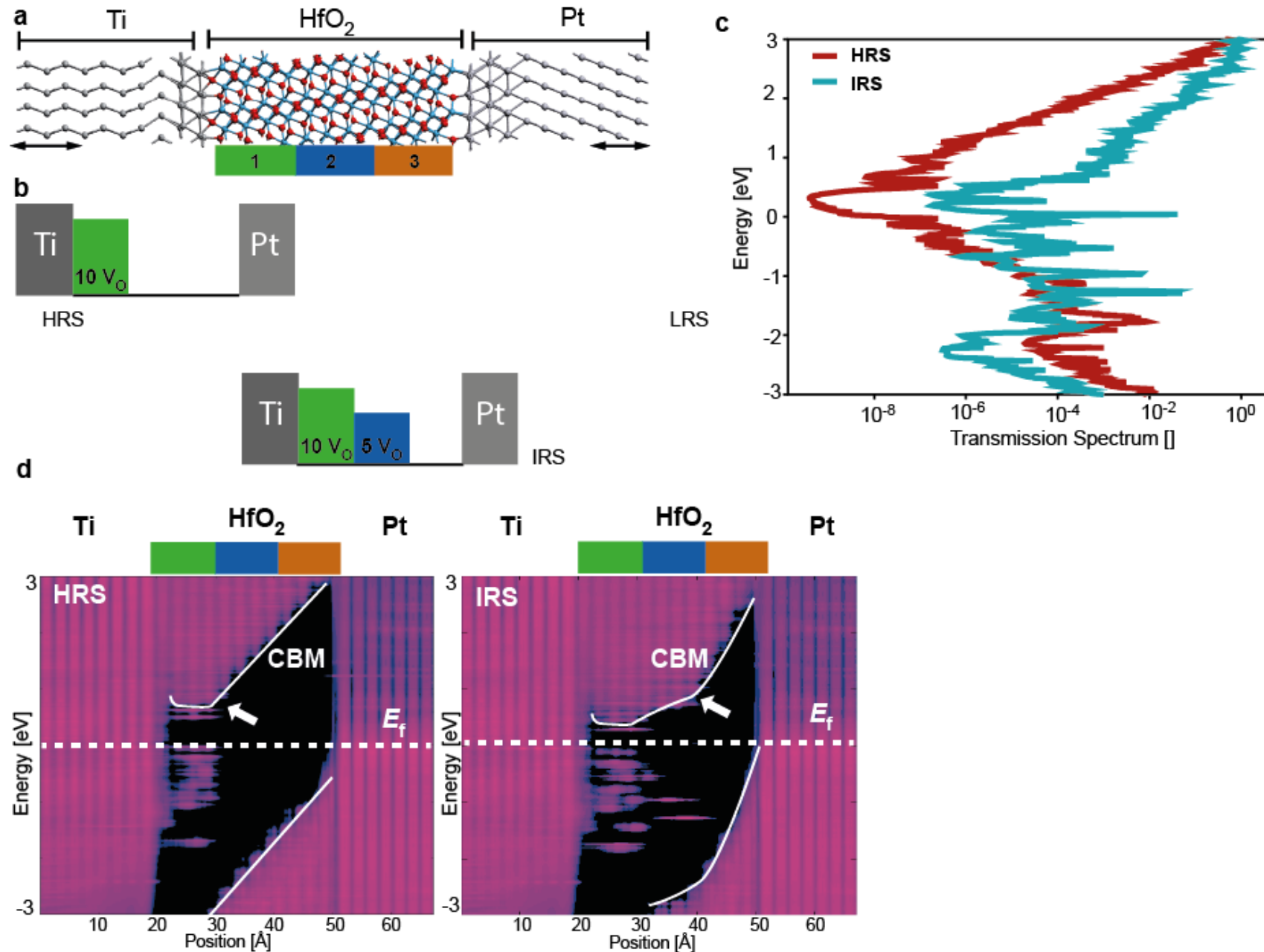
DFT-NEGF Simulation of the HRS

C. Funck, S. Menzel, *ACS Appl. Electron.*,
vol. 3, 3674-3692, (2021)



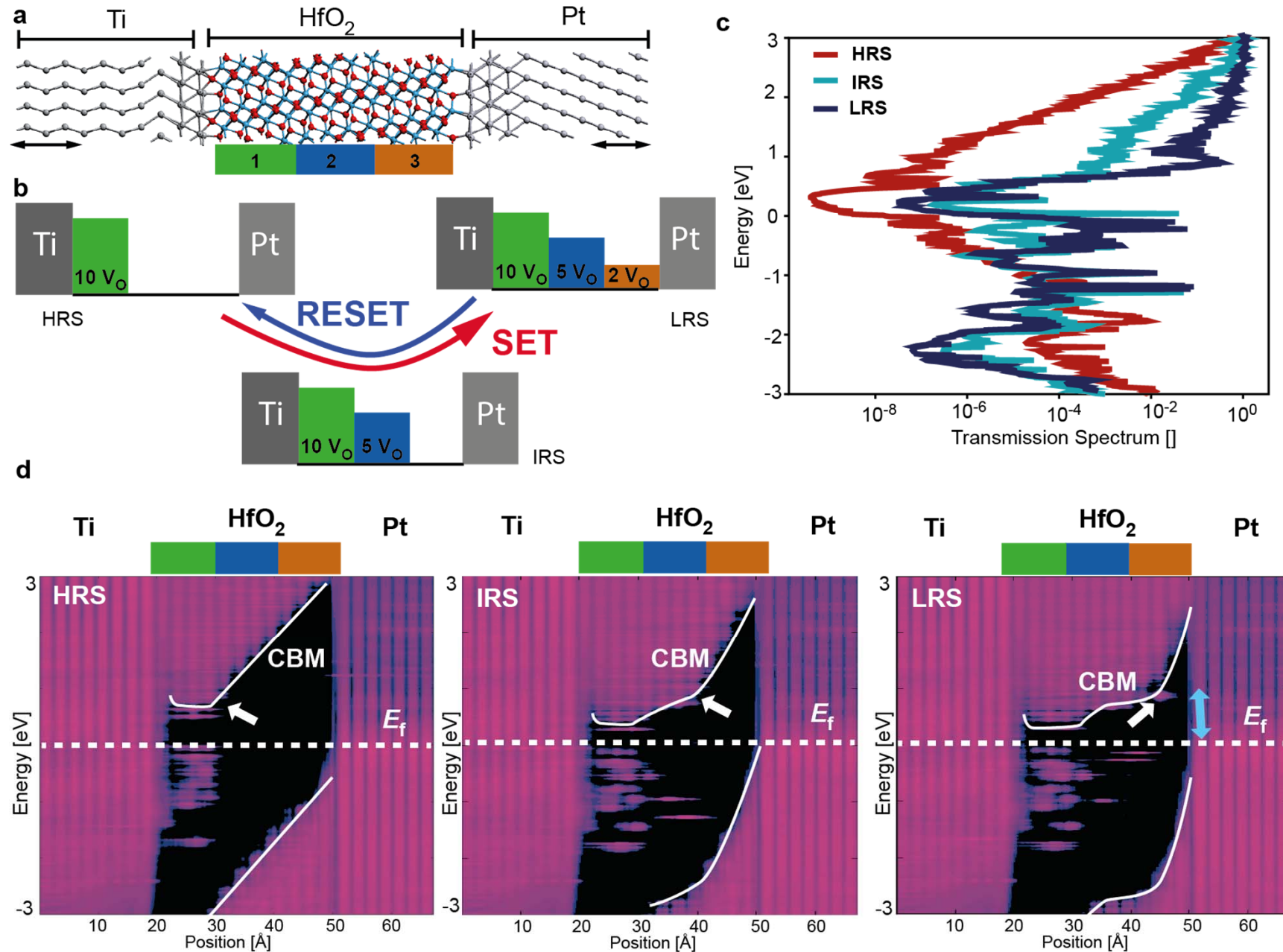
DFT-NEGF Simulation of an IRS

C. Funck, S. Menzel, *ACS Appl. Electron.*,
vol. 3, 3674-3692, (2021)

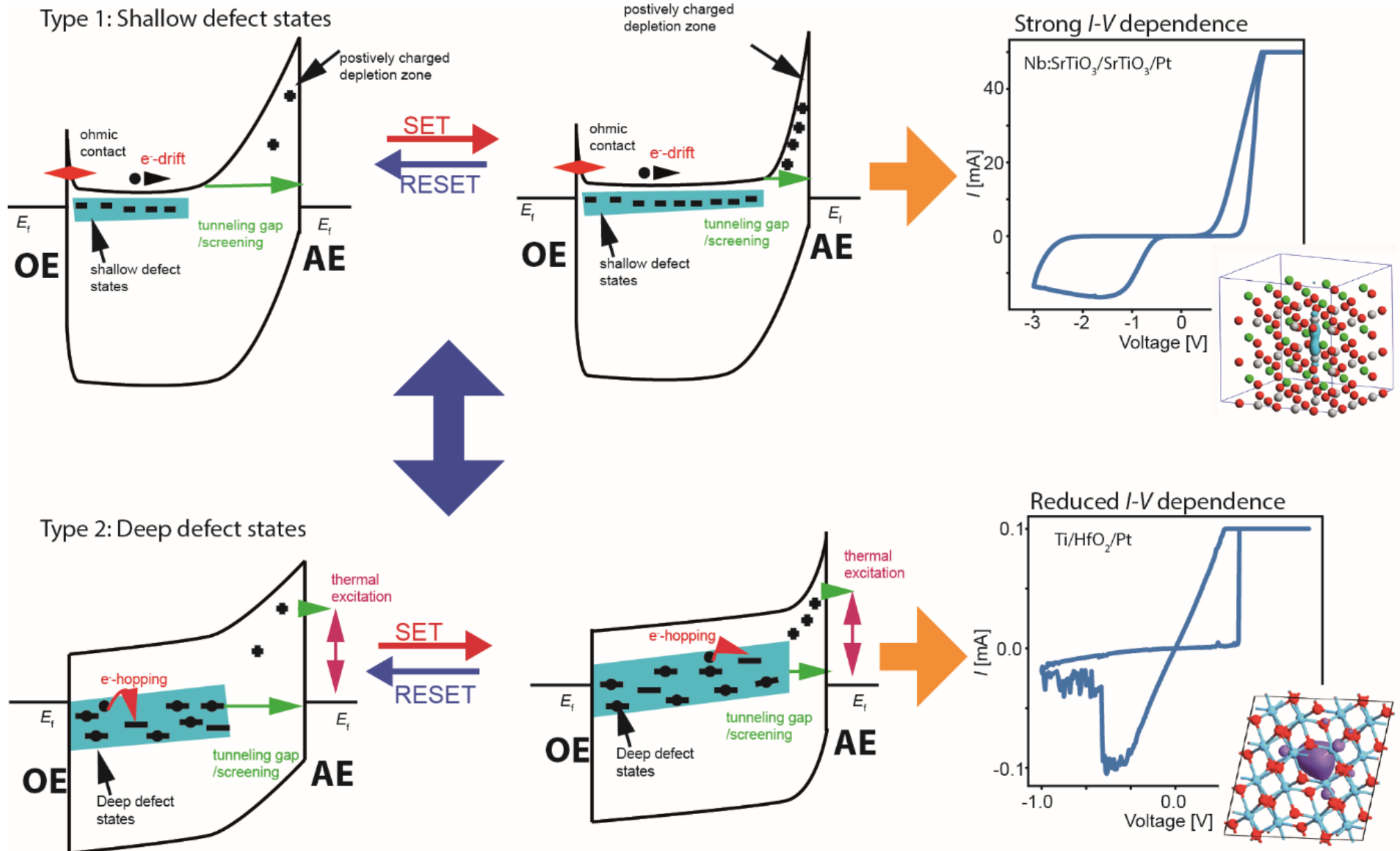


DFT-NEGF Simulation of the LRS

C. Funck, S. Menzel, *ACS Appl. Electron.*,
vol. 3, 3674-3692, (2021)



General Switching Mechanism



Outline



Motivation



Electronic Transport in VCM Cells:
A DFT-NEGF study



**Switching Variability of VCM Cells:
Kinetic Monte Carlo Modeling**



Switching Dynamics of VCM Cells:
Continuum Modeling



Towards Circuit Simulations:
VCM Compact Models (JART)



Array Level Modeling



Summary & Conclusion

KMC Model I: Electronic Model

Simulation geometry

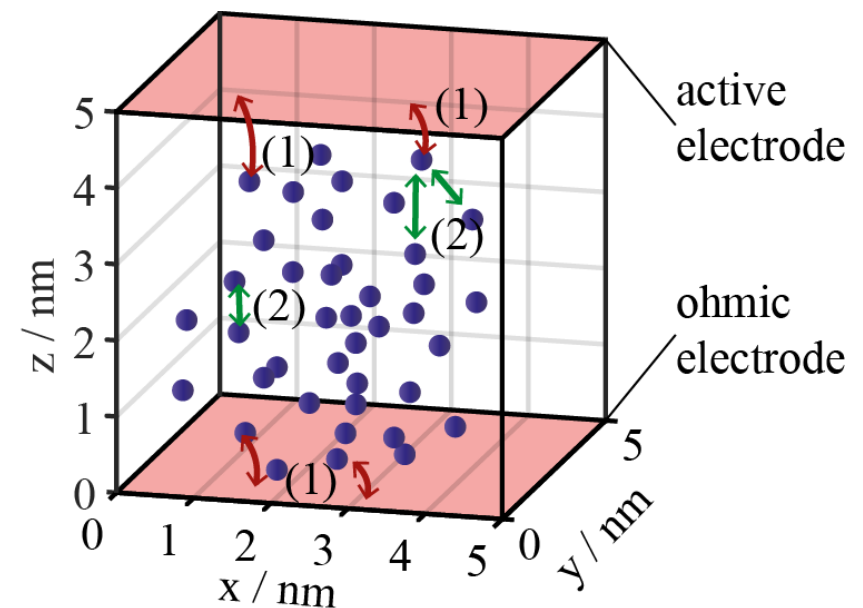
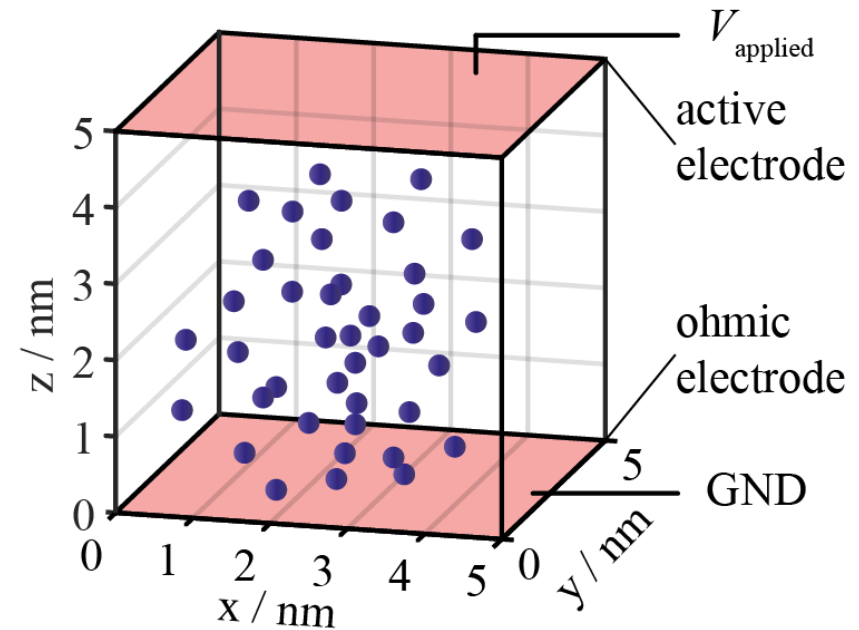
- Oxide cube of 5 nm x 5 nm x 5 nm
- Possible defect sites every 0.5 nm ($= a$)
- Active (AE) and ohmic electrode (OE)

Defects

- Oxygen vacancies $V_O^{\bullet\bullet}$
- Reduced cations close to $V_O^{\bullet\bullet}$ act as electron traps

Conduction mechanism (Type II)

- Trap assisted tunnelling
- (1) e^- tunneling between electrode & traps
- (2) e^- hopping between traps
- At high defect densities band conduction



KMC Model II: Ionic Model

Dynamic model

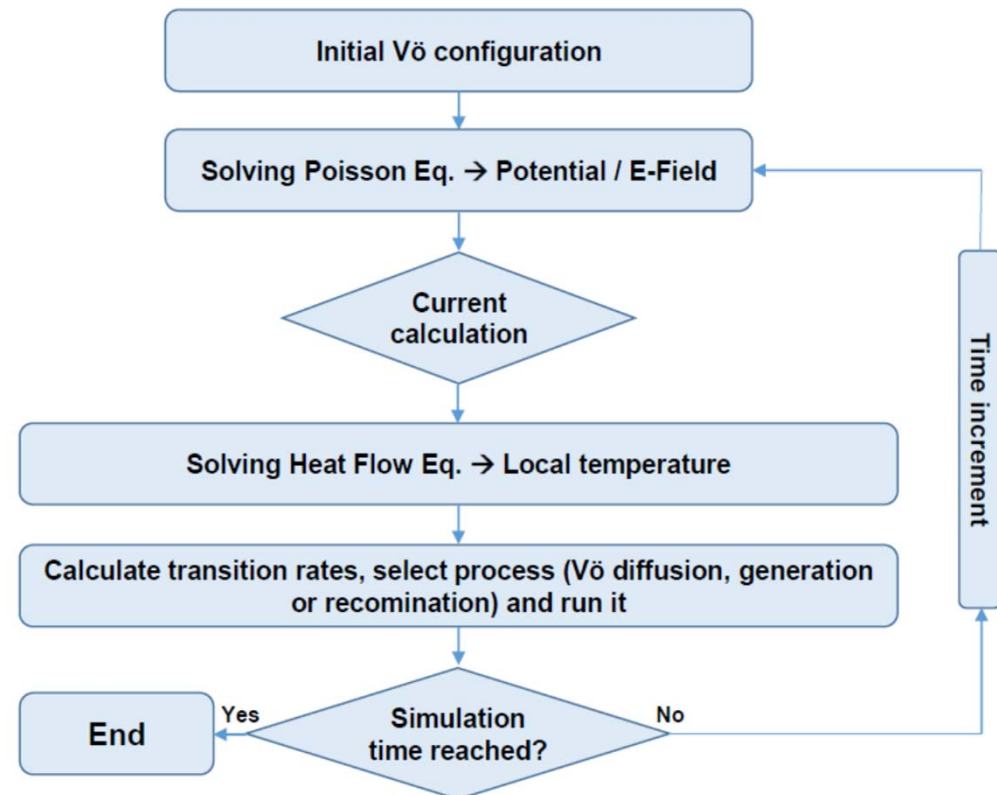
- Joule heating
- Oxygen exchange reaction at BE
- $V_O^{\bullet}$ hopping

$$\Gamma_{G,R,D} = \nu_0 \exp\left(-\frac{\Delta W_{G,R,D} - \alpha_i zE}{k_B T}\right)$$

