Analysis and Modeling of Conducting Filament in Nanoscale Resistive Switching Memory Devices

Dan Berco, 5th year PhD student, Department of Electronics Engineering and Institute of Electronics,
National Chiao Tung University, Advisor:Tseung-Yuen Tseng

Abstract

A numerical analysis method to investigate the conduction filament (CF) dynamics of a resistive switching nonvolatile metal-insulator-metal structured memory device is presented. This method, utilizes the Gibbs free energy criteria as a leading indicator and allow simulation of all memory operational phases (forming, set and reset).

The formation and rupture of an oxygen vacancies based CF are simulated to demonstrate a full cycle of operation allowing deeper understanding of the CF kinetics and introduce the concept of "hot spots" (HS), referring to random localized initial agglomeration of oxygen vacancies in which temperature surges is favored and contribute to initiate the formation process.

By basing the method on well known thermodynamic properties and the Metropolis algorithm, simulation reliability and efficiency are obtained. A study of the CF properties in monoclinic hafnium oxide (HfO_2) resistive switching layer (RSL) is presented as an example.

We also define a disorder parameter λ corresponding to the randomly generated initial distribution of metallic like OV defects in the RSL.

Formulation

The generation, hopping and recombination probabilities for the oxygen species are:

$$P_{g,n} = (1-C_n)\exp\left(-\frac{E_a - a_a Ze\xi_n}{k_B T_n}\right)$$

$$P_{h,n\to m} = C_n(1-C_m)\exp\left(-\frac{E_h - a_h Ze\xi_n}{k_B T_n}\right)$$

$$P_r = c_n \exp\left(-\frac{\Delta E_r}{k_B T_n}\right)$$

Mott variable range hopping model accounts for trap assisted tunneling through the RSL:

$$\sigma_{mn} = f_e \frac{e^2 c_m (1-c_n)}{d_{mn} k_B T_n}\exp\left(-\frac{2d_{mn}}{\alpha}\right)\exp\left(-\frac{e\left|\nabla\varphi_{mn}\right|}{k_B T_n}\right)$$

The Fermi integral represents the number of filled states (F_{in}), with respect to the empty trap level in the injecting electrode, and the number of empty states (F_{out}), with respect to the occupied trap level in the collecting electrode :

$$F_{in,n} = \int_{\Delta E_e - e\varphi_n}^{\infty} f[E_{fe} - (E - e\varphi(x,0))]dE$$

$$F_{out,n} = \int_{-\infty}^{\Delta E_o - e\varphi_n} \{1 - f[E_{fe} - (E - e\varphi(x,L))]\}dE$$

The *in* and *out* e^- flux probabilities between the RSL and the control electrodes are calculated according to WKB approximation:

$$P_n^{out} = c_n \exp\Big[-\frac{2}{\hbar}\sum_{\substack{m\neq n \\ m(y)>n(y)}} \sqrt{2m_e^*(\Delta E_o - e\varphi_{mn})}\Big]$$

$$P_n^{in} = (1-c_n)\exp\Big[-\frac{2}{\hbar}\sum_{\substack{m\neq n \\ m(y)>n(y)}} \sqrt{2m_e^*(\Delta E_e - e\varphi_{mn})}\Big]$$

The *carrier continuity* and *steady state Fourier* equations are solved to determine the temperature, potential and conduction:

$$\nabla\cdot\sigma_n\nabla\varphi_n = 0$$

$$-\nabla\cdot k_{th,n}\nabla T_n = \sigma_n\left|\nabla\varphi_n\right|^2$$

The density of the O species within the resistive layer is determined by solving the continuity drift diffusion equation:

$$\Delta N_{o,n} = \frac{1}{f_o}\nabla\cdot\left(D_n\nabla N_{o,n} - \frac{eD_n}{k_B T_n}\nabla\varphi_n N_{o,n}\right)$$

