Consistent Modelling of Instability and Retention Phenomena in Filamentary Valence Change Memories

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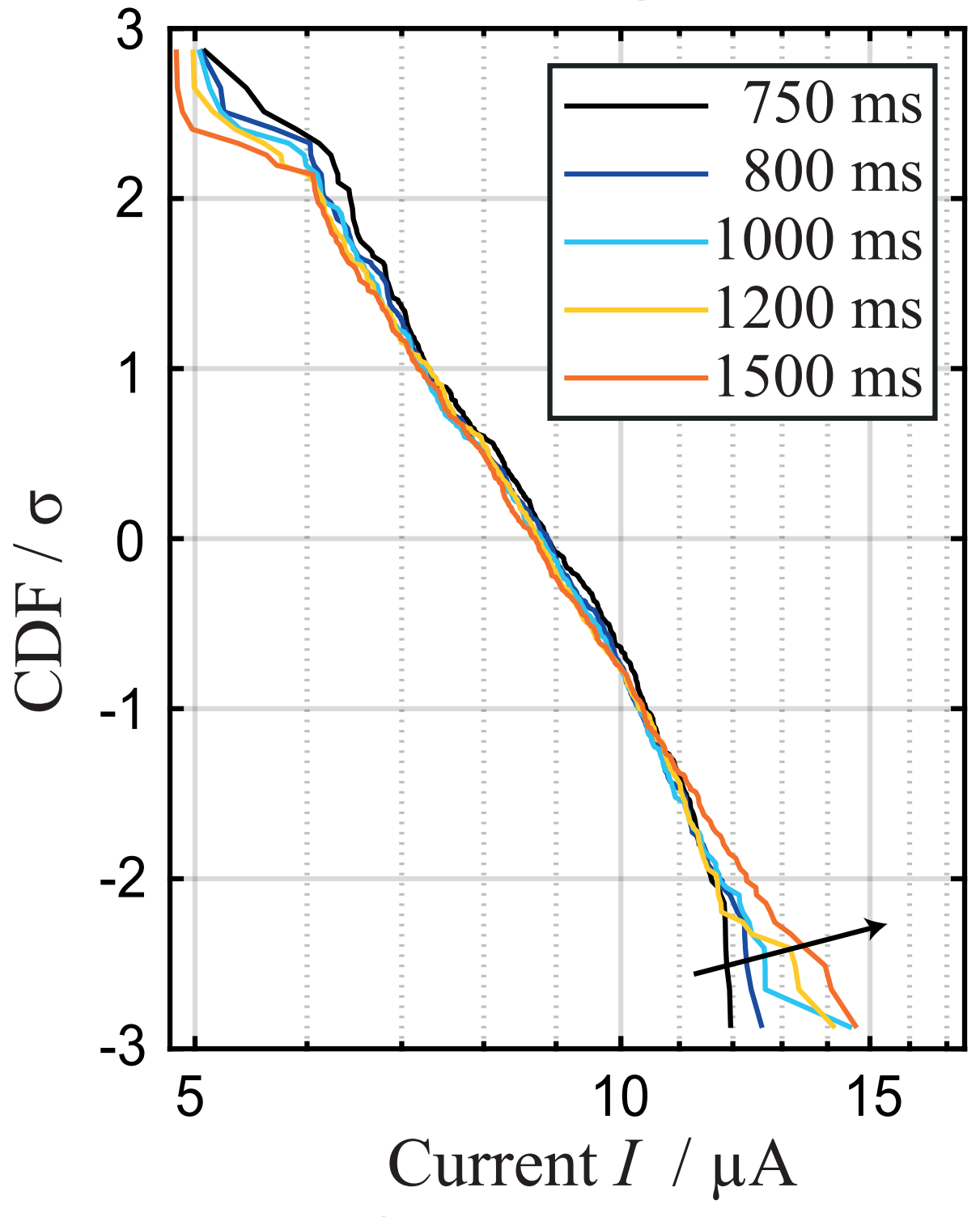
Motivation