- Weighted random selection of process
- Time increment

$$\Delta t = -\frac{\ln(\Gamma_i)}{\Gamma_{\text{total}}}$$

Simulation flow

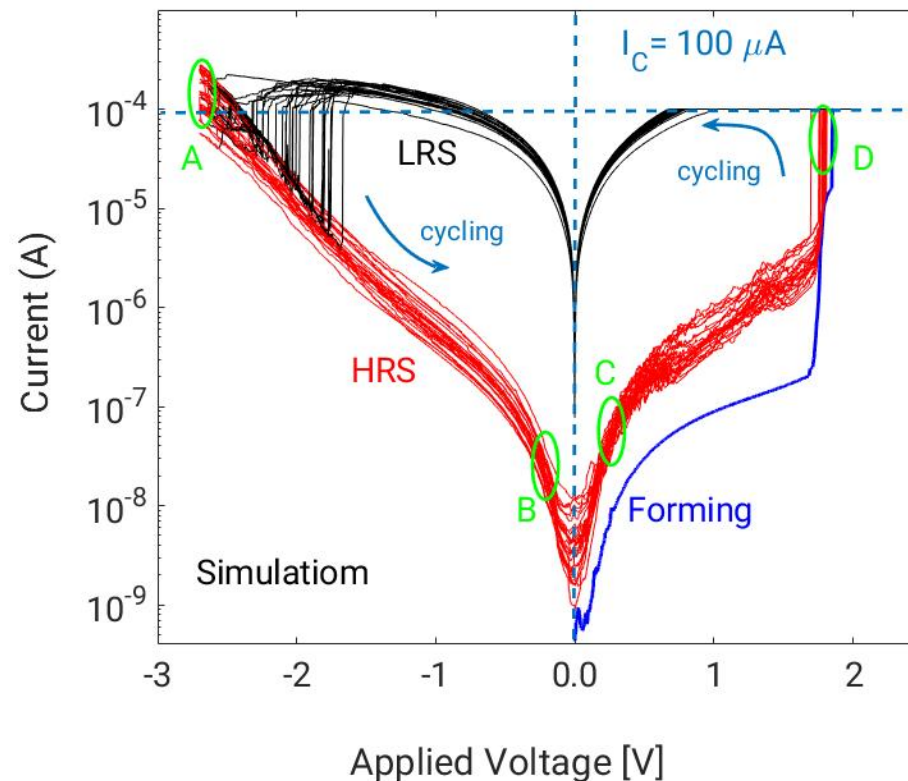


E. Abbaspour, S. Menzel, C. Jungemann et. al,
IEEE Trans. Nanotechnology, vol. 17, no. 6, pp. 1181-1188 (2018)

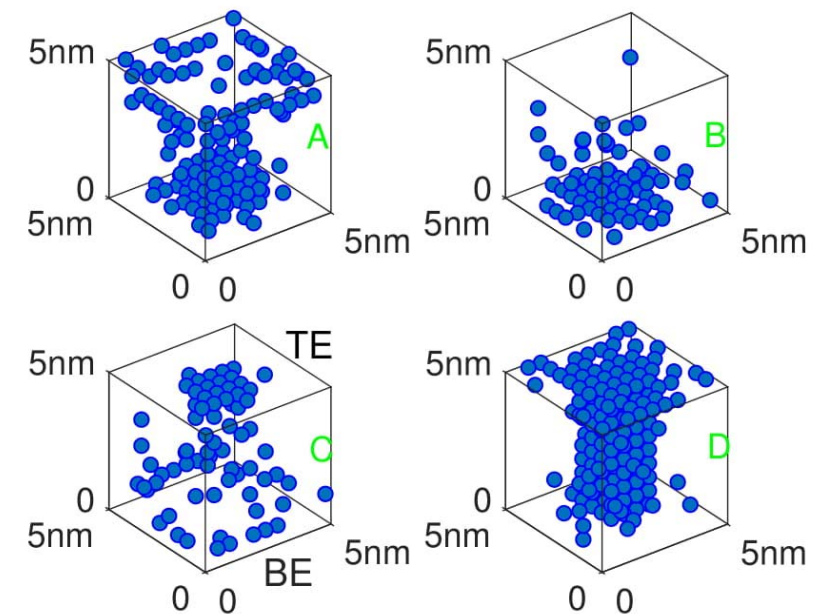
E. Abbaspour, S. Menzel, C. Jungemann, *Journal of Computational Electronics*, vol. 19, pp. 1426-1432 (2020)

Origin of the Switching Variability: Stochasticity

Simulation of 100 I - V cycles



Filament evolution

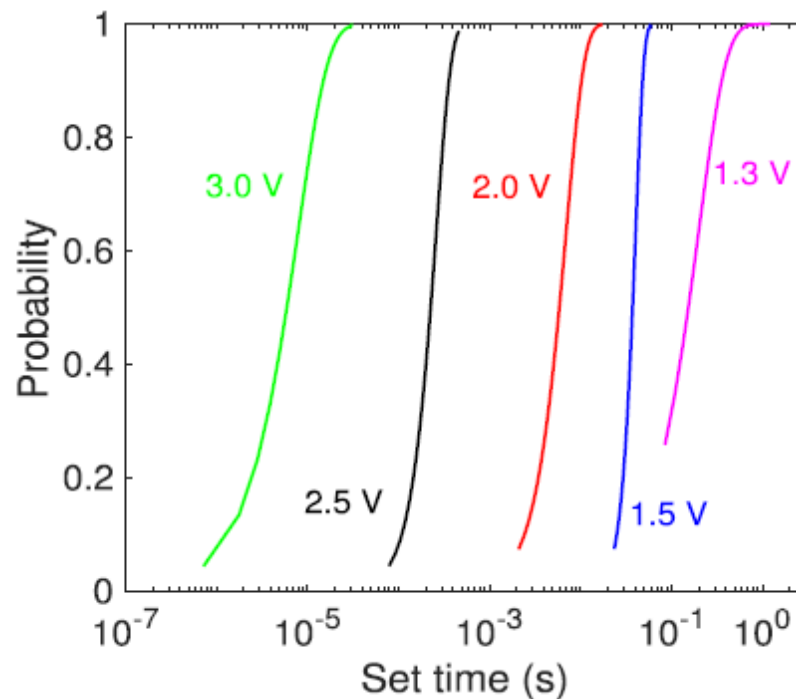


→ Typical SET/RESET switching obtained

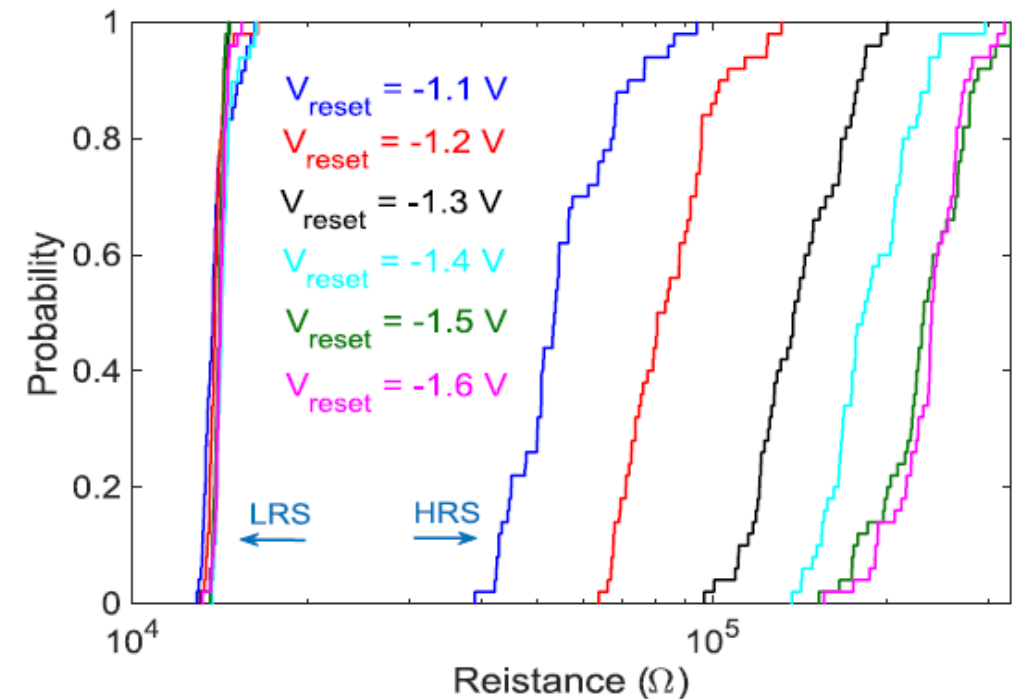
E. Abbaspour, S. Menzel, C. Jungemann et. al,
IEEE Trans. Nanotechnology, vol. 17, no. 6, pp. 1181-1188 (2018)

Origin of the Switching Variability: Stochasticity II

SET switching probability



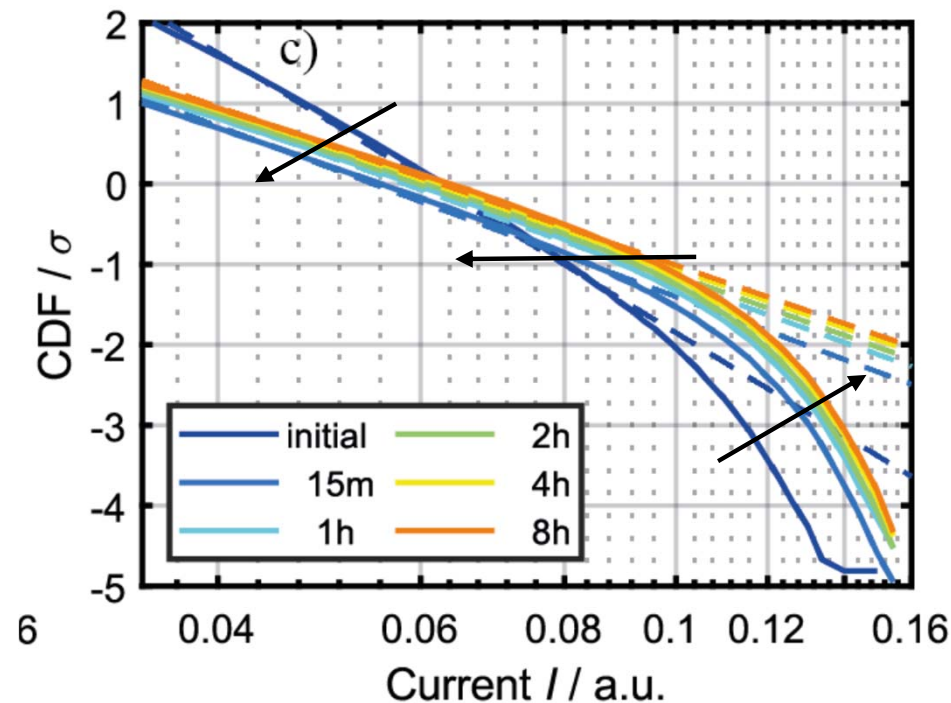
HRS/LRS distributions



- Distributions tighter than in experiment
- Stochasticity is not sufficient to explain variability

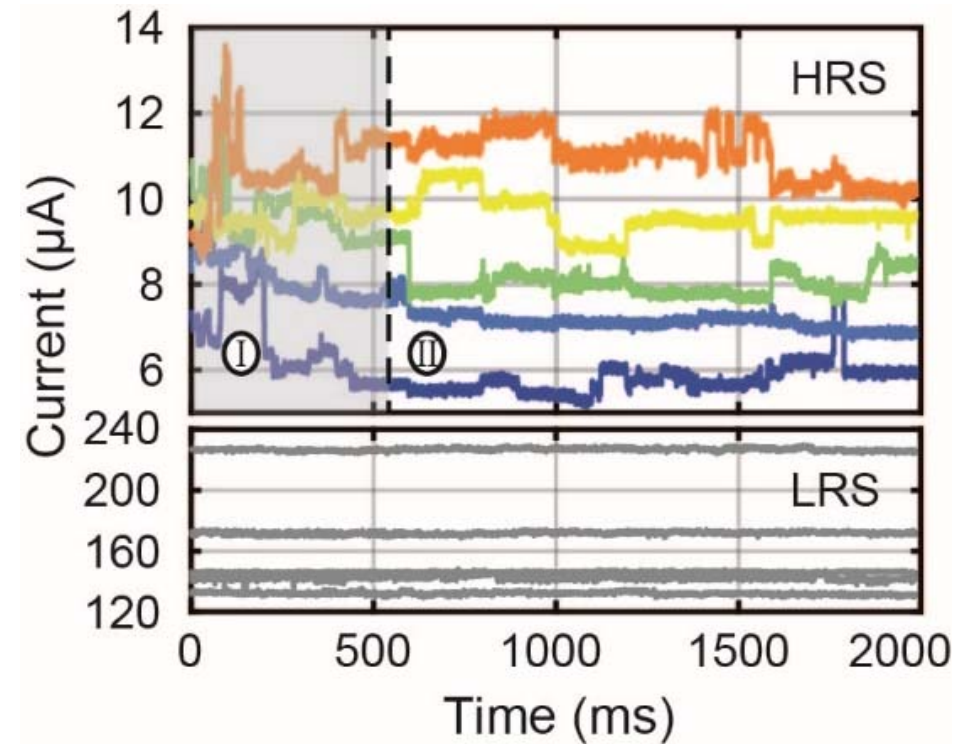
Relation between Read Instability & Retention

Retention (shifts & tilts)



S. Wiefels, S. Menzel et al.,
IEEE IMW (2020)

Read instability

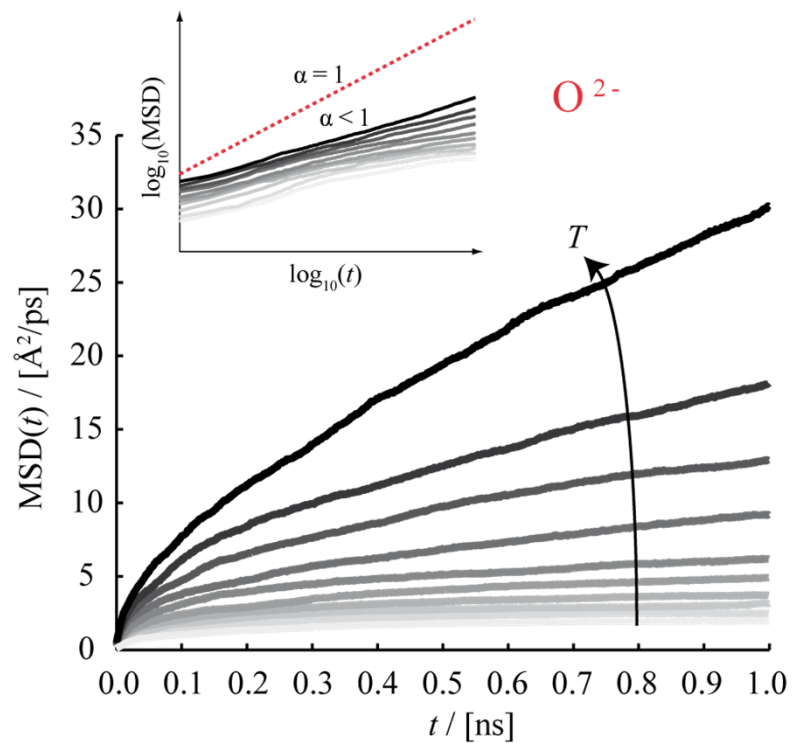


S. Wiefels, S. Menzel et al., *IEEE T-ED*,
vol. 67, no. 10, pp. 4208-4215 (2020)

→ Both processes depends on ionic motion,
but occur on different timescales !?

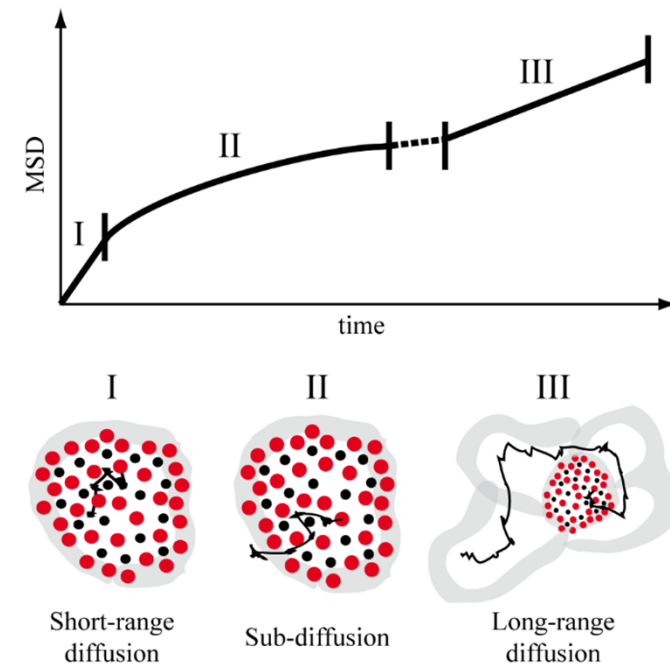
Physical Model Idea

MD Simulation of ion transport in amorphous HfO_2



M. Schie, R. de Souza et al., *J. Chem. Phys.*, vol. 9, no. 146, 94508 (2017)

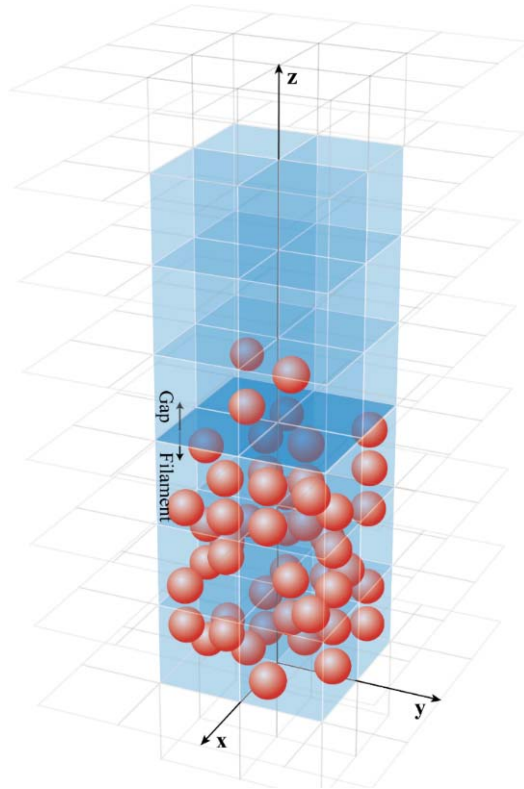
Sub-diffusive transport



→ Different diffusive regions

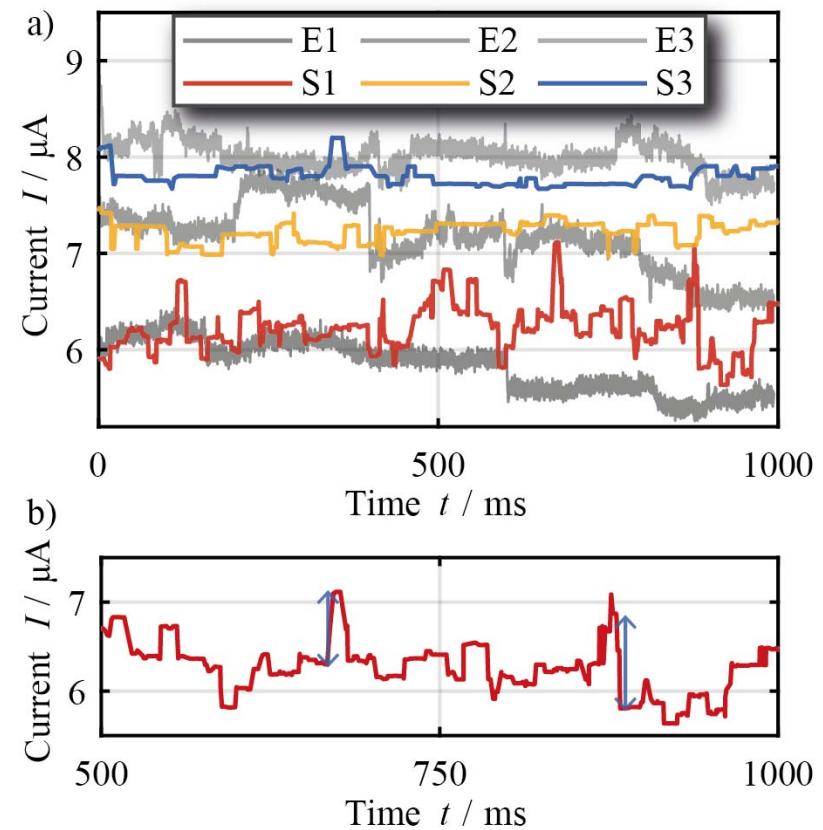
KMC Multi-Domain Model I

Model



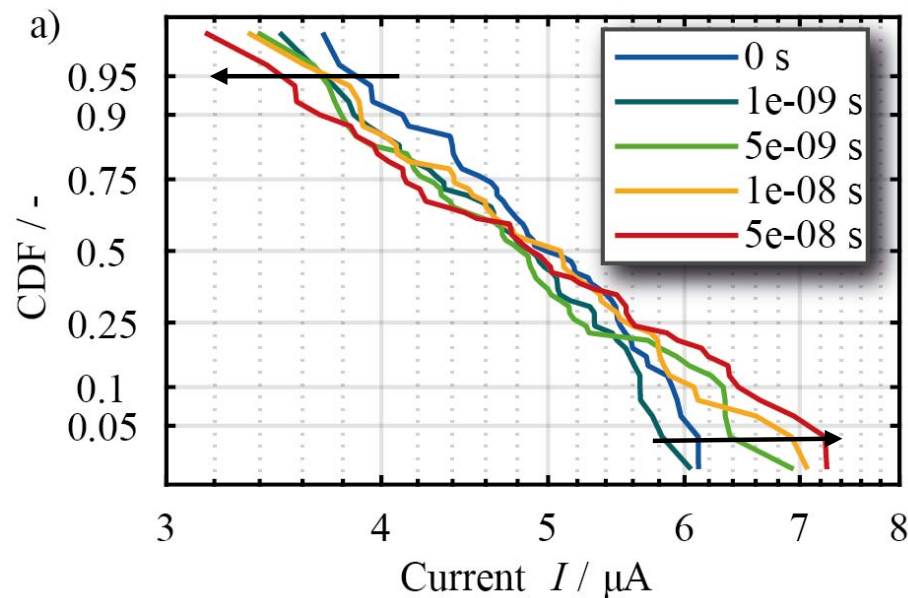
→ Read instability due to jumps in the boxes