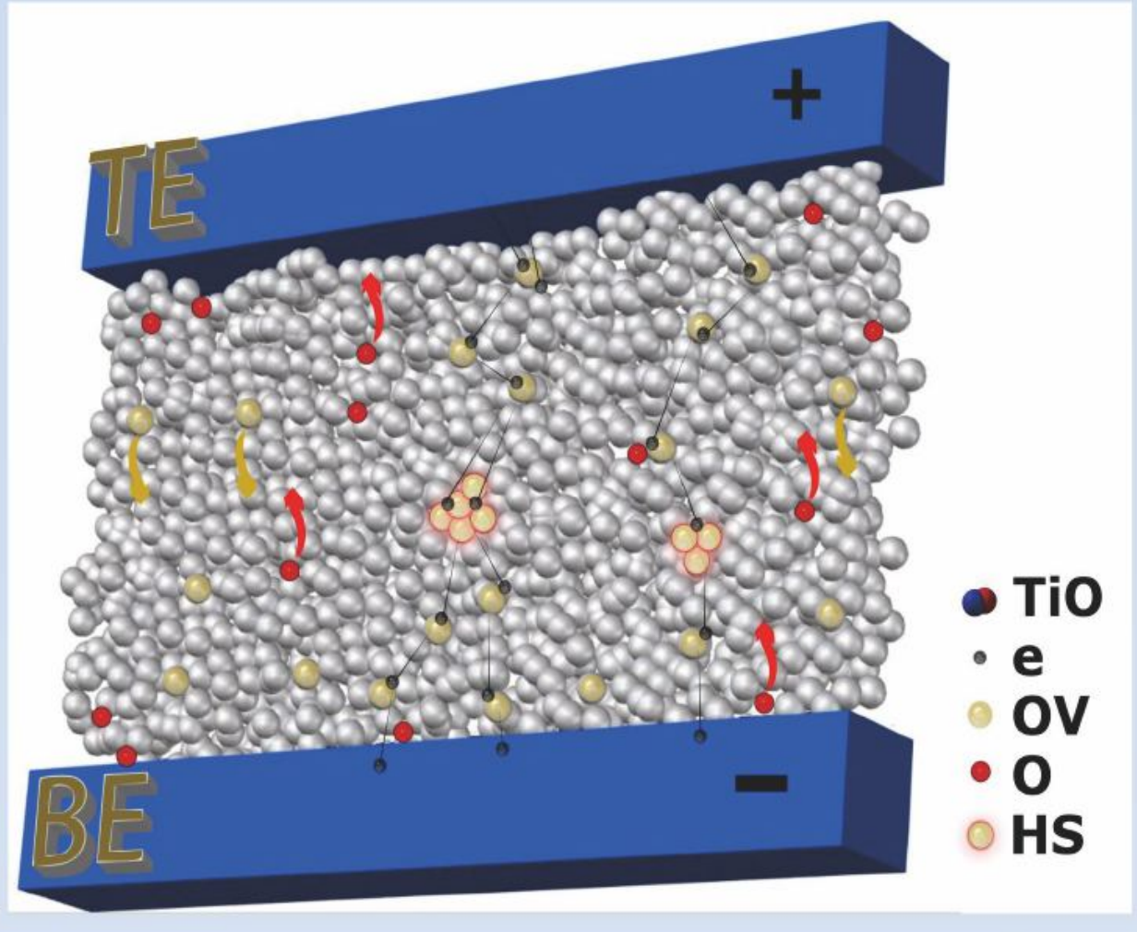
$$D_n = D_o \exp\left(-\frac{E_h}{k_B T_n}\right)$$

The differential change in the Gibbs free energy during the simulation progress is given by:

$$\Delta E_n = \mu\Delta N_{ov,n} - S\Delta T_n$$

Results

Schematic illustration during initial forming stages. Random high initial OV concentration spots attract more hopping electrons and yield "hot spots".