Instability



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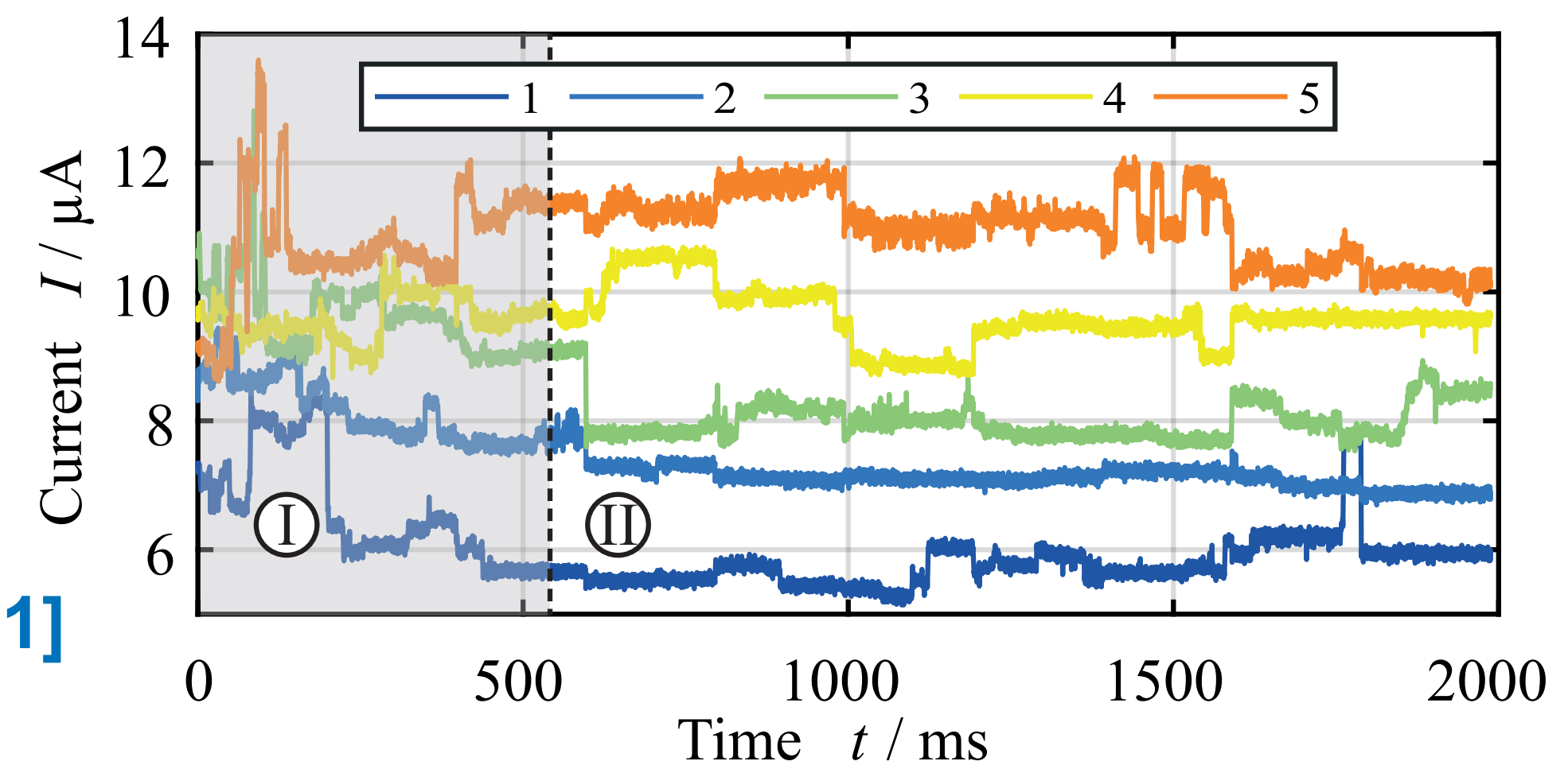
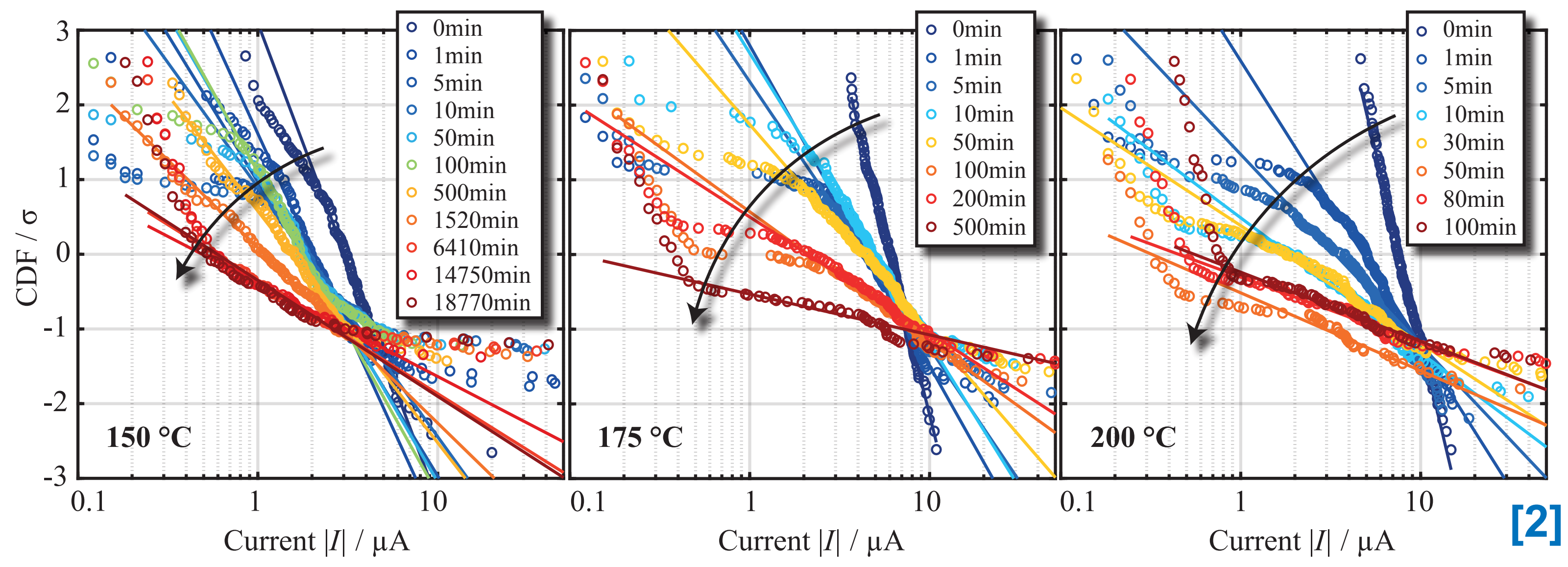


- Experimental read current of ZrO_2 based VCM ReRAM in the high resistive state (HRS)
- Overall current distribution stable over time, current of single devices changes and jumps between discrete levels