Read Instability

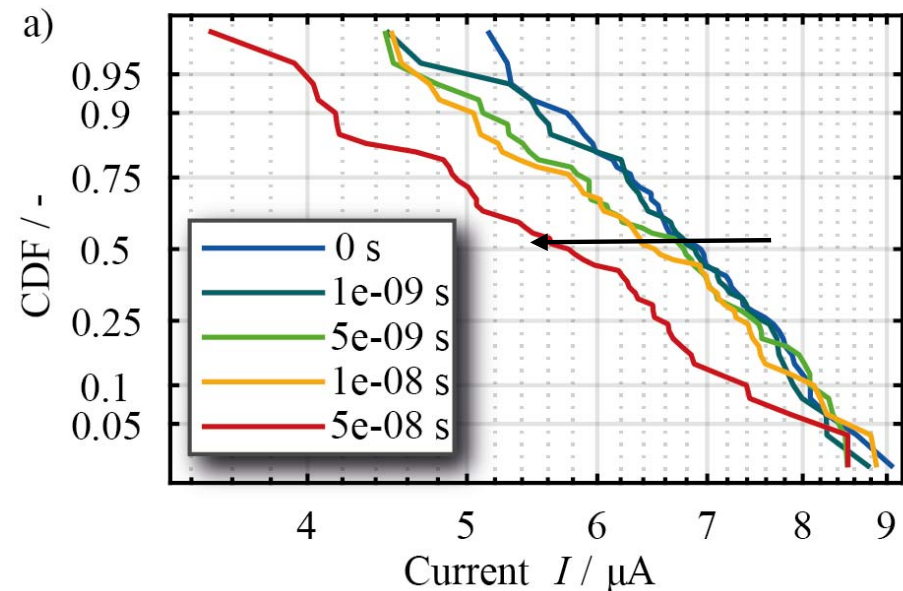


KMC Multi-Domain Model II

Tilting of the distribution



Shift of the distribution



- Retention due to jumps out of the boxes
- depends on initial state

Outline



Motivation



Electronic Transport in VCM Cells:
A DFT-NEGF study



Switching Variability of VCM Cells:
Kinetic Monte Carlo Modeling



**Switching Dynamics of VCM Cells:
Continuum Modeling**



Towards Circuit Simulations:
VCM Compact Models (JART)



Array Level Modeling



Summary & Conclusion

VCM Continuum Model I: Equation system

Non-isothermal drift-diffusion equation for doubly charged V_O

$$\frac{\partial N_{V_O}^{2+}}{\partial t} - \nabla \left(\mu_{V_O} N_{V_O}^{2+} \nabla \psi + D_{V_O} \nabla N_{V_O}^{2+} - N_{V_O}^{2+} D_{TV_O} \nabla T \right) = -R_{V_O,2}$$

Drift-diffusion equation for electrons (Type I)

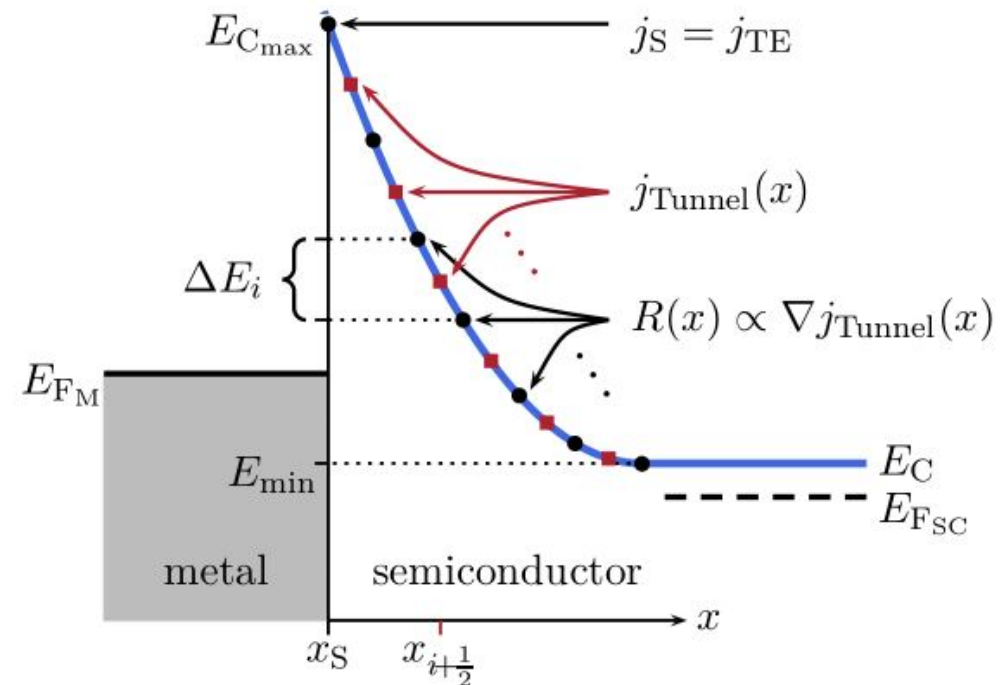
$$\nabla \left(\mu_n n \nabla \psi - D_n \nabla n + e D_{Tn} \nabla T \right) = \pm \frac{\partial j_{n,tunnel}}{\partial x}$$

Poisson equation

$$\nabla (\varepsilon \nabla \psi) = -e (n - N_{V_O}^+ - 2N_{V_O}^{2+})$$

Heat equation

$$-\nabla (k \nabla T) = jF$$



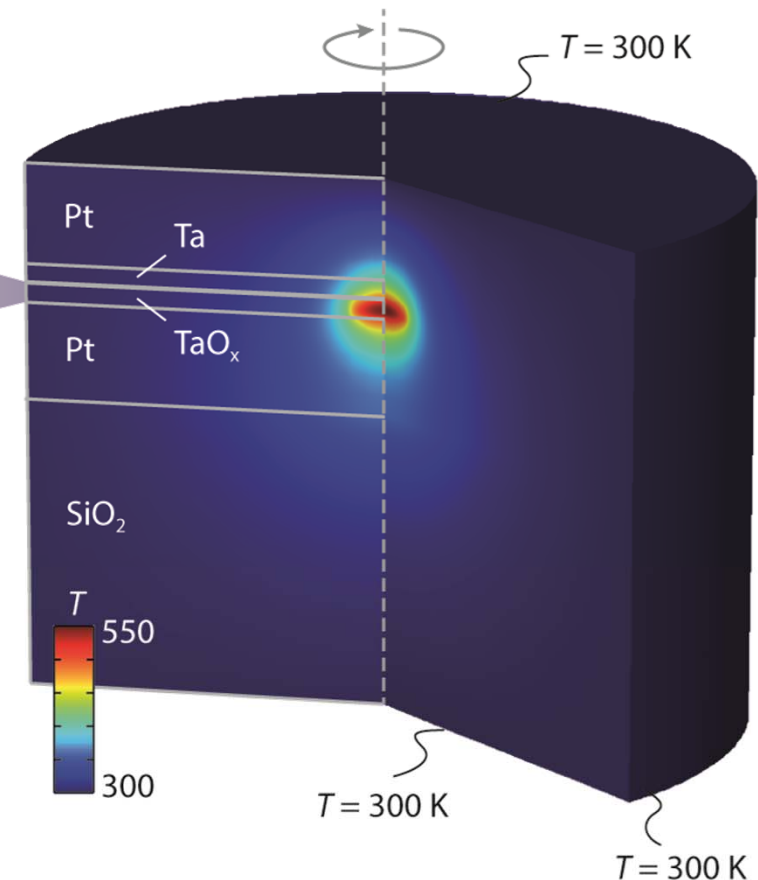
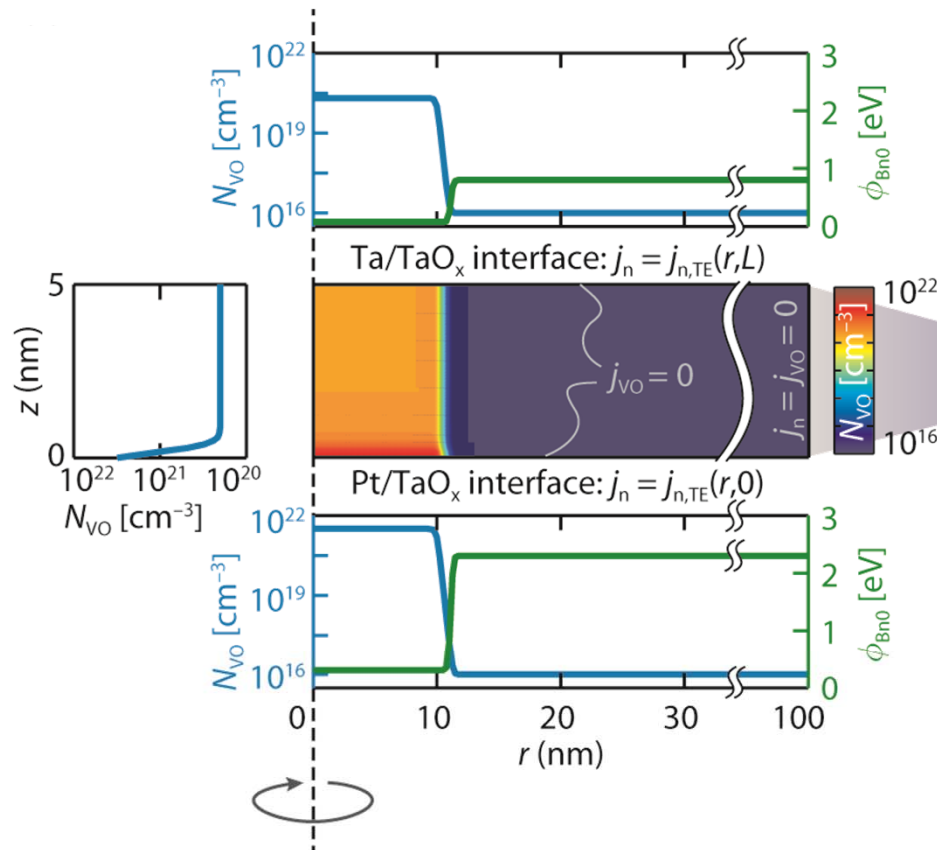
A. Marchewka, S. Menzel et al.,
Adv. Electron. Mater., 2016, vol. 2, no. 1

A. Marchewka, S. Menzel et al., SISPAD (2015)

VCM Continuum Model II: 2D Domains and Initial Conditions

Drift-diffusion equation

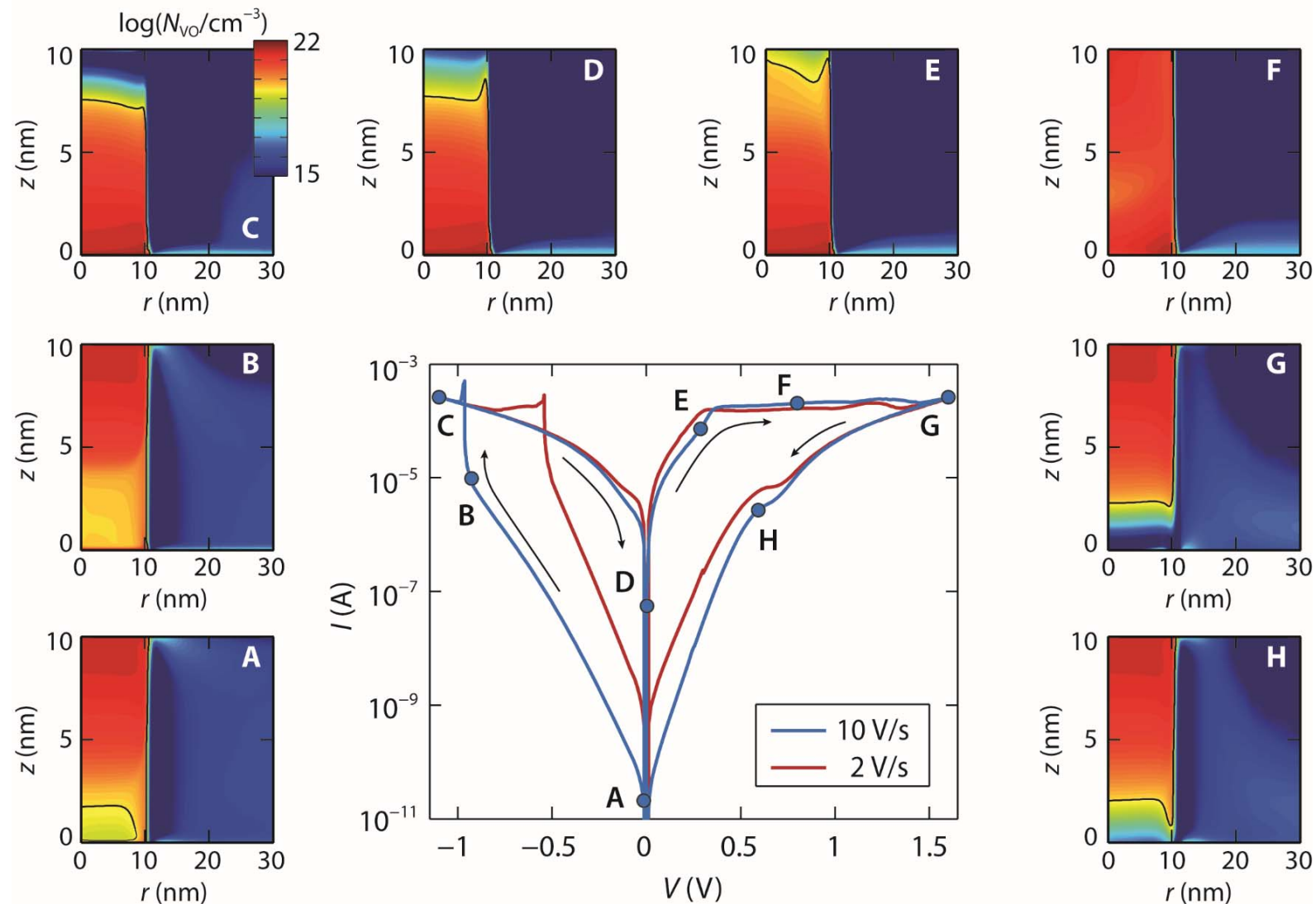
Heat transfer equation



A. Marchewka, S. Menzel et al.,
Adv. Electron. Mater., vol. 2, no. 1, 1500233 (2016)

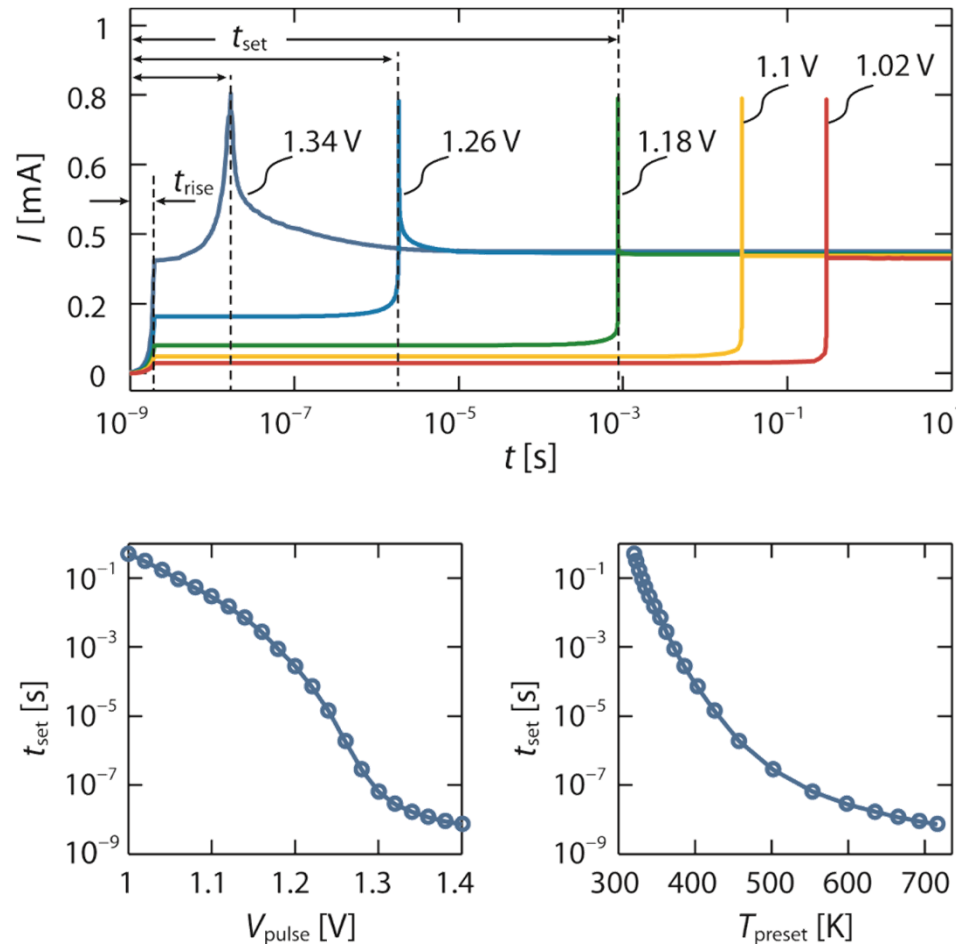
Simulated I - V Characteristics

A. Marchewka, S. Menzel et al.,
SISPAD 2016

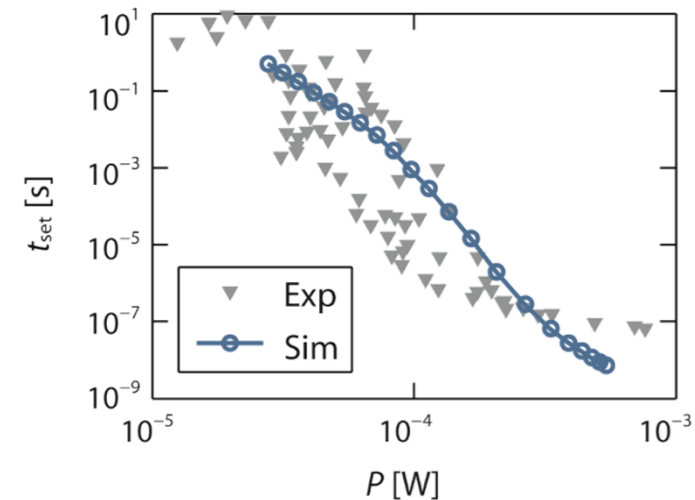


→ Bipolar c8w-switching due to asymmetric barriers
(change of concentration in front of active electrode dominant)