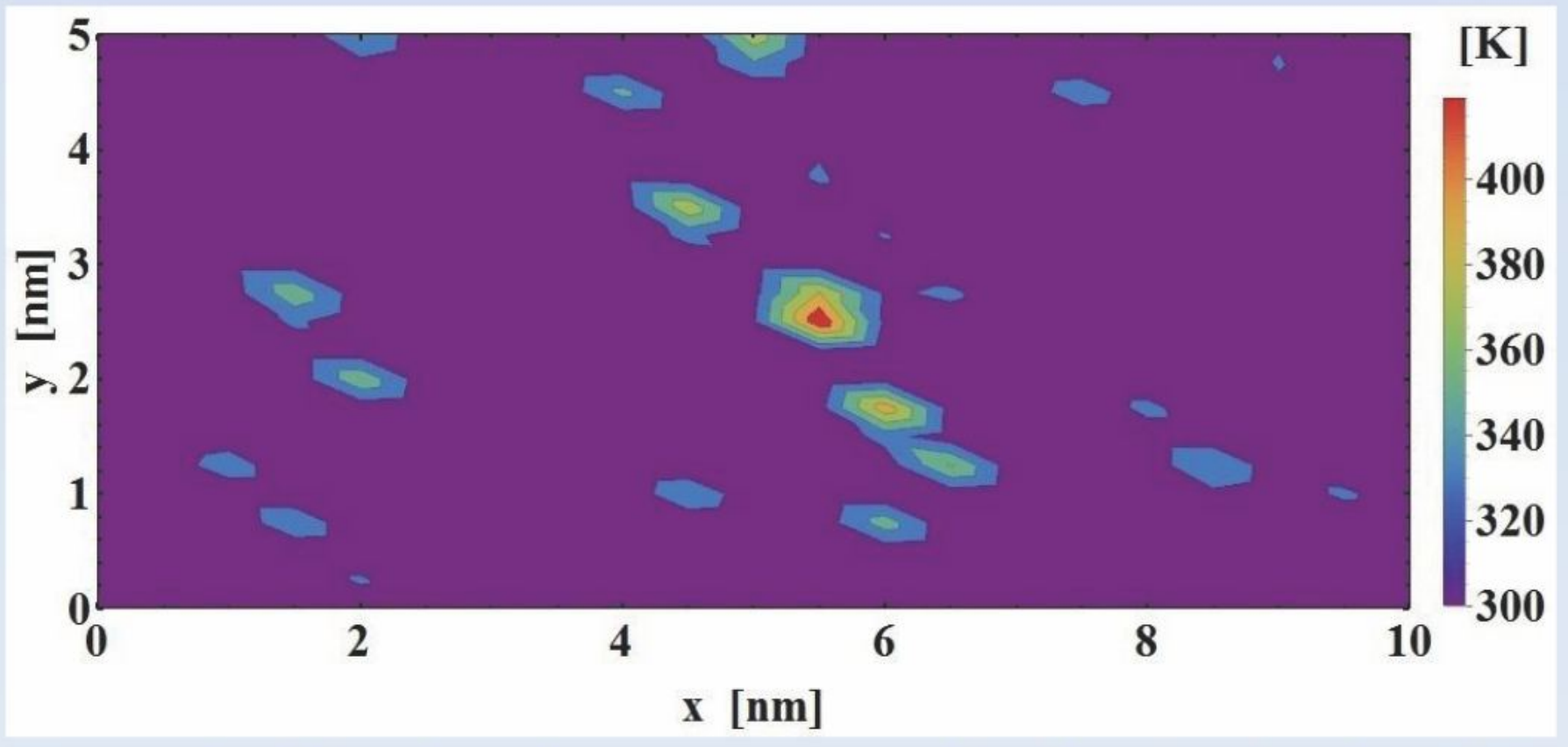
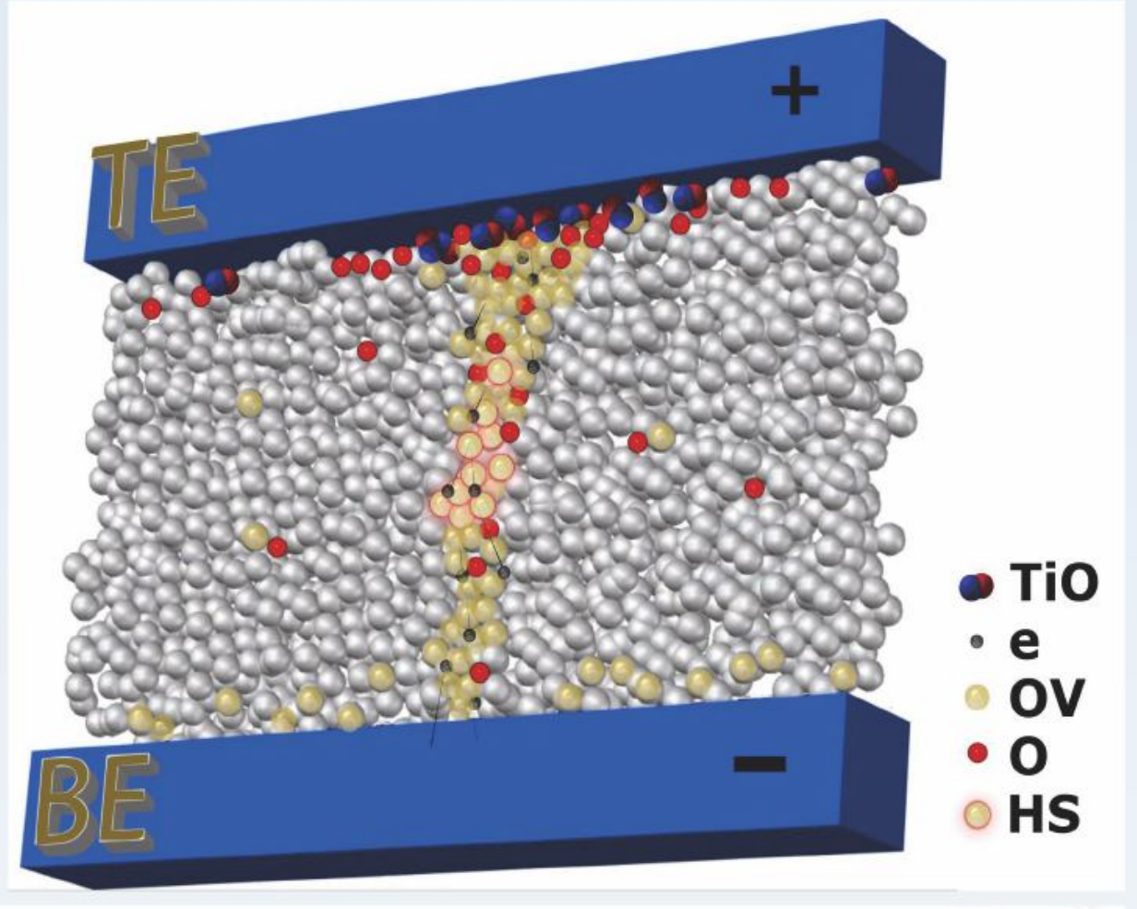