- Failure of shaping algorithms trying to widen read window

► Current distribution always reverts to intrinsic distribution

Retention



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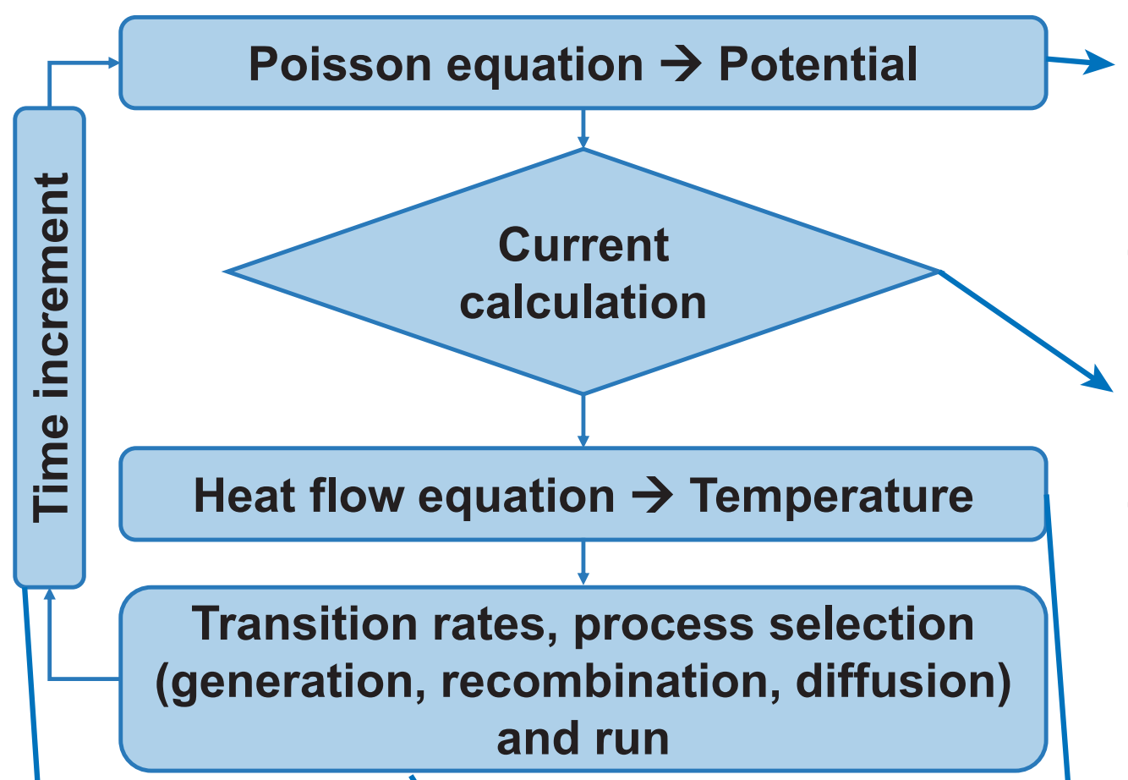
- Current distribution not stable at comparably large timescales
- Thermally accelerated retention experiments
- Tilt (broadening) and shift of current distribution observed during 'baking'

► Read window becomes smaller

KMC Model



$$\Delta t = \frac{-ln(r_1)}{R_{\mathrm{total}}}$$

Generation rate:

$$R_G = \nu_0\, e^{-\frac{E_G - \alpha a q F}{k_B T}}$$

Recombination rate:

$$R_R = \nu_0\, e^{-\frac{E_R - (1-\alpha) a q F}{k_B T}}$$

Diffusion rate:

$$R_D = \nu_0\, e^{-\frac{E_D}{k_B T}}$$

3D Poisson eq.: $\Delta\Phi = -\frac{\rho}{\epsilon_0\,\epsilon_r}$

Drift Diffusion (DD):

DD current continuity eq.: $\nabla \cdot j = 0$

DD current density: $j = -q\mu_n(n\nabla V - V_T\nabla n)$

Trap Assisted Tunneling (TAT):

Trap→Trap, Abraham-Miller:

$$h_{ij} = \begin{cases} \nu_{0n} exp\left(-\frac{d_{ij}}{a_0} + \frac{q(V_i^H - V_j^H)}{k_B T}\right) & V_i^H \le V_j^H \\ \nu_{0n} exp\left(-\frac{d_{ij}}{a_0}\right) & V_i^H > V_j^H \end{cases}$$

WKB approximation: $T_r = e^{-2\int_{x_m}^{x_t}\frac{1}{\hbar}\sqrt{2m^*(q\Phi_B - E_e)}\,dx}$

Electrode→Trap, Hopping rate: $P_{Ei} = P_0 T_r \int_{E_t^e}^{\infty} F(E)\rho(E)dE$

Occupational probability:

$$(1-p_i)\sum_{j=1,j\neq i}^{N} p_j h_{ij} - p_i \sum_{j=1,j\neq i}^{N}(1-p_j)h_{ij} + (P_{Ci} + P_{Ai})(1-p_i) - (P_{iC} + P_{iA})p_i = 0$$