Continuum Modeling of SET Dynamics



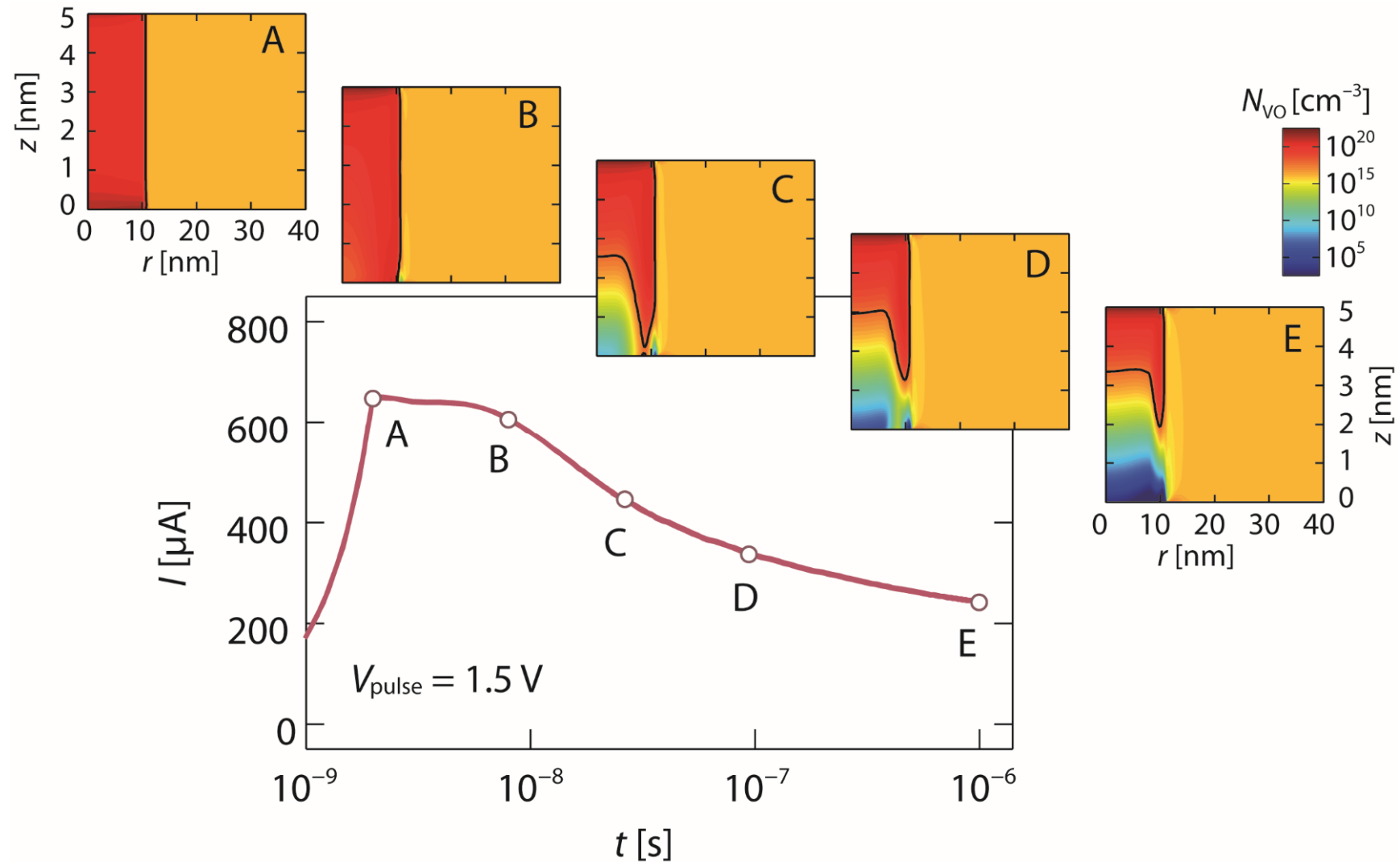
Comparison to Pt/SrTiO₃/Ti cell



A. Marchewka, S. Menzel et al.,
SISPAD (2015)

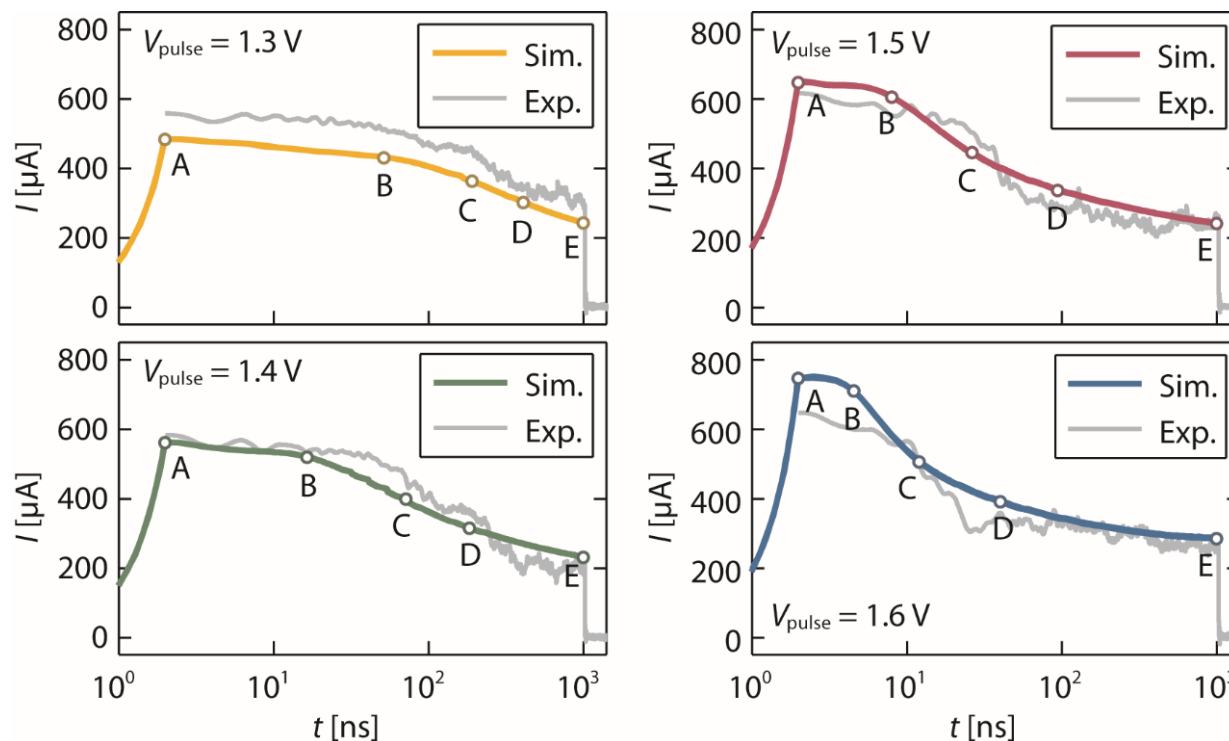
- Simulated current transients reproduce experimental behavior
- Simulation model reproduces experimental power dependence

RESET Kinetics I: Simulation Results

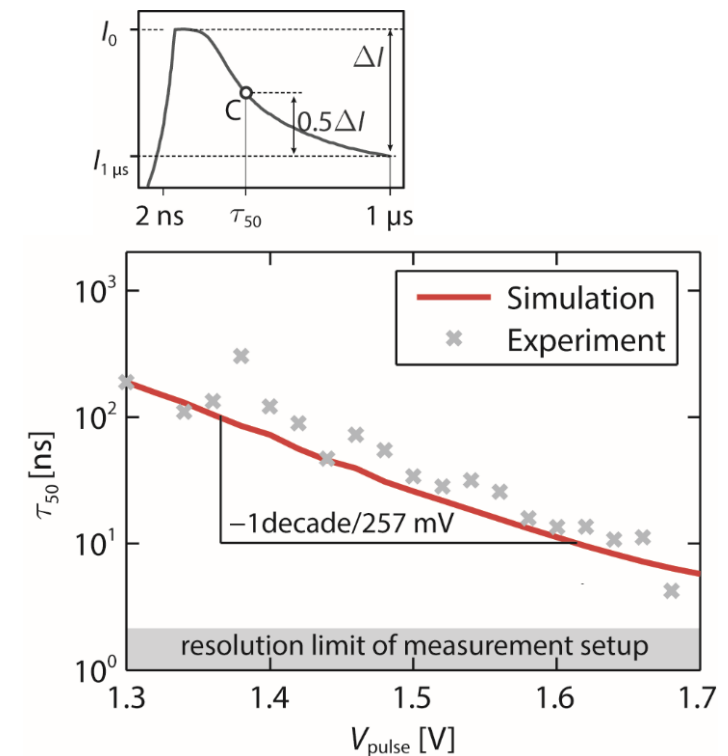


RESET Kinetics II: Simulation Results

Transient currents



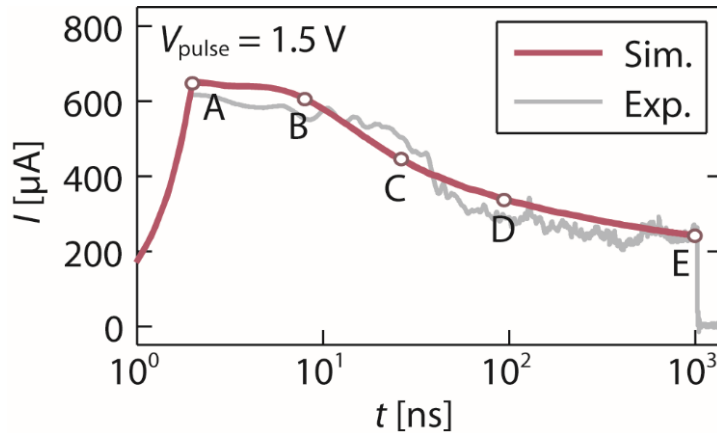
Decay times



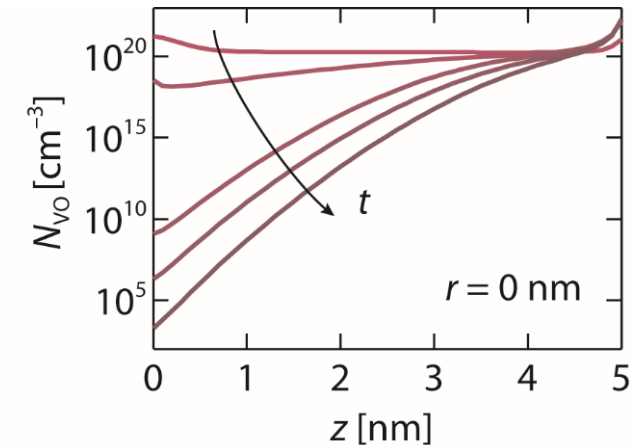
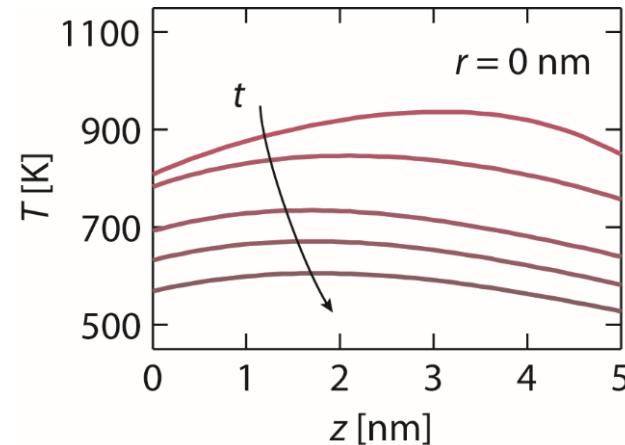
→ RESET kinetics can be explained by ion migration

VCM RESET Kinetics III: Simulation Results (2D)

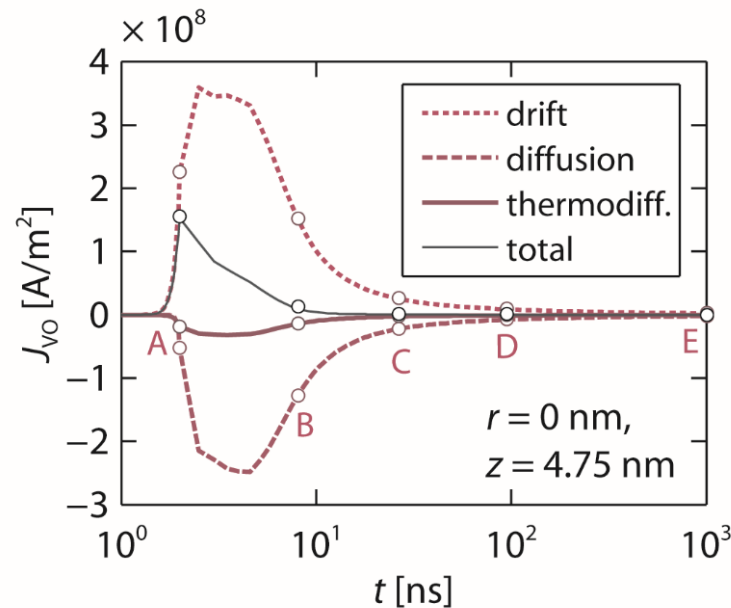
Transient current



Temperature and vacancy distributions



Transient vacancy current density



→ Gradual RESET due to balance between drift and diffusion

A. Marchewka, S. Menzel et al., *Adv. Electron. Mater.*, vol. 2, no. 1, 1500233 (2016)

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**Towards Circuit Simulations:
VCM Compact Models (JART)**



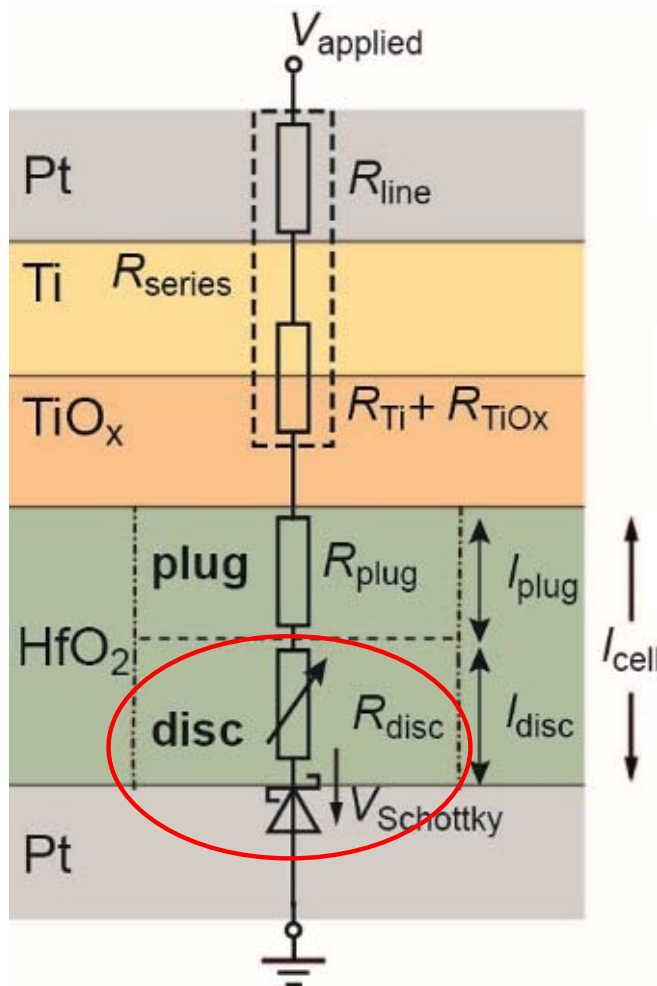
Array Level Modeling



Summary & Conclusion

C. Bengel, S. Hoffmann-Eifert,
S. Menzel et al., *IEEE T-CAS I*, vol.
67, no. 12, pp. 4618-4630 (2020)

Equivalent circuit diagram



Series resistance

$$\begin{aligned} R_{\text{series}} &= R_{\text{line}} + R_{\text{TiOx}} \\ &= R_{\text{TiOx}} + R_0 \left(1 + \alpha_{\text{line}} R_0 I^2 R_{\text{th, line}} \right) \end{aligned}$$

Plug resistance

$$R_{\text{plug}} = \frac{l_{\text{cell}} - l_{\text{var}}}{z_{\text{Vo}} e \mu_n A N_{\text{plug}}}$$

Disc resistance

$$R_{\text{disc}} = \frac{l_{\text{var}}}{z_{\text{Vo}} e \mu_n A N_{\text{disc}}}$$

MI interface (V_{schottky})

Forward direction: Thermionic emission (TE)

Reverse direction: Thermionic field emission (TFE)

→ Conductance is defined by defect concentration close to the Pt electrode N_{disc}

JART VCM v1 Model II: Ionic Model

Driving force for is ionic current

$$\frac{dN_{\text{disc}}}{dt} = -\frac{I_{\text{ion}}}{ez_{\text{Vo}}Al_{\text{var}}}$$

$$I_{\text{ion}} = ez_{\text{Vo}}c_{\text{Vo}}a_{\text{Vo}}F_{\text{limit}}A \cdot \left(\exp\left(-\frac{\Delta W_{\text{min}}}{k_{\text{B}}T}\right) - \exp\left(-\frac{\Delta W_{\text{max}}}{k_{\text{B}}T}\right) \right)$$

$$= f(E, T)$$

Electric field

$$\text{FB: } E = (V_{\text{disc}} + V_{\text{Schottky}} + V_{\text{plug}}) / l_{\text{cell}}$$

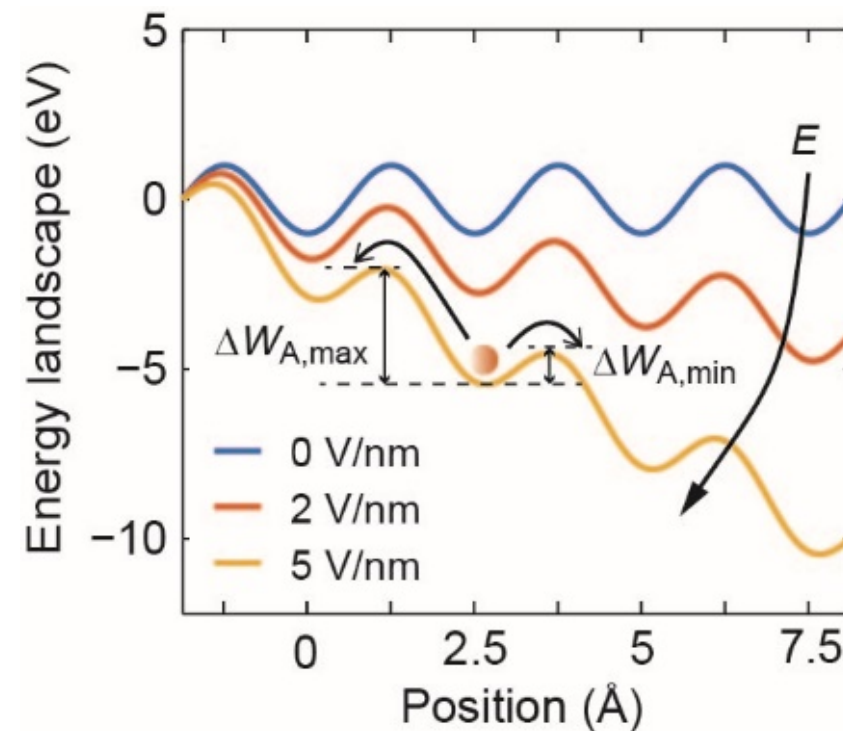
$$\text{RB: } E = V_{\text{disc}} / l_{\text{disc}}$$