Figure 1: Simulated temperature distribution in the RSL during the initial forming stages, hot spots are evident.

Schematic illustration of the formed CF within the RSL. The HS area along with the high concentration of OV are shown.



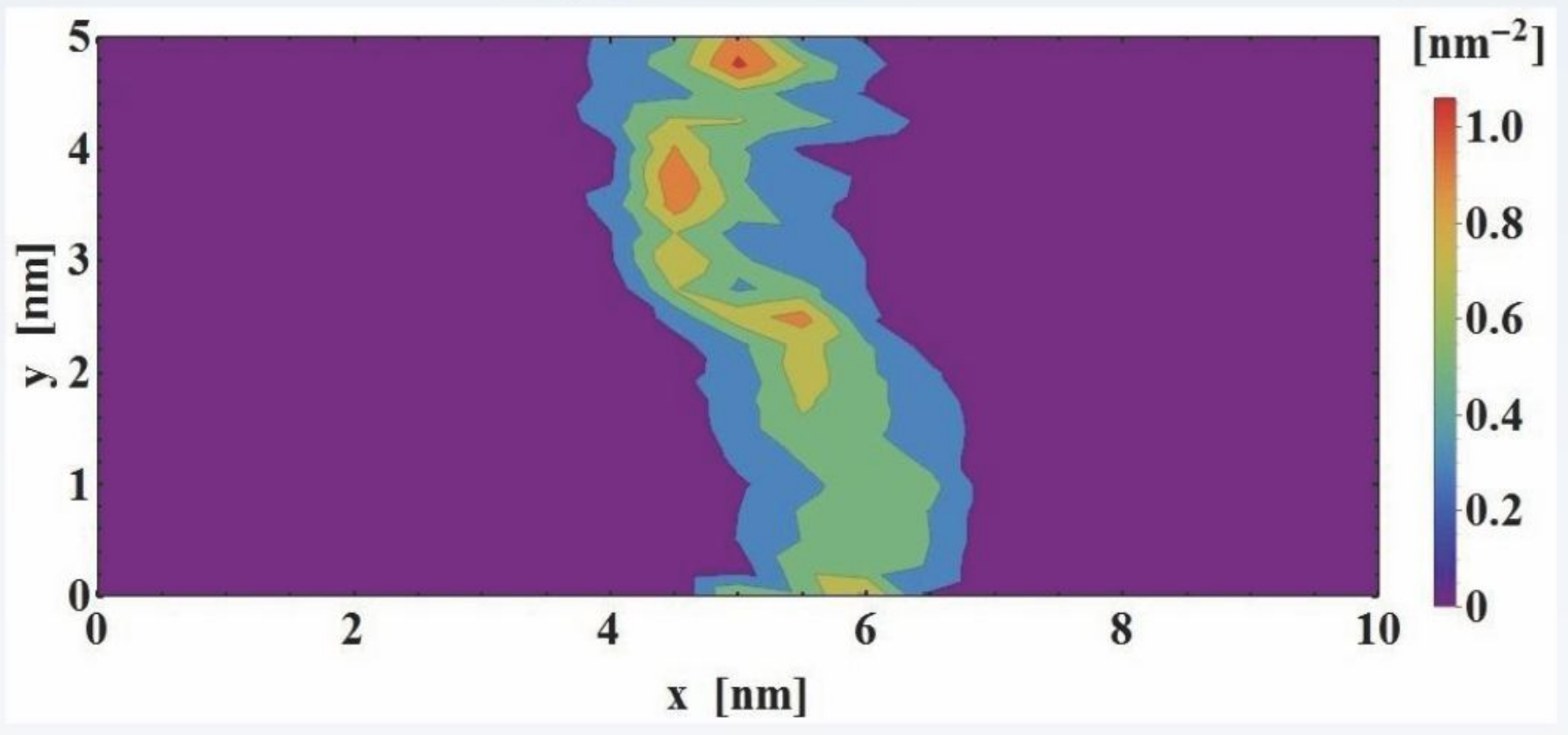