Tunneling current: $I_{TAT} = e\sum_{i=1}^{N}[p_i P_{iE} - (1-p_i)P_{Ei}]$

Fourier's heat flow eq.: $\nabla \cdot (k_{th}\,\nabla T) = -g$

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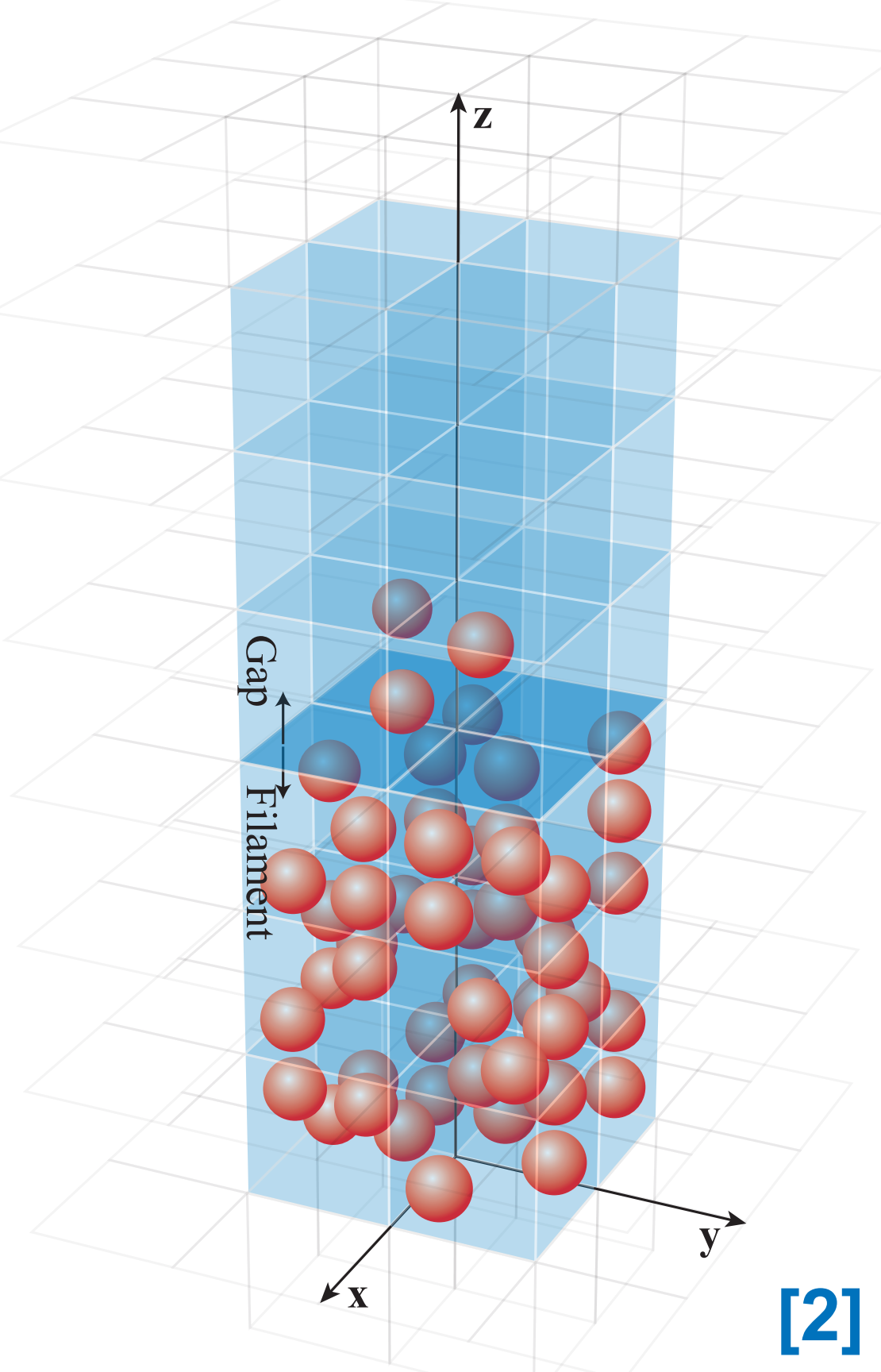
Multi Domain Model



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- Different diffusion regimes observed in molecular dynamics simulations for oxygen vacancies in HfO_2 [4]

► Introduction of diffusion-limiting domains

► Modelled by boxes with 'easy' diffusion inside, but hindered diffusion of oxygen vacancies from box to box