Joule heating

$$T = T_0 + R_{\text{th,SET}} P_{\text{device}} \quad \text{SET}$$

$$T = T_0 + R_{\text{th,RESET}} P_{\text{device}} \quad \text{RESET}$$

Ion in periodic lattice

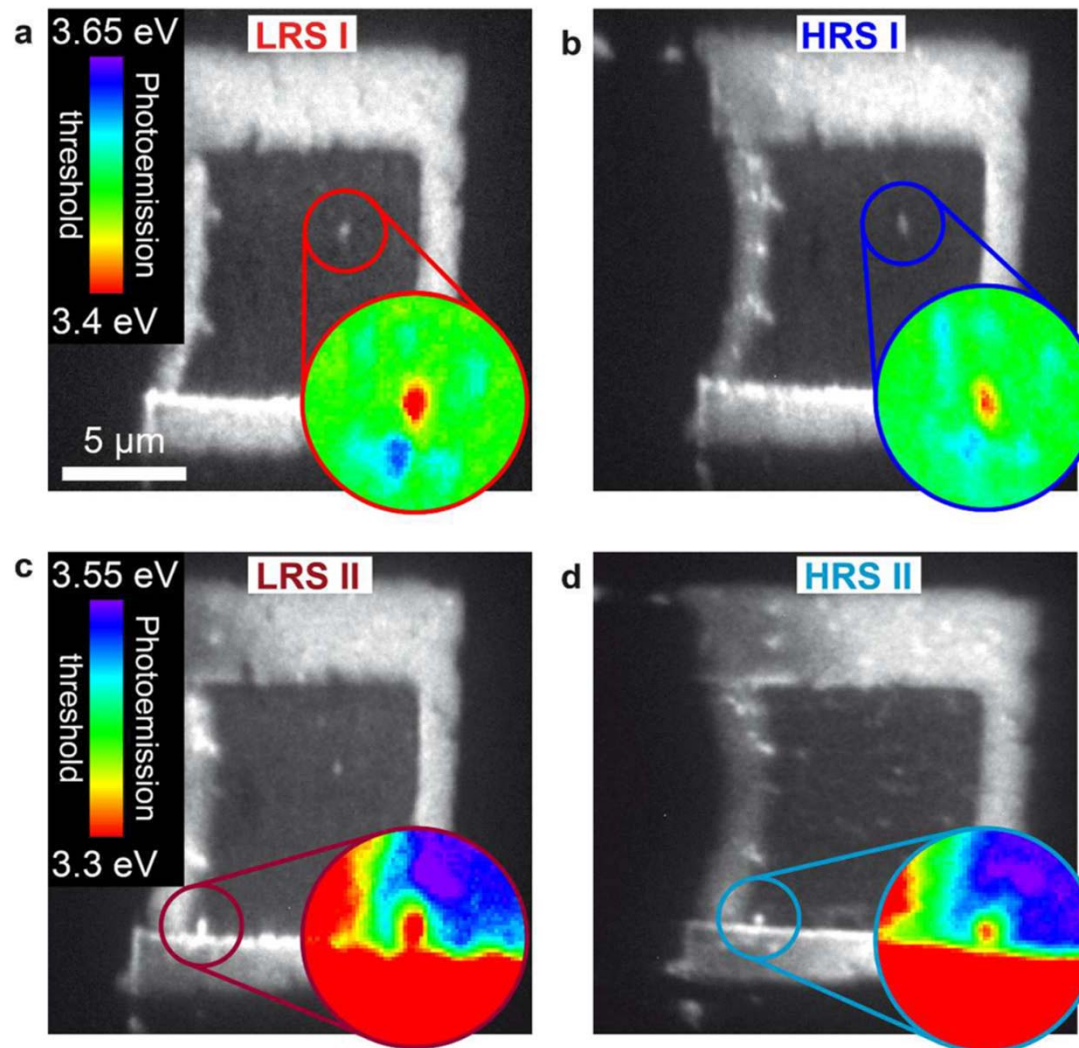


S. Menzel et al., *Faraday Discussions*
vol. 213, pp. 197-213 (2018)

A. Genreith-Schrieffer, et al., *Phys. Rev. B*
vol. 94, no. 22, pp. 224304 (2016)

Physical Origin of the Switching Variability

PEEM analysis of SrTiO_3 -based cells



→ Parallel growth of multiple filaments

→ One filament „wins“ during SET

→ Variability due to change of filament location and geometry

C. Baeumer, R.Dittmann, et al., *ACS Nano*, vol. 11, no. 7, pp. 6921-6929 (2017)

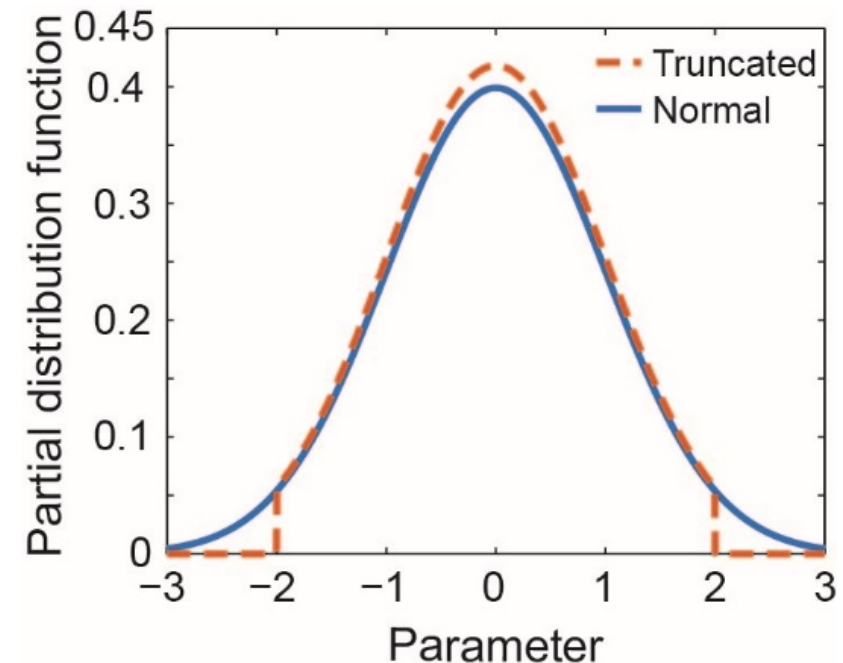
JART VCM v1: Modeling the Switching Variability I

→ Variability due change in filament properties

Device-to-device variability

Parameter are chosen randomly from a truncated Gaussian distribution

- Minimum disc concentration $N_{\text{disc,min}}$
- Maximum disc concentration $N_{\text{disc,max}}$
- Filament radius r
- Disc length l



C. Bengel, S. Hoffmann-Eifert, S. Menzel et al.,
IEEE T-CAS I, vol. 67, no. 12, pp. 4618-4630 (2020)

JART VCM v1: Modeling the Switching Variability II

Cycle-to-cycle variability

Random walk algorithm is used to change the parameters from c2c

$$\xi_k = \xi_{k-1} (1 \pm \Delta \xi_{\max} \cdot P) \quad P \in (0,1)$$

Change of r , and l depends on N_{disc}

SET

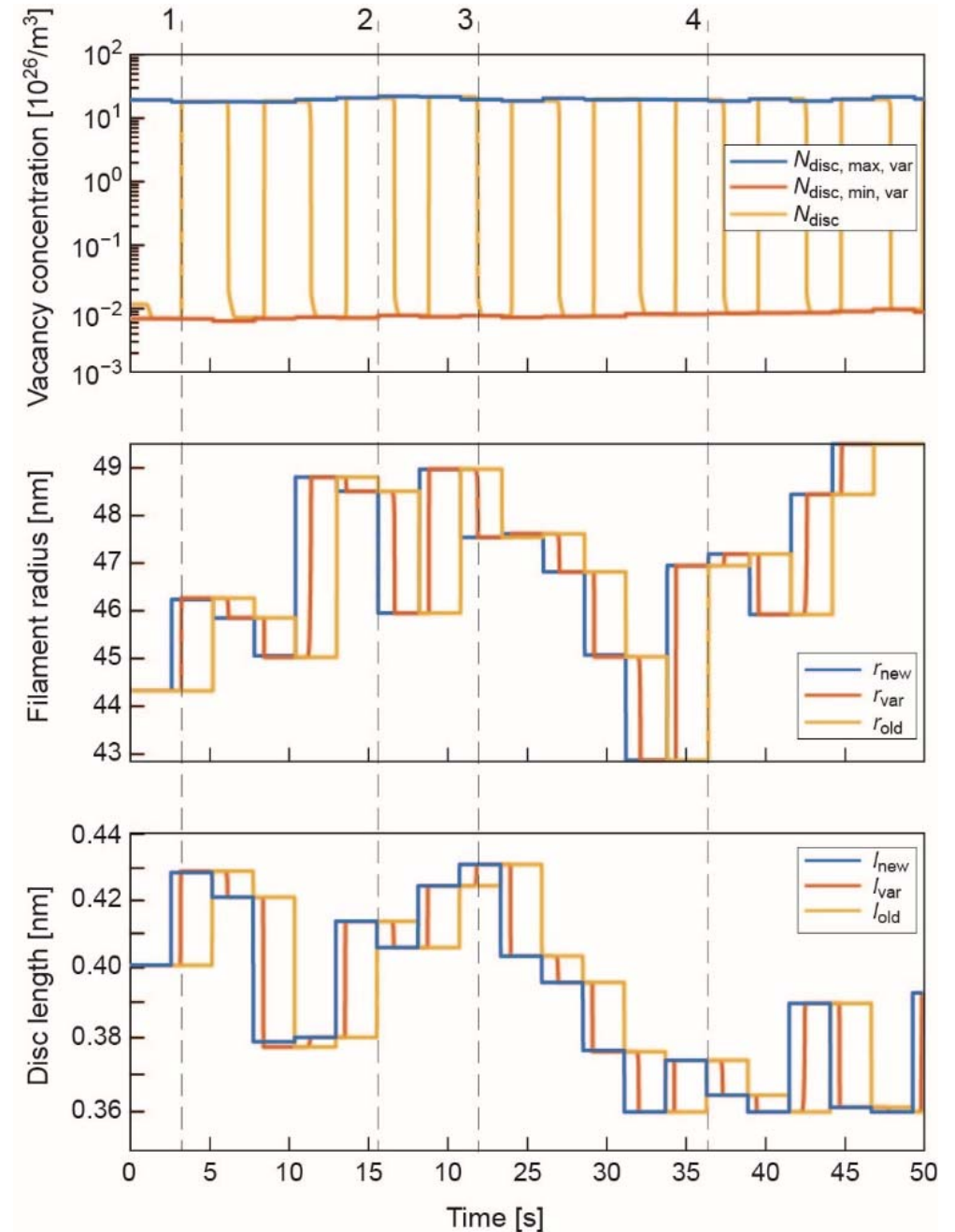
$$r_{\text{var}} = r_{\text{old}} + (r_{\text{new}} - r_{\text{old}}) \left(\frac{N_{\text{disc}} - N_{\text{disc,old}}}{N_{\text{disc,max,var}} - N_{\text{disc,old}}} \right)$$

$$l_{\text{var}} = l_{\text{old}} + (l_{\text{new}} - l_{\text{old}}) \left(\frac{N_{\text{disc}} - N_{\text{disc,old}}}{N_{\text{disc,max,var}} - N_{\text{disc,old}}} \right)$$

RESET

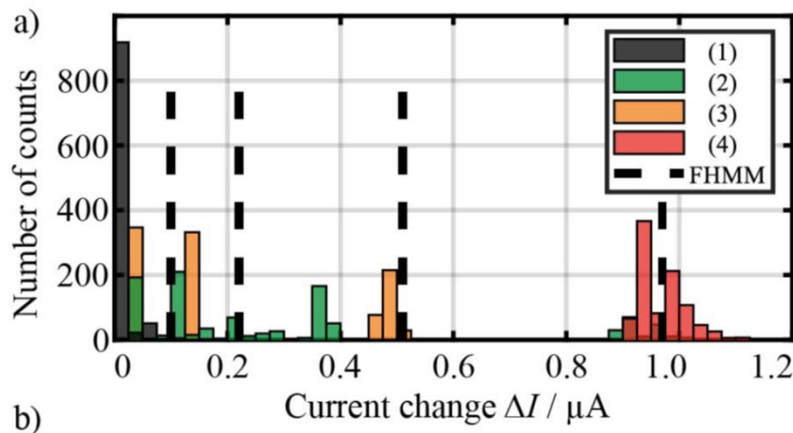
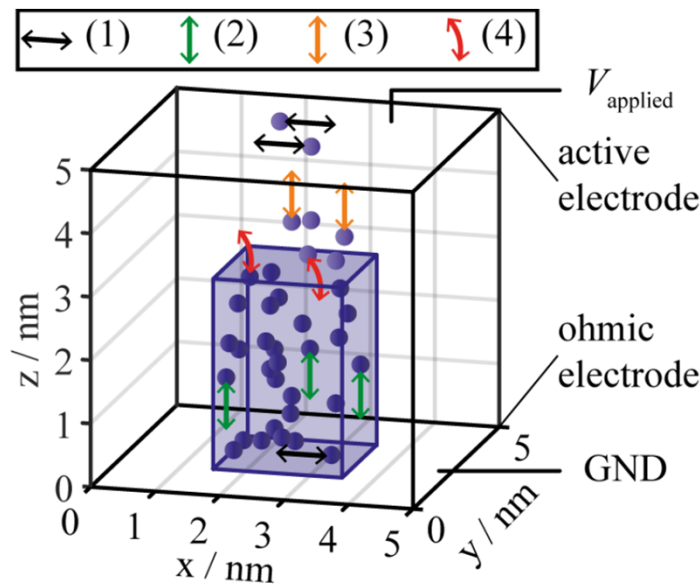
$$r_{\text{var}} = r_{\text{old}} + (r_{\text{new}} - r_{\text{old}}) \left(\frac{N_{\text{disc,old}} - N_{\text{disc}}}{N_{\text{disc,old}} - N_{\text{disc,min,var}}} \right)$$

$$l_{\text{var}} = l_{\text{old}} + (l_{\text{new}} - l_{\text{old}}) \left(\frac{N_{\text{disc,old}} - N_{\text{disc}}}{N_{\text{disc,old}} - N_{\text{disc,min,var}}} \right)$$



JART VCM v1: Modeling Read Noise

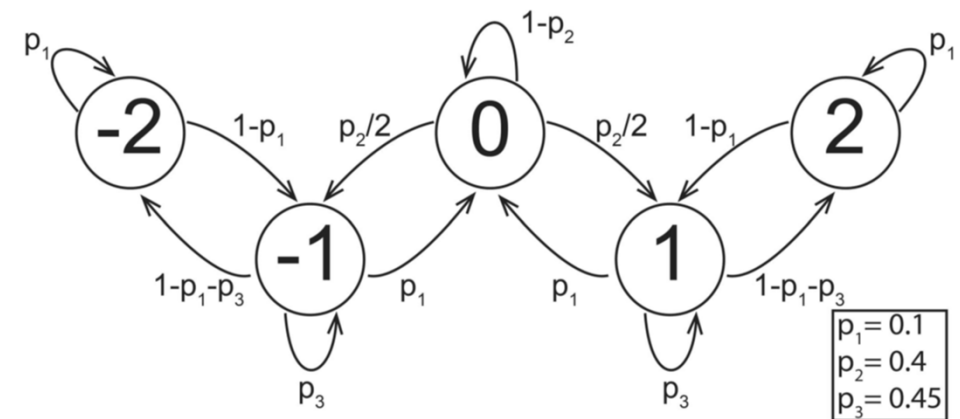
Physical Origin



Read instability model

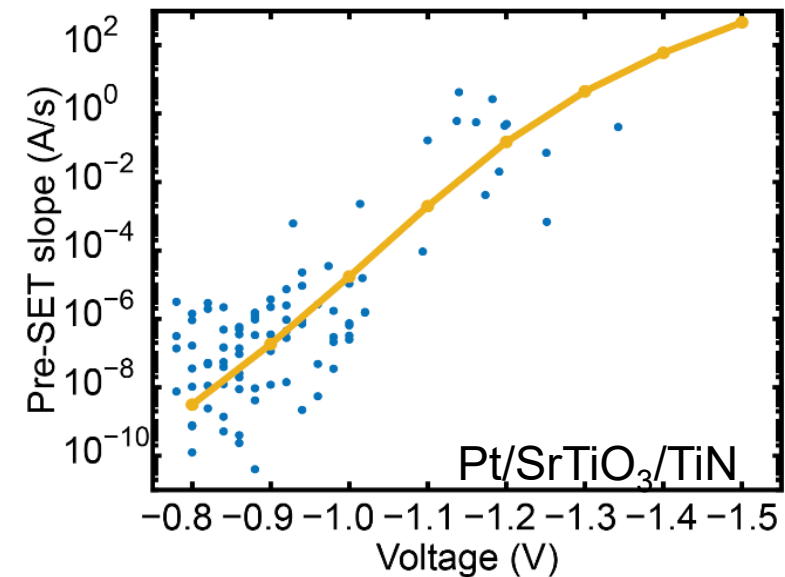
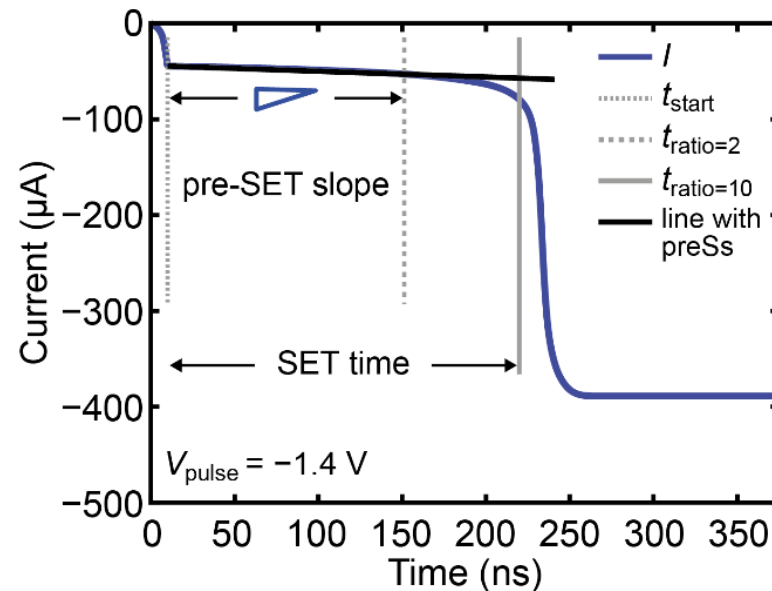
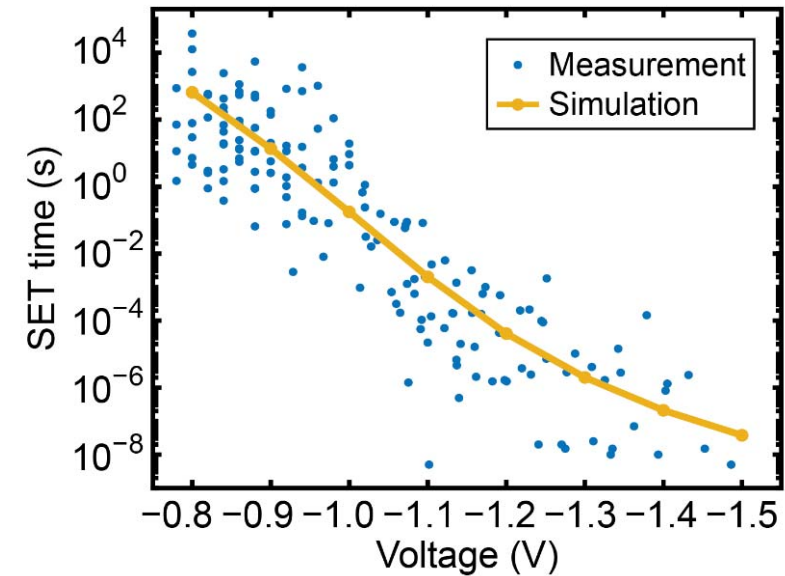
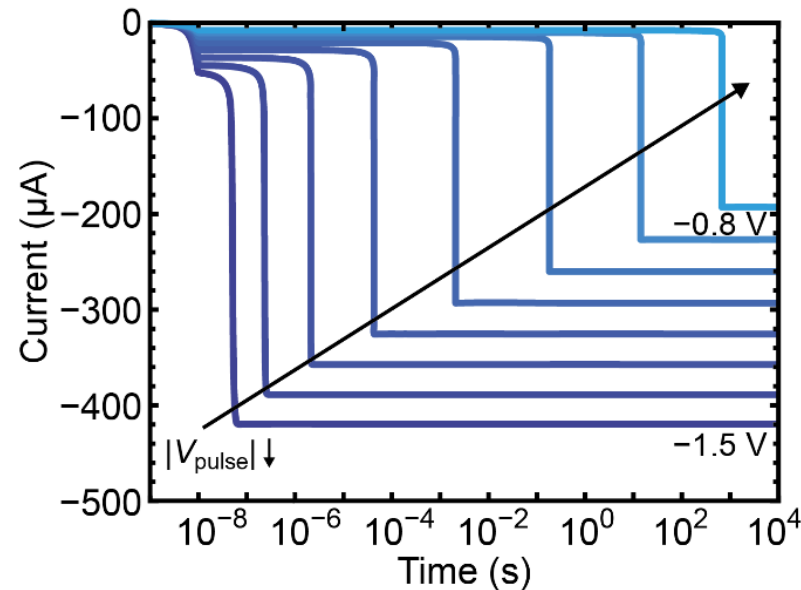
- Most important jump between plug to disc
- Change of N_{disc} by $\pm 1, \pm 2$ defects