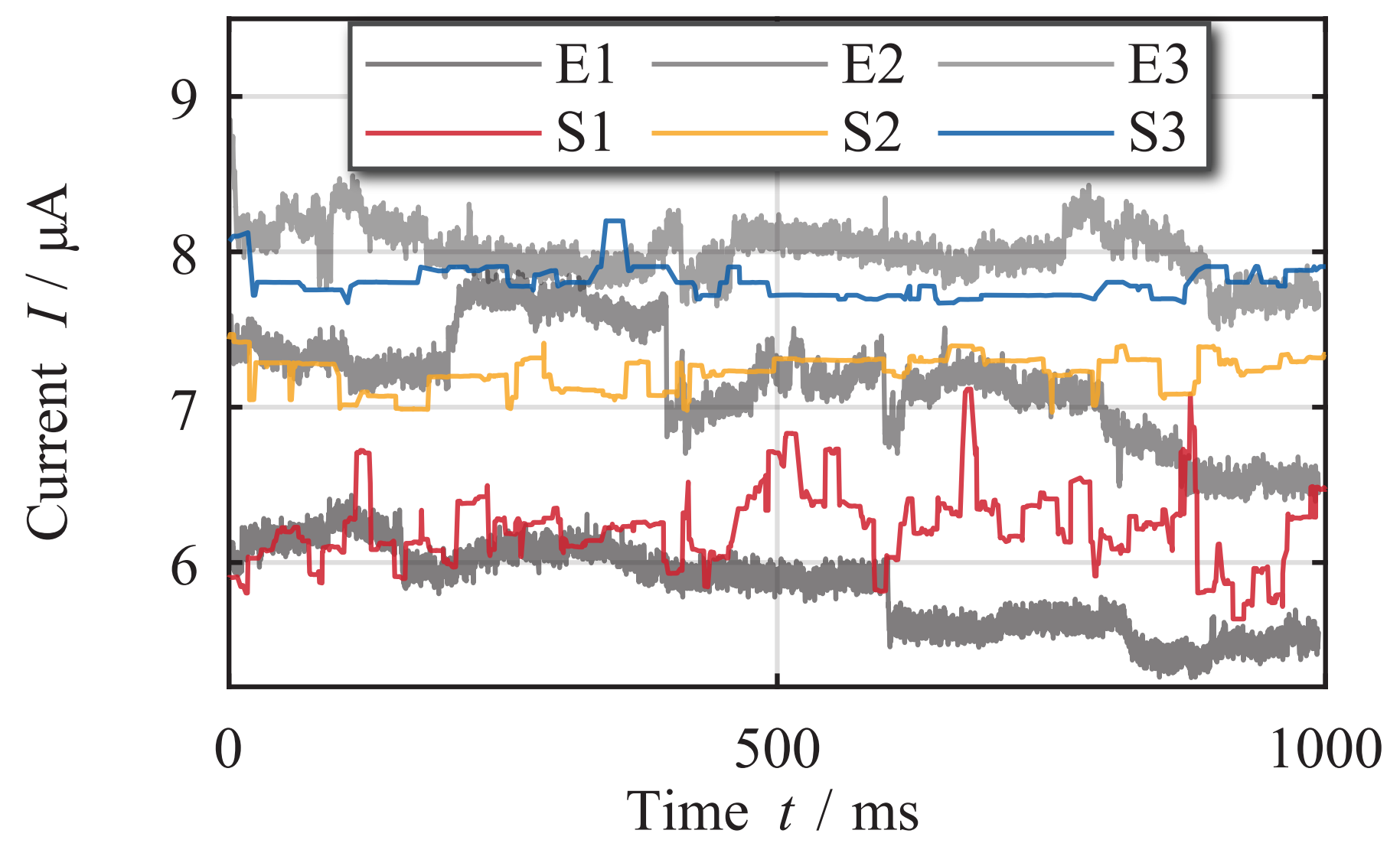
- Investigation of HRS which is most susceptible to instability and retention failures
- Modelled by comparably low number of defects in filament with large gap between filament and electrically active top electrode

- Goal: Explain short-term instability and long-term retention phenomena in the same model by the same physical processes (random distribution and diffusion of oxygen vacancies)

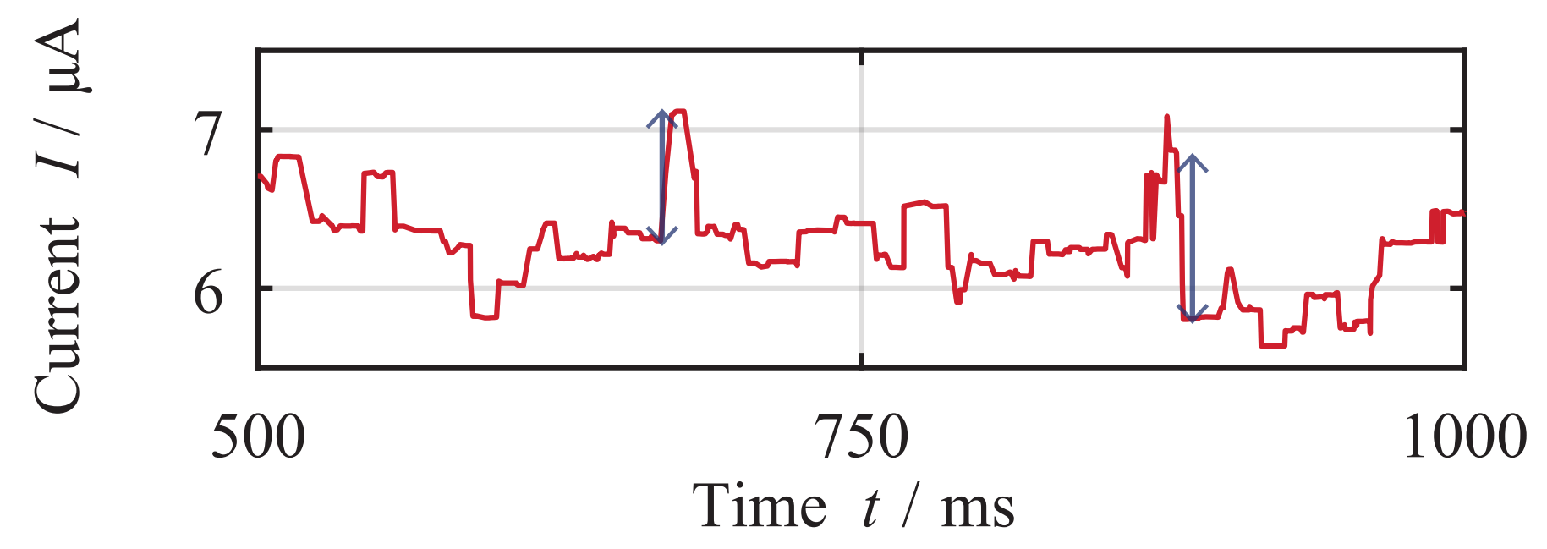
Results

Instability

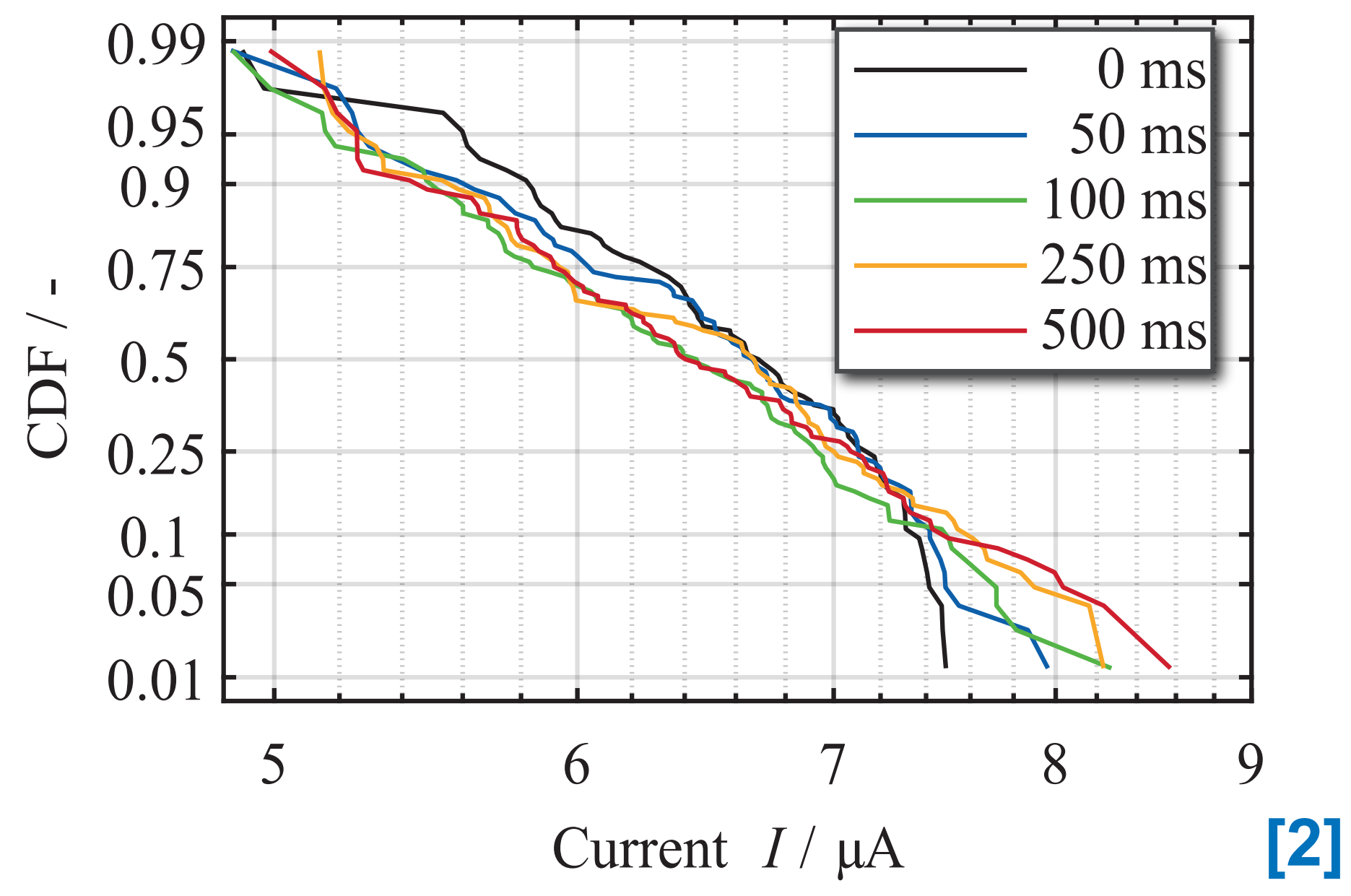
- Read current investigation at room temperature
- Defects jump and rearrange inside boxes, but cannot overcome high barriers (no structural changes)
- Discrete random jumps of current of single cells due to oxygen vacancy diffusion



- Highest current jumps originate from oxygen vacancy jumps close to filament-gap interface



- Read current distribution stable over time
- Shaping failure can be modelled and explained by the random redistribution of oxygen vacancies
- Random diffusion of oxygen vacancies leads to intrinsic lognormal current distribution



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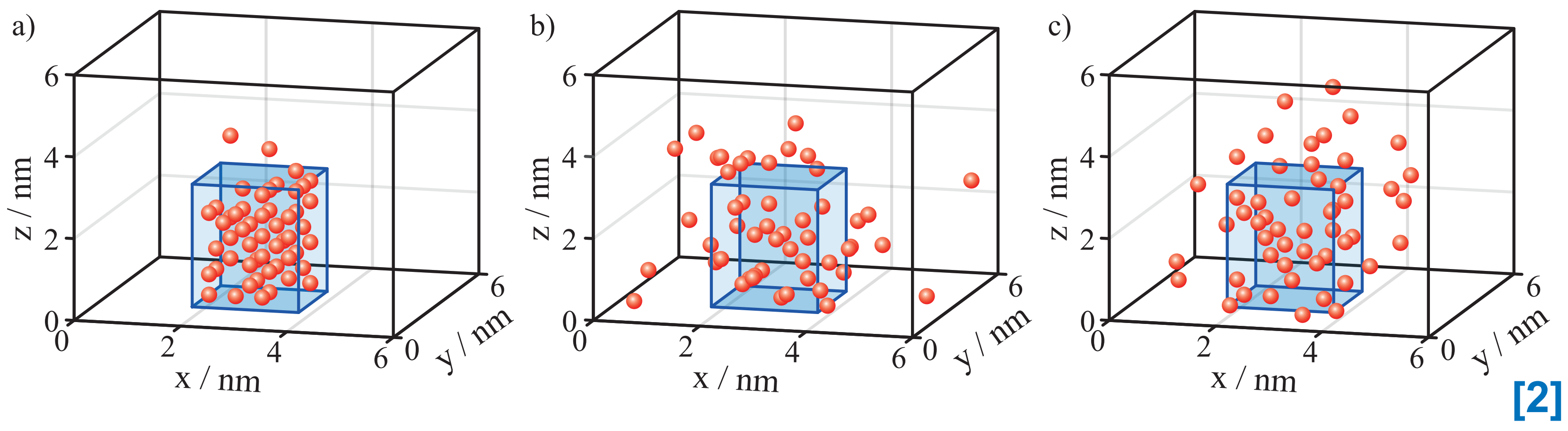
Retention