Implemented using state machine



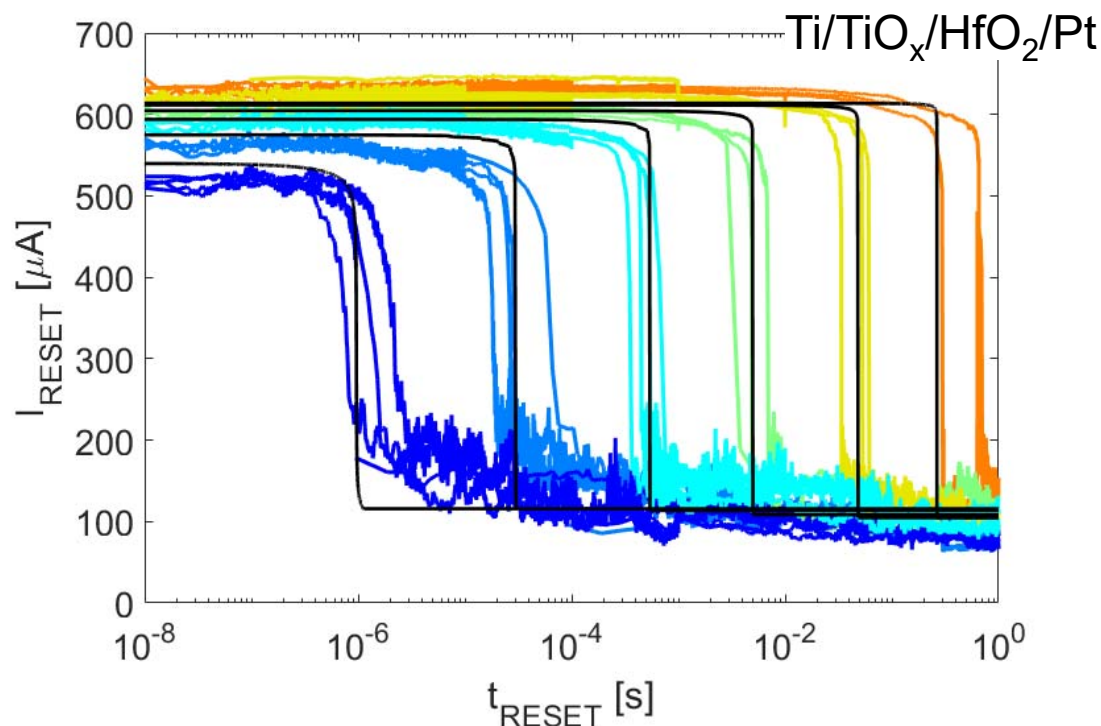
S. Wiefels, S. Menzel et al., *IEEE T-ED*,
vol. 67, no. 10, pp. 4208-4215 (2020)

Compact Modeling of SET Dynamics

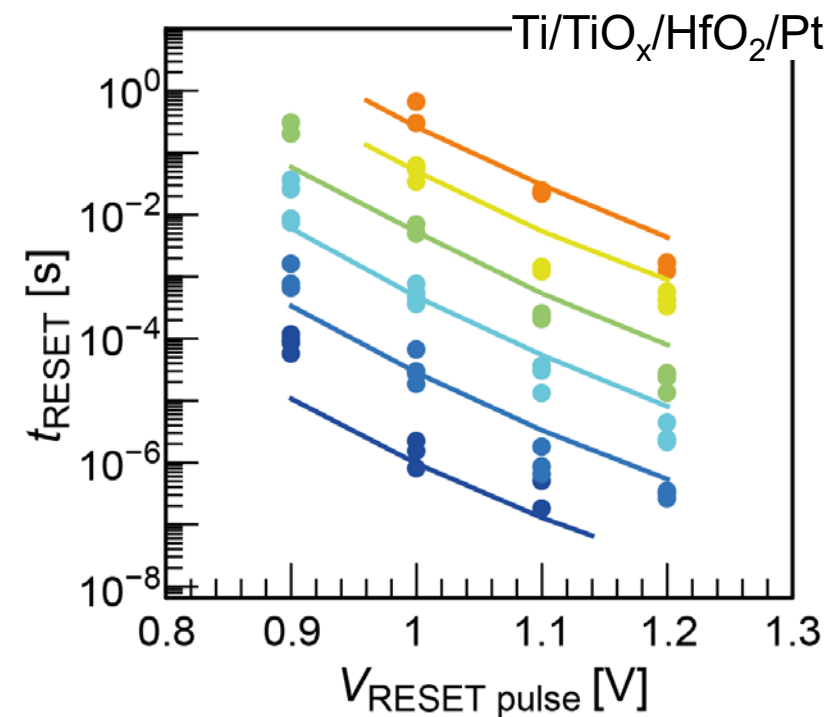


Compact Modeling of RESET Dynamics

RESET transients



RESET kinetics



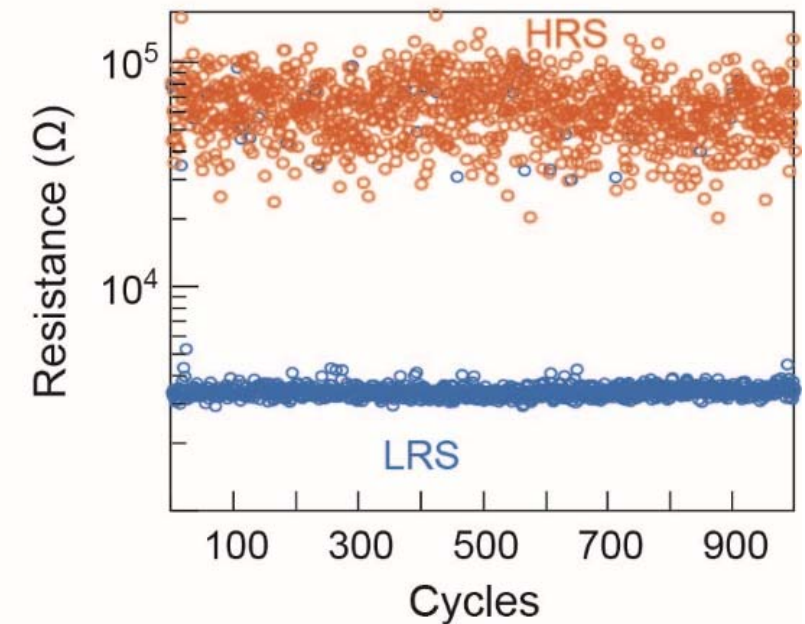
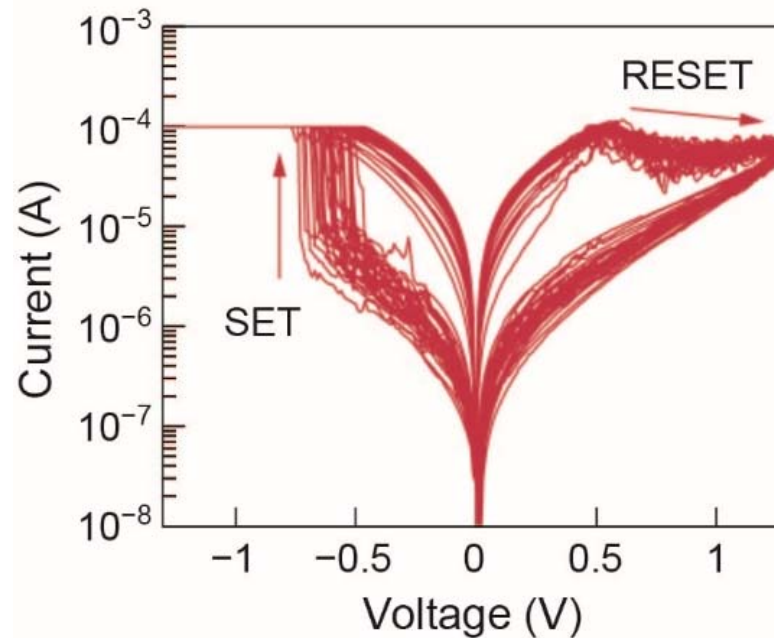
→ Voltage-divider between series resistance and actual device leads to strong state-dependence

Switching Variability I

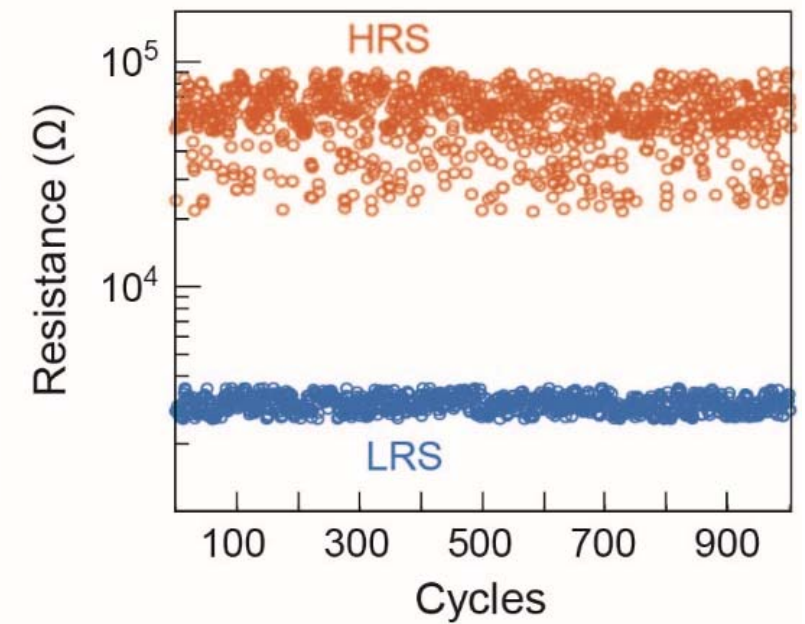
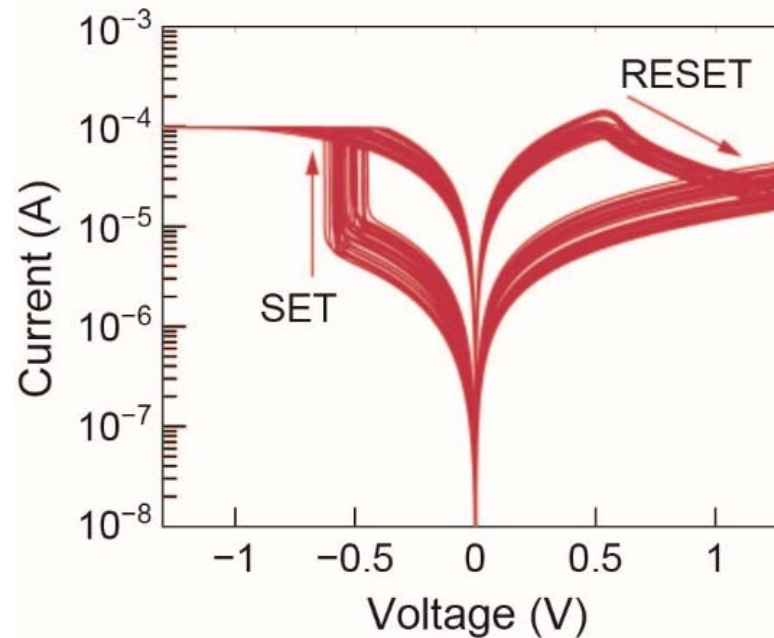
C. Bengel, S. Menzel et al., *IEEE T-CAS I*,
vol. 67, no. 12, pp. 4618-4630 (2020)

Experiment

Ti/TiO_x/HfO₂/Pt



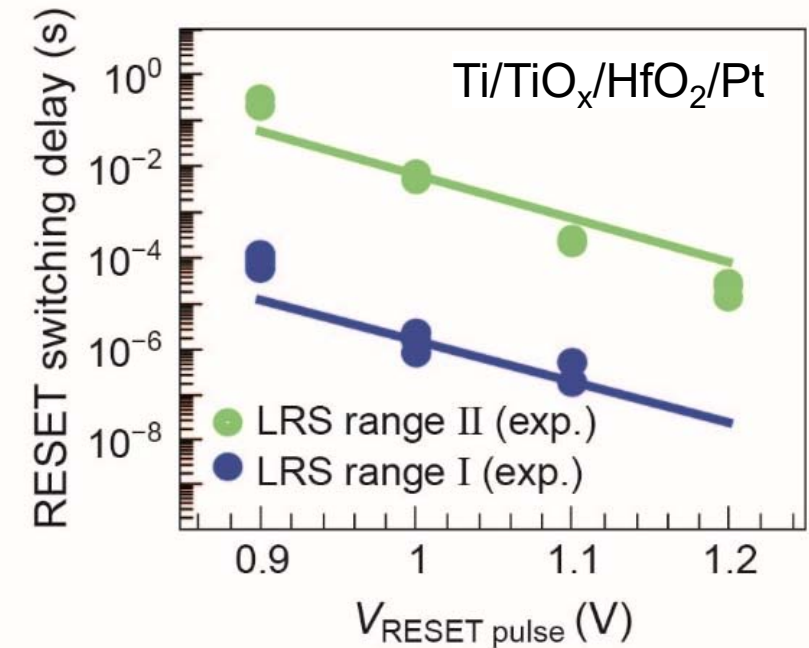
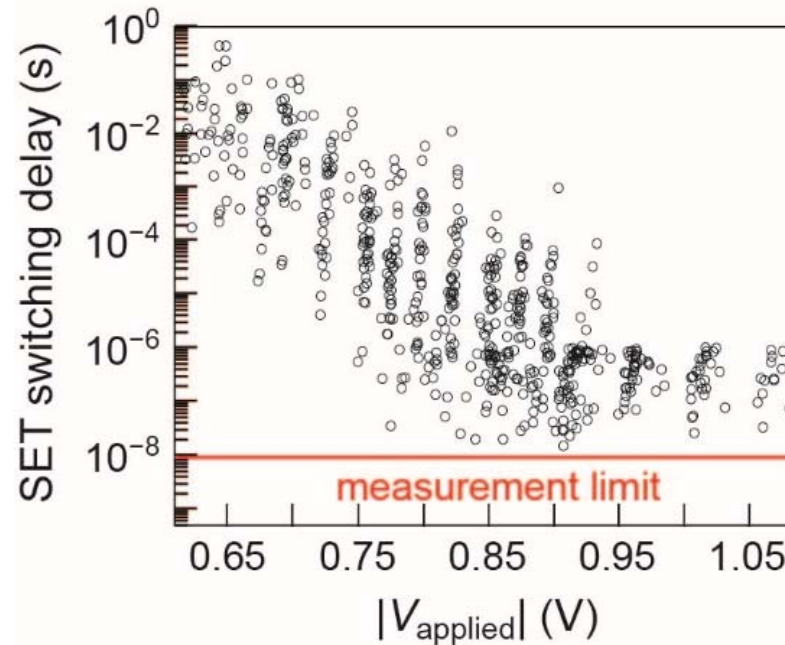
Simulation



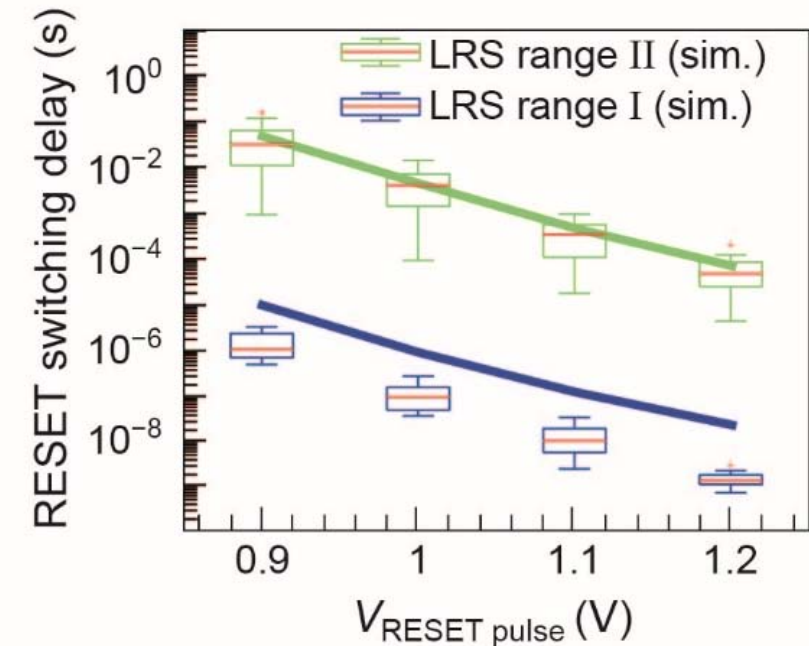
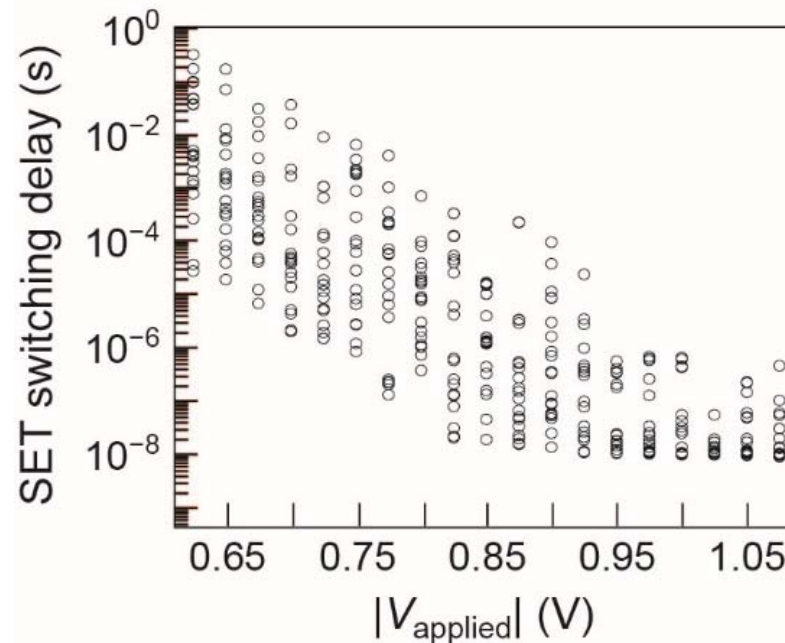
Switching Variability II