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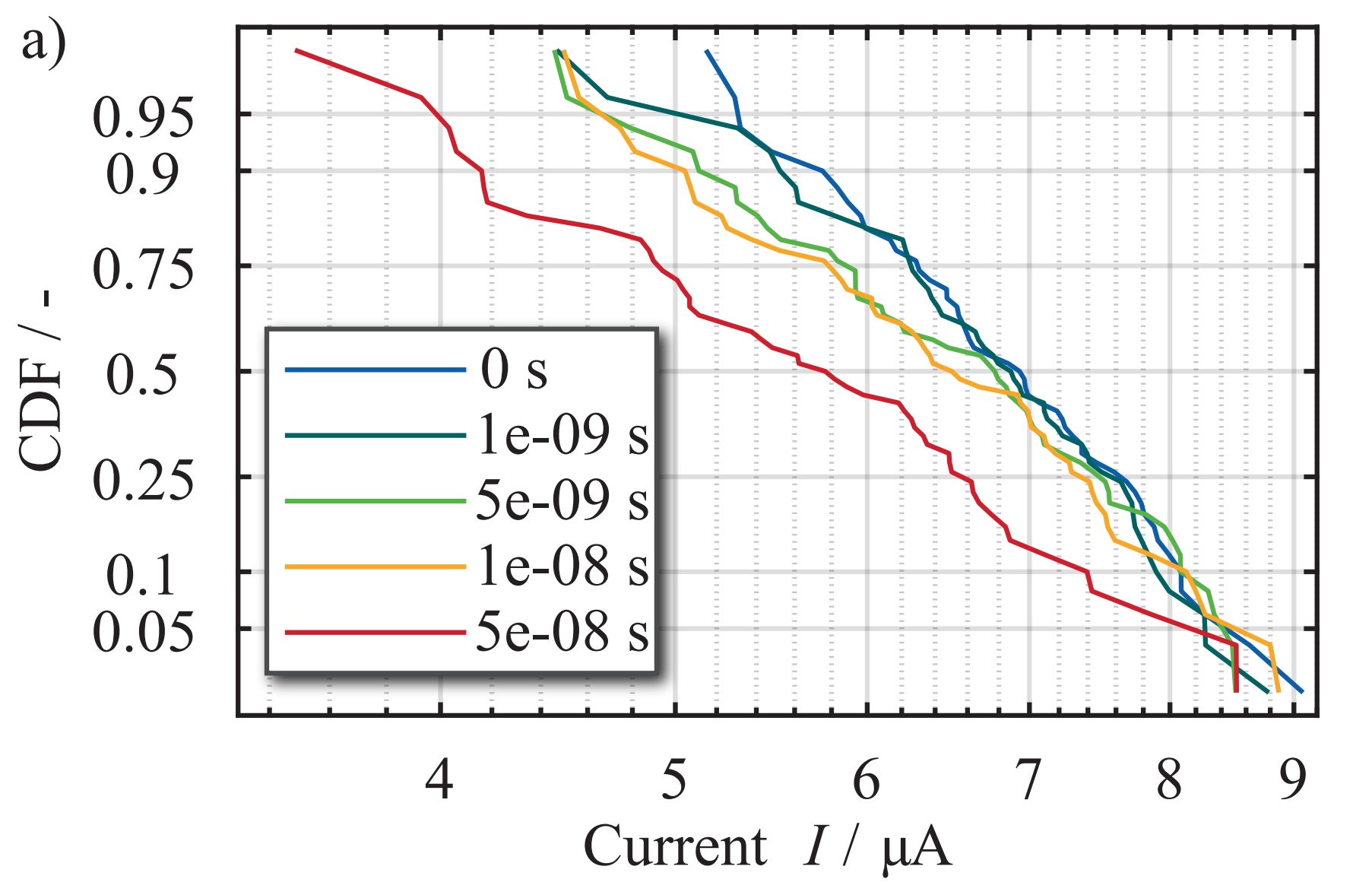
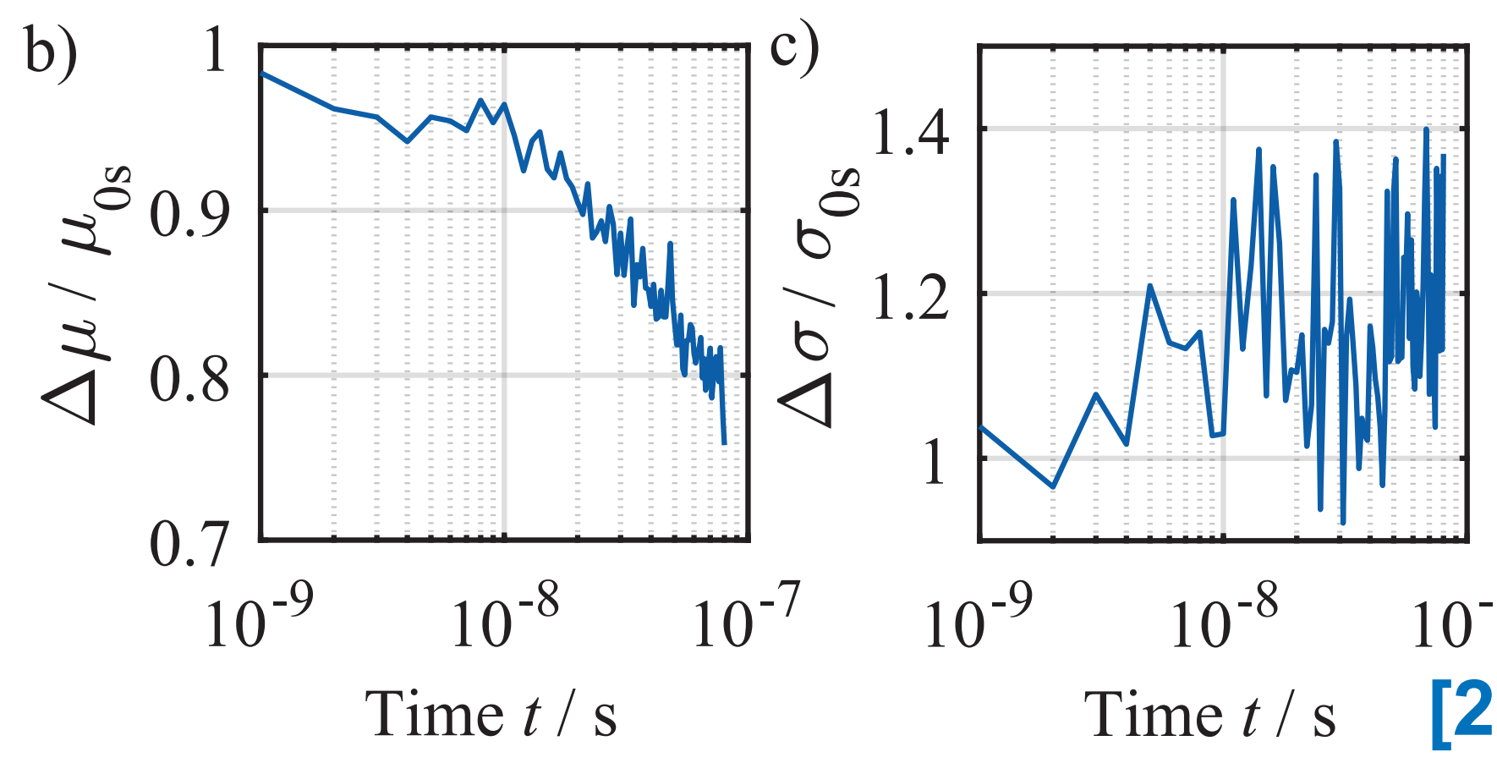
- Simulation of retention phenomena at highly elevated temperatures
- Oxygen vacancies can overcome barriers and also jump from box to box (structural changes)
- Radial diffusion (b) or vertical diffusion closing the gap (c) can be reached from initial state (a)
- Usually, superposition of both processes



- Tilt of distribution (always) and shift of distribution depending on which process dominates (radial diffusion or closing gap)

► Diffusion of oxygen vacancies sufficient to explain retention phenomena



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Conclusion

- Different possible sources of retention effects in VCM ReRAMs have been investigated. Regions with different diffusion energy barrieres have been introduced - here, both instability and retention effects can be explained by one consistent model.
- Due to the random fluctuations, the read current follows intrinsic statistics. A transition from log-normal to normal statistics is observed from HRS towards LRS. The origin of the intrinsic statistics will be further investigated. Connection to the conduction mechanism: localized vs delocalized electrons, area vs filamentary switching. Read noise in different oxides will be compared.

[1] S. Wiefels, C. Bengel, N. Kopperberg, K. Zhang, R. Waser and S. Menzel, "HRS Instability in Oxide-Based Bipolar Resistive Switching Cells," in IEEE Transactions on Electron Devices, vol. 67, no. 10, pp. 4208-4215, Oct. 2020, doi: 10.1109/TED.2020.3018096.

[2] N. Kopperberg, S. Wiefels, S. Liberda, R. Waser., S. Menzel; A Consistent Model for HRS Short-Term Instability and Long-Term Retention Mechanisms in Filamentary VCM ReRAM; ACS Applied Materials & Interfaces 2021 13(48), 58066-58075, doi: 10.1021/acsami.1c14667.

[3] E. Abbaspour, S. Menzel, A. Hardtdegen, S. Hoffmann-Eifert, C. Jungemann. "KMC Simulation of the Electroforming, Set and Reset Processes in Redox-based Resistive Switching Devices". In: *IEEE Trans. Nanotechnol.* 17.6 (2018), pp.1181-1188

[4] M. Schie, M. P. Müller, M. Salinga, R. Waser, R. A. De Souza. "Ion Migration in Crystalline and Amorphous HfOx". In: *The Journal of Chemical Physics* 146, 094508 (2017).