C. Bengel, S. Menzel et al., *IEEE T-CAS I*,
vol. 67, no. 12, pp. 4618-4630 (2020)

Experiment



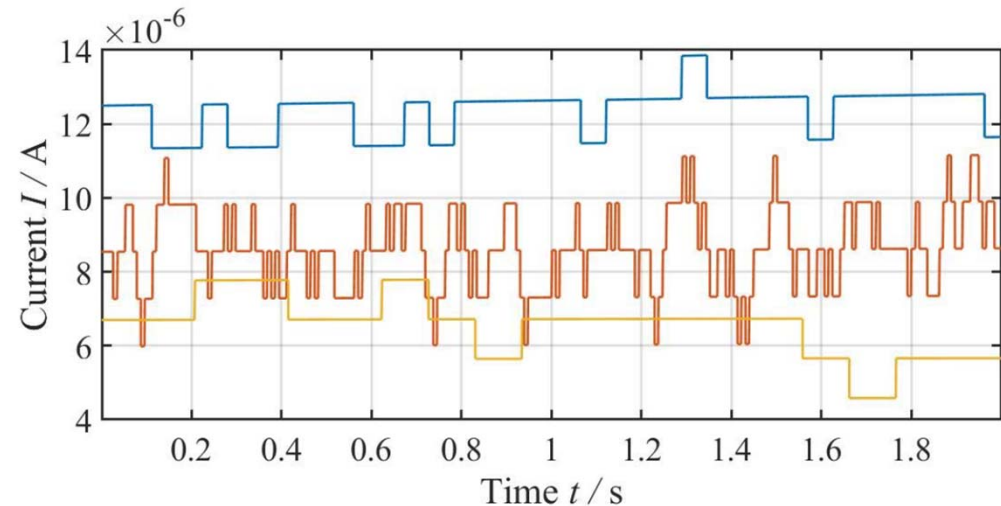
Simulation



Simulation of Read Instability: JART VCM 1b

Simulated I - t curve

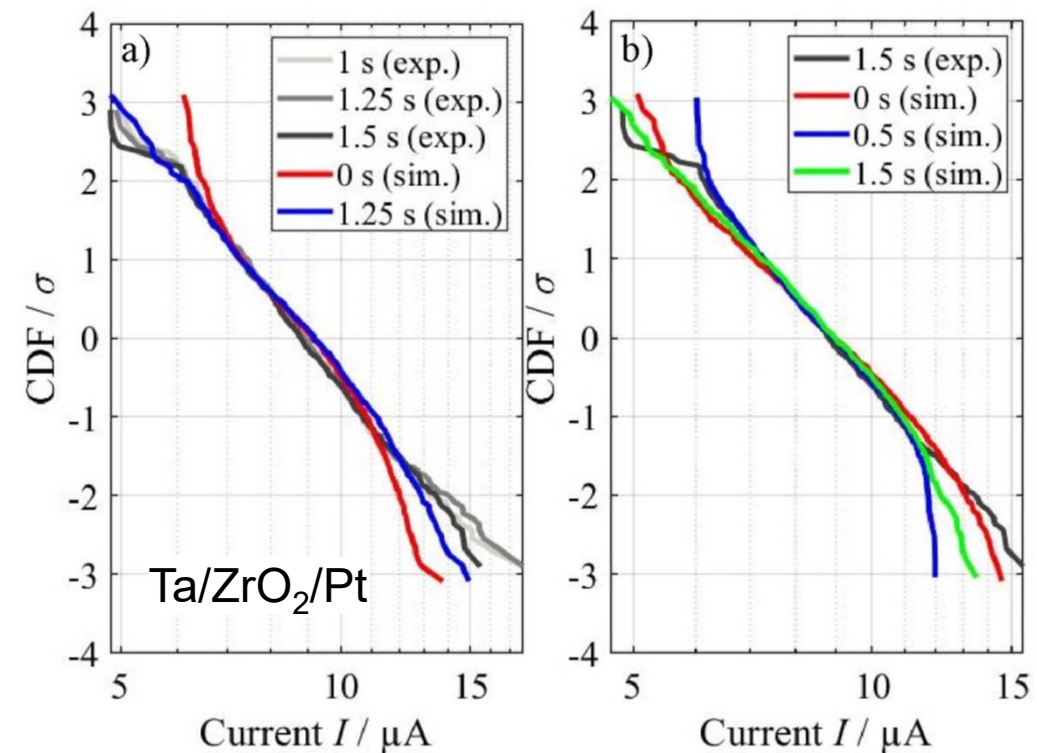
Observed current jumps similar to experimental ones



Simulated and experimental read distribution

- Log-normal distribution observed
- Log-normal distribution recovers after shaping experiment

S. Wiefels, S. Menzel et al., *IEEE T-ED*, vol. 67, no. 10, pp. 4208-4215 (2020)



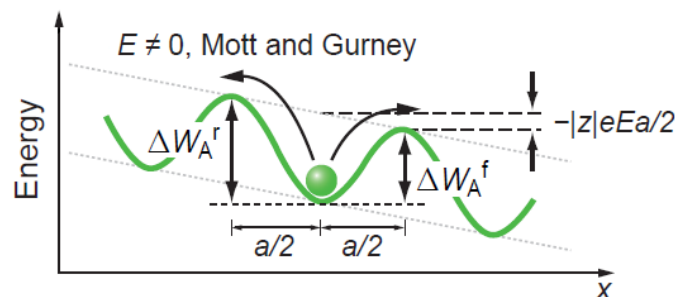
JART VCM: A 1D Kinetic Monte Carlo Approach

Based on *JART VCM 1.0* Compact model

Ion movement

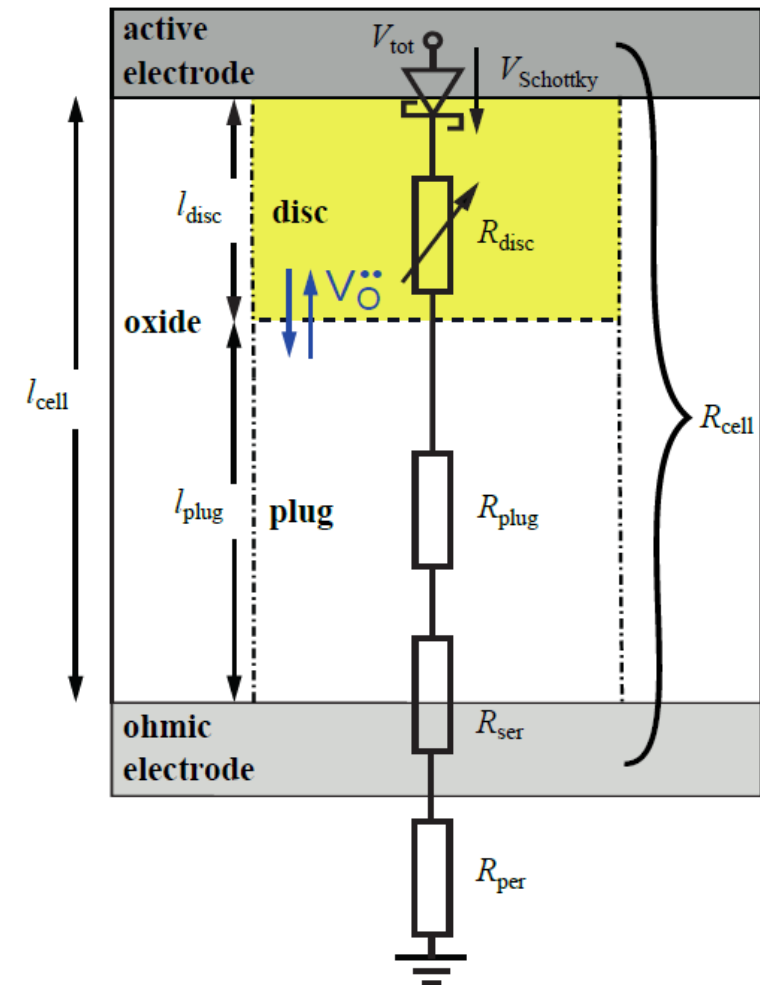
- Mott-Gurney law extended by KMC method
- V_{O} jump: plug $\leftrightarrow$ disc

$$R^{f,r} = v_0 \times \exp\left(-\frac{\Delta W_A^{f,r}}{k_B T}\right)$$



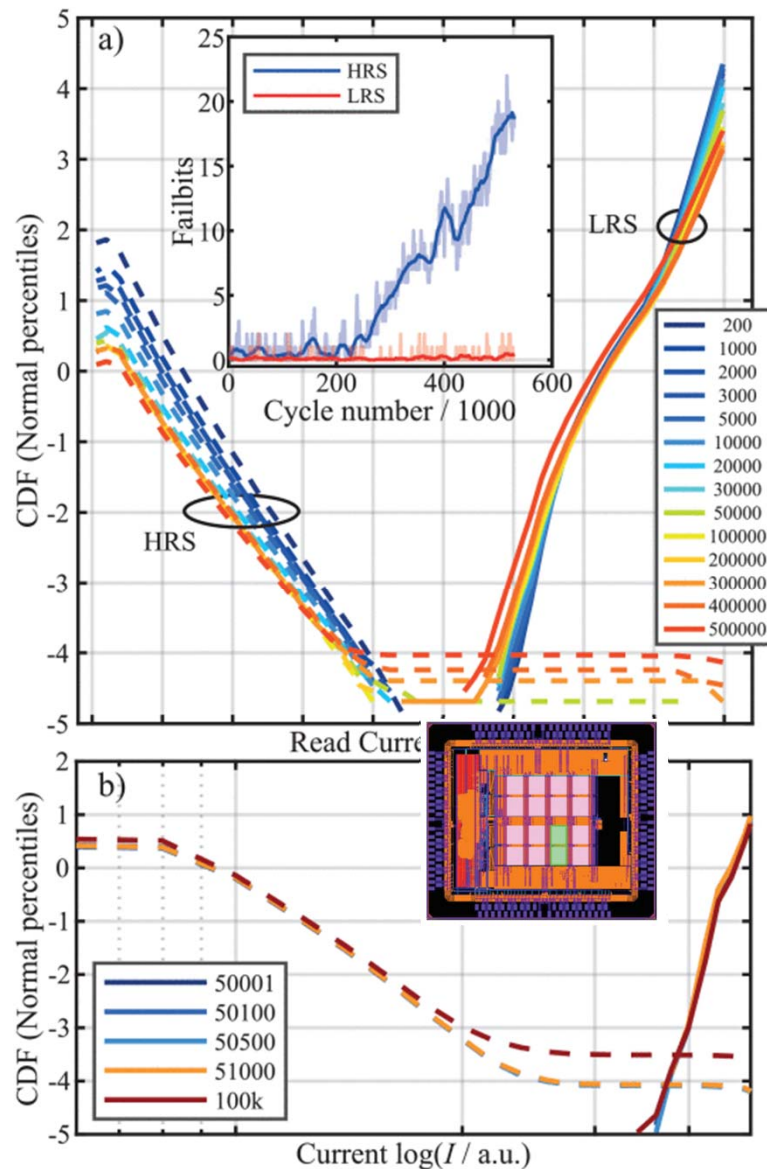
- Weighted, random process selection
- Time update

$$t_{\text{jump}} = \frac{\ln(\text{rand})}{R^f + R^r}$$

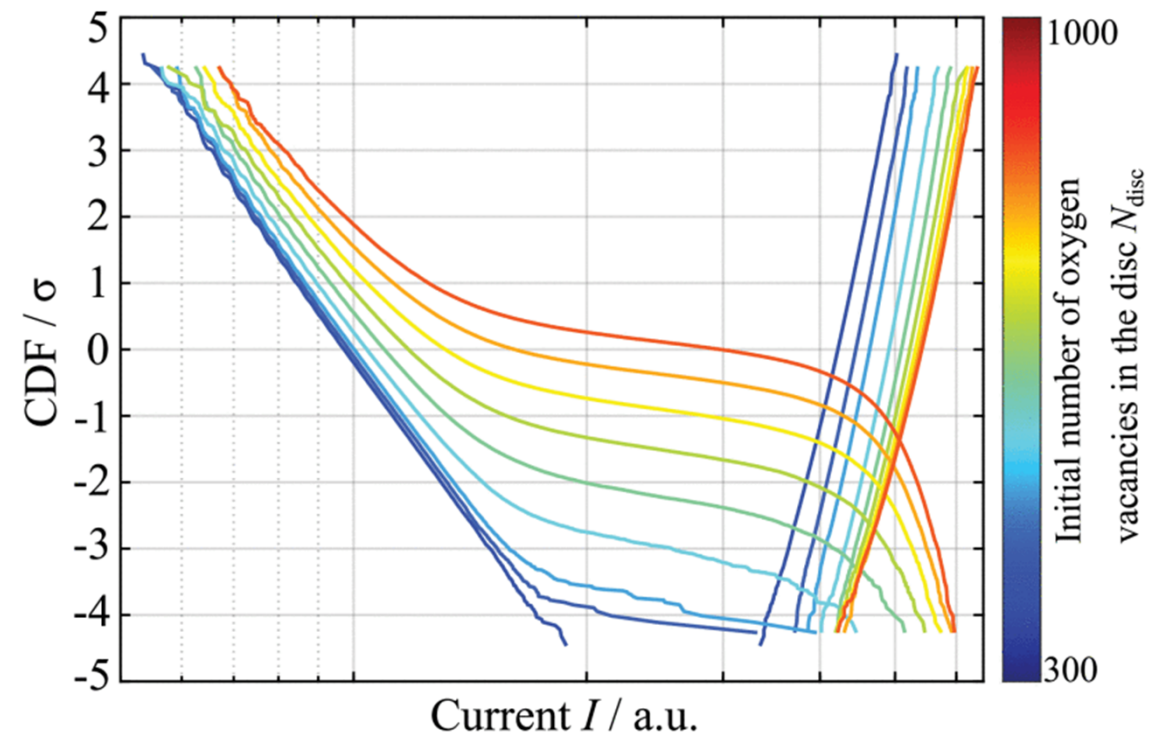


Stuck-at-LRS Failure in Test Chips

Endurance Data on 2 Mbit Cells



Simulated Failure using 1D KMC Model



→ Decreased RESET probability due to voltage divider effect

N. Kopperberg, S. Menzel et al., *IEEE Access*, vol. 10, pp. 122696 – 122705 (2022)

JART VCM: Further Model Simplification I

Fitting the state equation and state-dependent's Ohm's law using logistic functions

$$I = f(N_{\text{disc}}, V_{\text{app}}, r_{\text{fil}}, l_{\text{disc}})$$

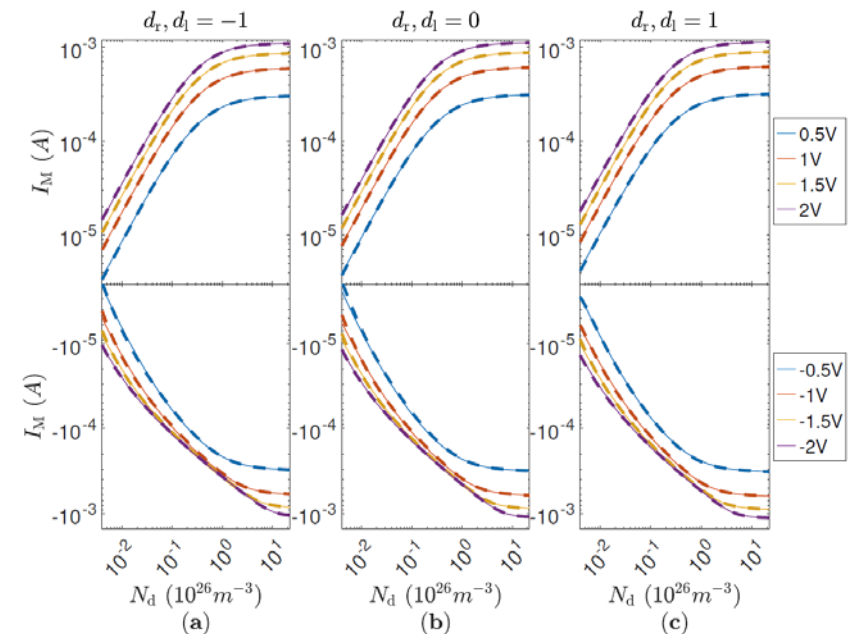
$$\frac{dN_{\text{disc}}}{dt} = f(N_{\text{disc}}, V_{\text{app}}, r_{\text{fil}}, l_{\text{disc}})$$

- Higher number of fitting parameters
- Parameters purely empirical

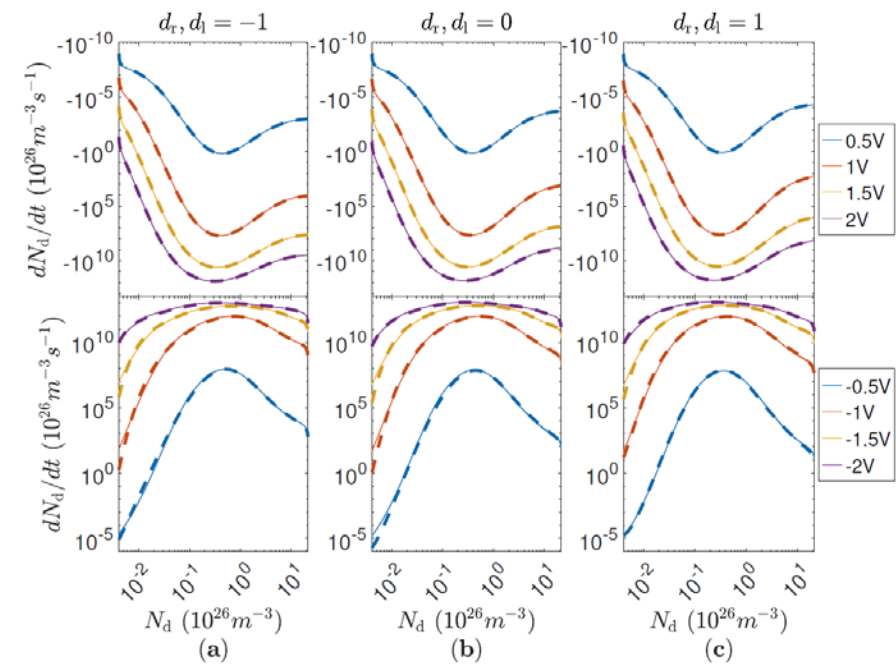
V. Ntinis, S. Menzel, R. Tetzlaff et al.
IEEE TCAS-II, vol. 14, no. 8, 2473 – 2477 (2023)

V. Ntinis, S. Menzel, R. Tetzlaff et al.,
Int. Conf. *SMACD'23* (2023)

Device current

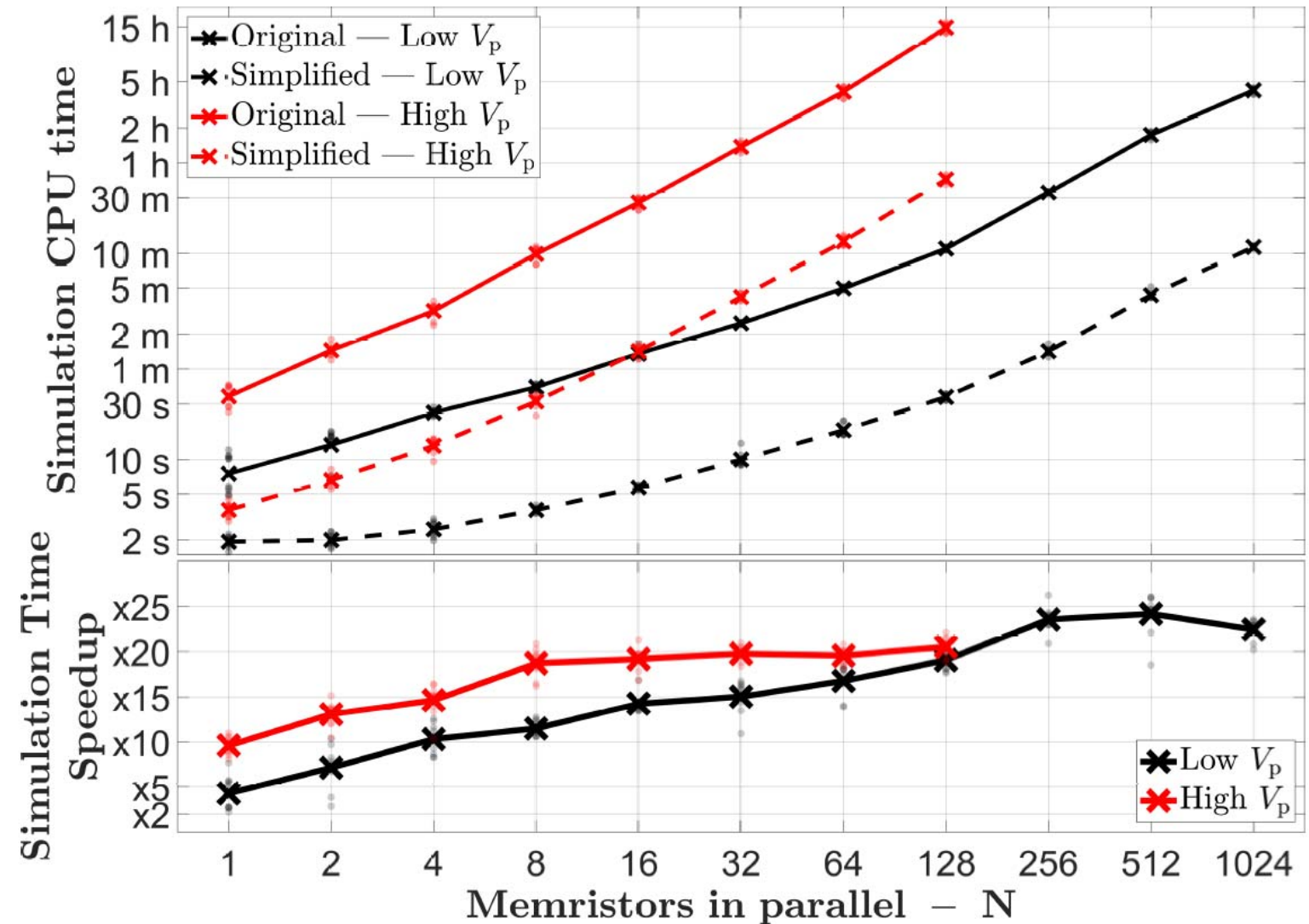


Dynamic route map



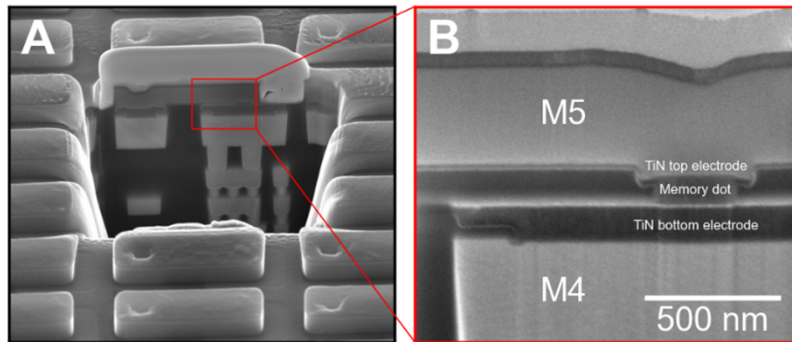
JART VCM: Further Model Simplification II

Simulation time
scaling over the
number of
parallel
memristors



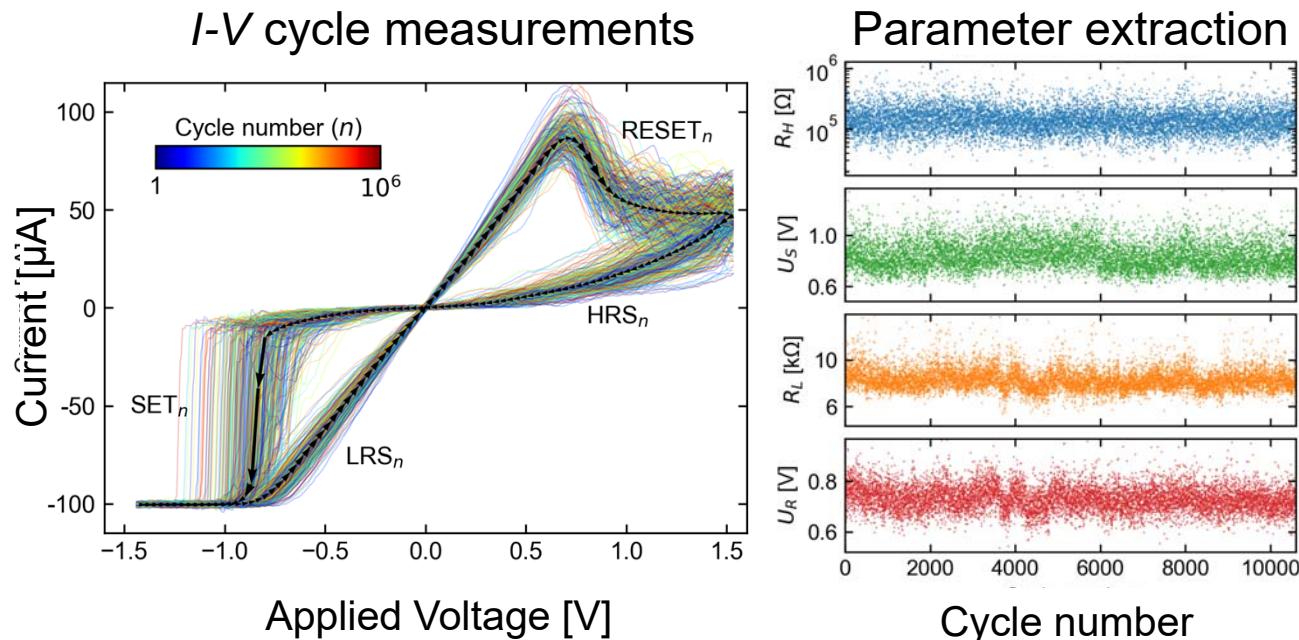
A Data-Driven Modeling Approach

Real-world measurement data



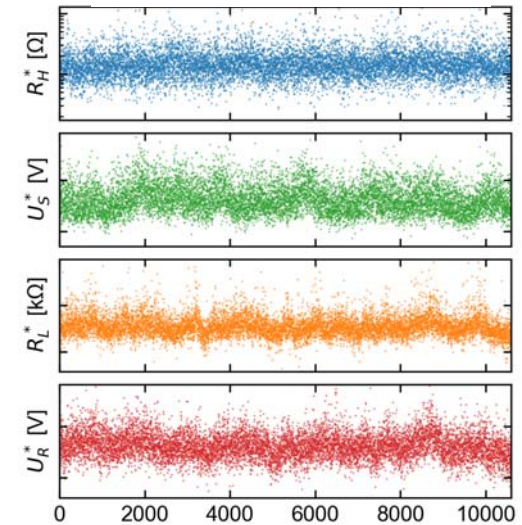
Training

Generative device model



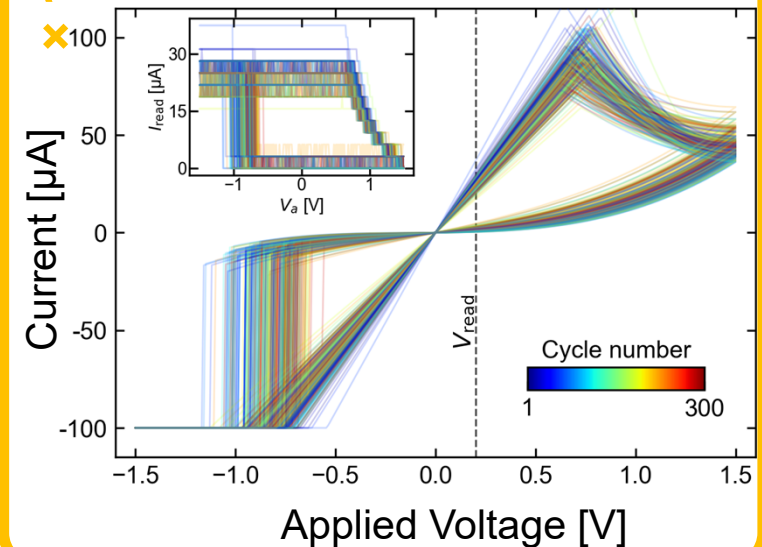
× 1 billion devices in memory!

Parameter generation



Cycle number

I-V cycle reconstruction



Outline



Motivation



Electronic Transport in VCM Cells:
A DFT-NEGF study



Switching Variability of VCM Cells:
Kinetic Monte Carlo Modeling



Switching Dynamics of VCM Cells:
Continuum Modeling



Towards Circuit Simulations:
VCM Compact Models (JART)

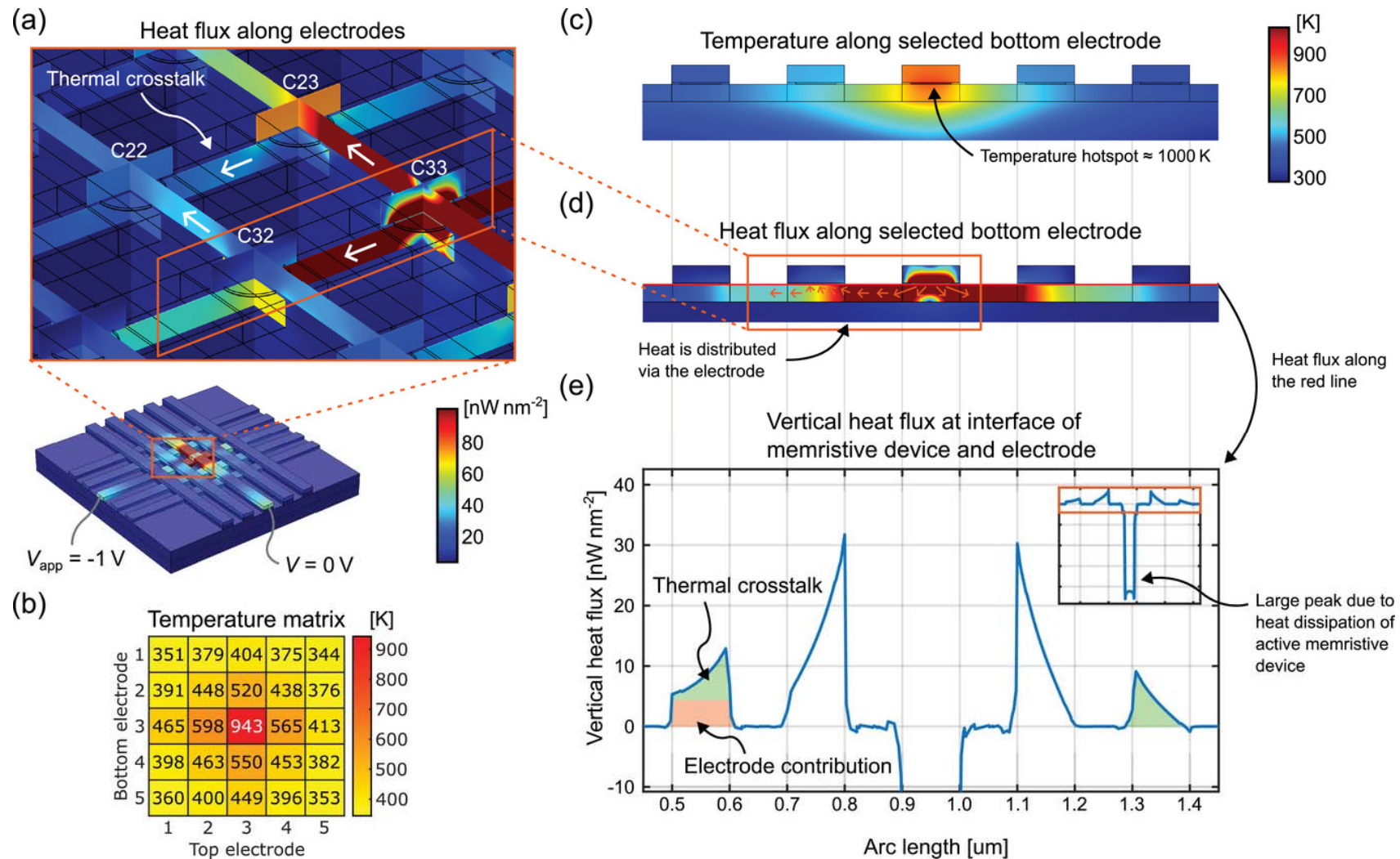


Array Level Modeling



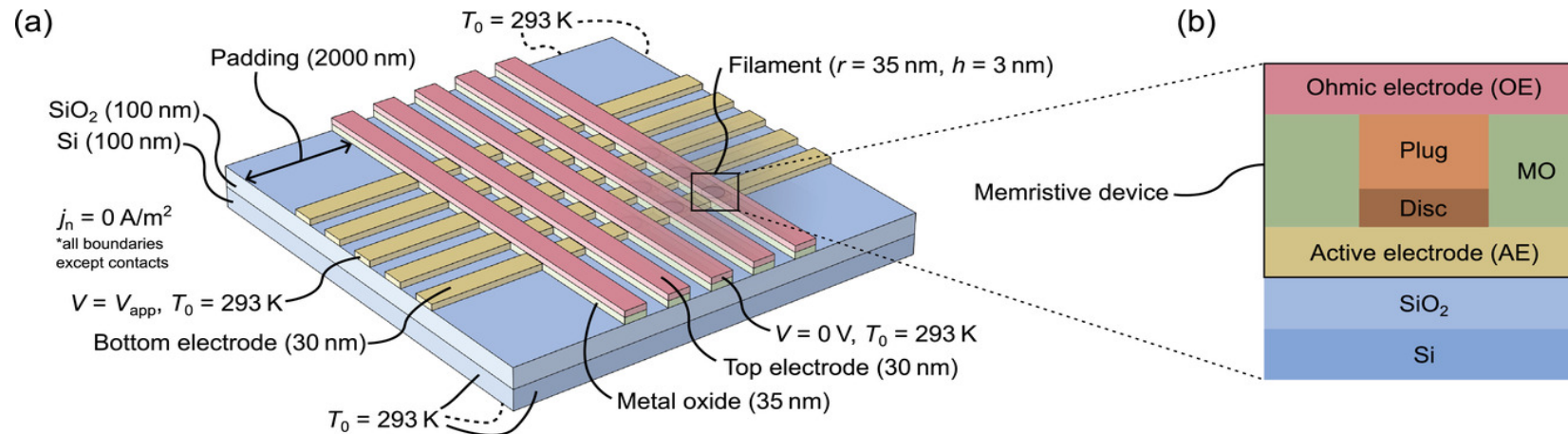
Summary & Conclusion

Modeling Thermal Crosstalk

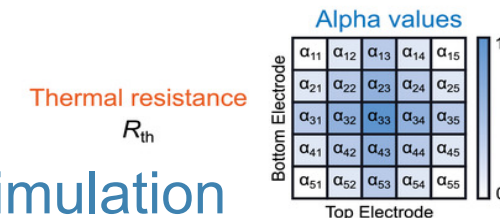
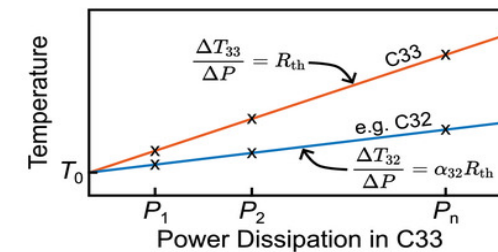
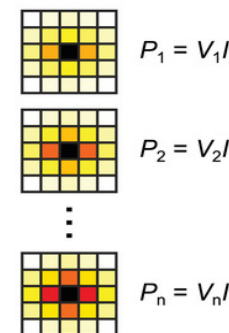
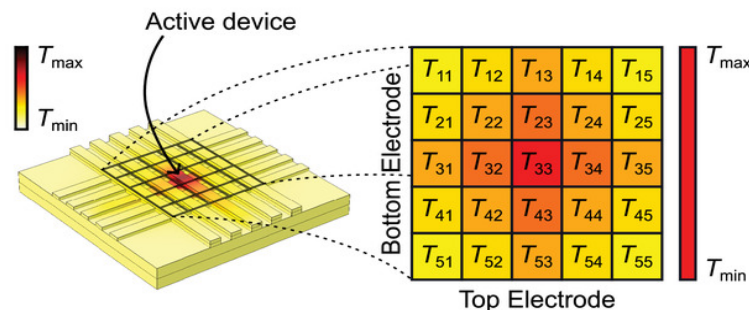


→ Thermal crosstalk via electrodes

Array-level Simulations including Thermal Crosstalk



- (c) Simulation steps:
- ① Electrothermal simulation of a memristive crossbar array
 - ② Map of device temperatures in a temperature matrix
 - ③ Performing a voltage sweep to obtain temperature matrices
 - ④ Determination of thermal resistance and alpha values

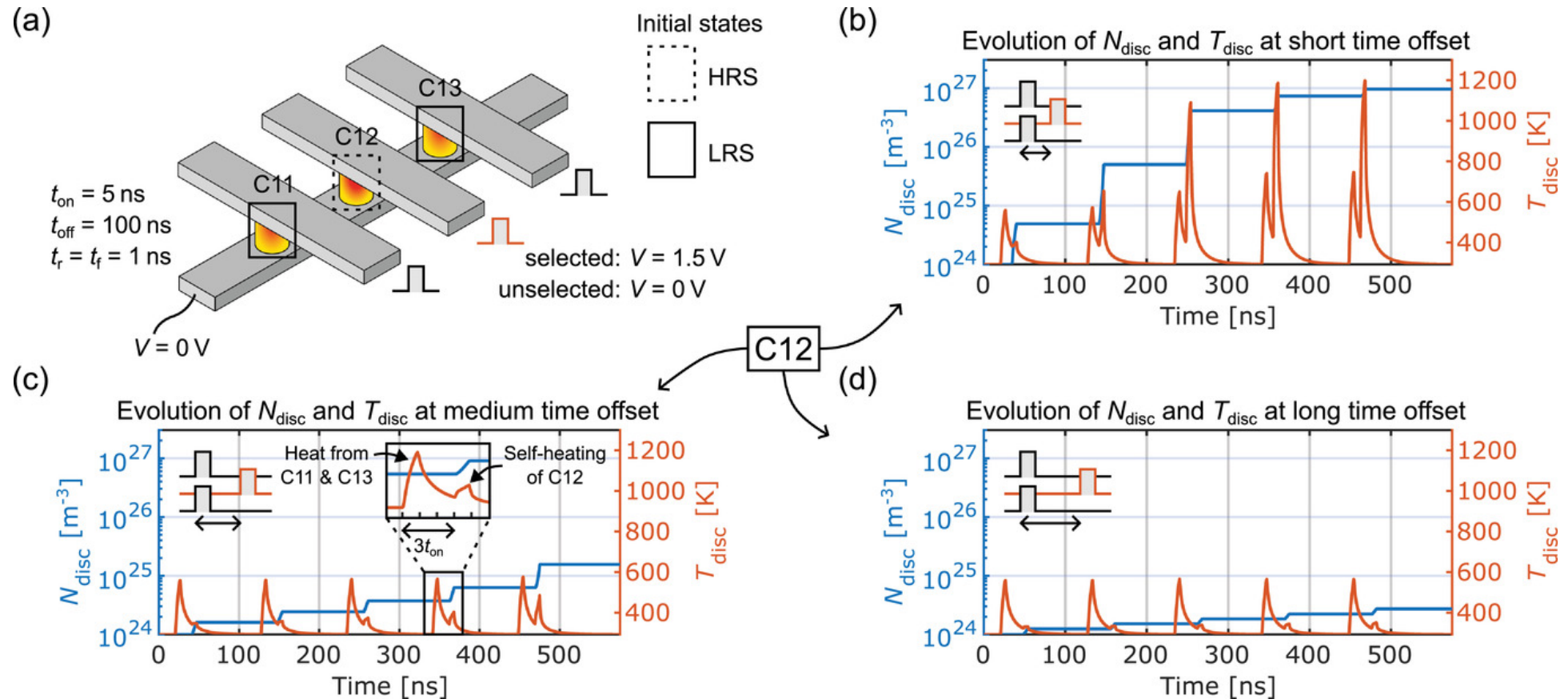


→ Alpha matrices can be incorporated in circuit simulation

D. Schön, S. Menzel et al., *Adv. Funct. Mater.*, <https://doi.org/10.1002/adfm.202213943> (2023)

F. Staudigl, S. Menzel, R. Leupers et al., *DATE 2022*

Spatio-temporal Correlations in Crossbar Arrays



→ For Δt smaller t_{RC} adjacent cells can switch

Outline



Motivation



Electronic Transport in VCM Cells:
A DFT-NEGF study



Switching Variability of VCM Cells:
Kinetic Monte Carlo Modeling



Switching Dynamics of VCM Cells:
Continuum Modeling



Towards Circuit Simulations:
VCM Compact Models (JART)



Array Level Modeling



Summary & Conclusion

Summary

Electronic Transport in VCM Cells is Injection Limited

Type I conduction: injection into conduction band

Type II conduction: injection into defect levels

Switching Variability

Stochasticity causes only minor part of the variability

(major contribution is state-dependence of switching)

Read instability due to random ionic jumps into the “gap” region

Multi-domain model could explain different time regimes of ionic noise and retention

Switching Dynamics

Abrupt SET in filamentary VCMs due to a thermal runaway

Gradual RESET due to a non-isothermal drift-diffusion balance

Compact Modeling

JART Models including variability presented

Array Level Modeling

Combination of FEM and compact modeling → extraction of crosstalk



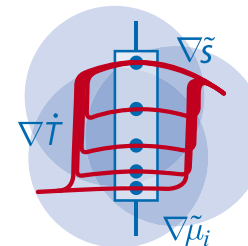
Funded by
DFG Deutsche
Forschungsgemeinschaft
German Research Foundation

Thank you for your attention!

www.emrl.de/JART.html



FKZ:
16ES1133K
16ES1134



SFB 917
Nanoswitches