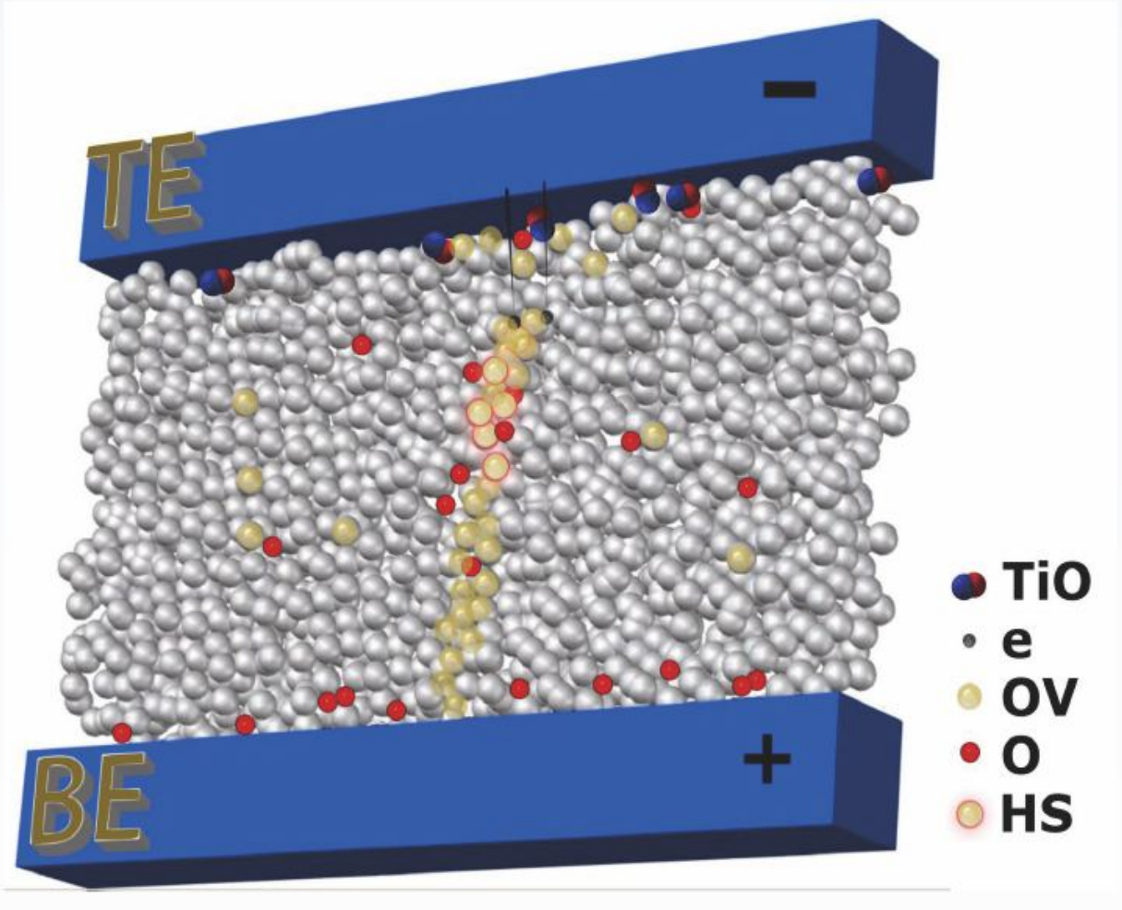


Figure 2: simulation results of OV concentration within the RSL depicting a formed CF as evolved from the HS.

Schematic illustration of the ruptured CF. The ruptured area is close to the TE due to O reservoir like behavior of the TE.



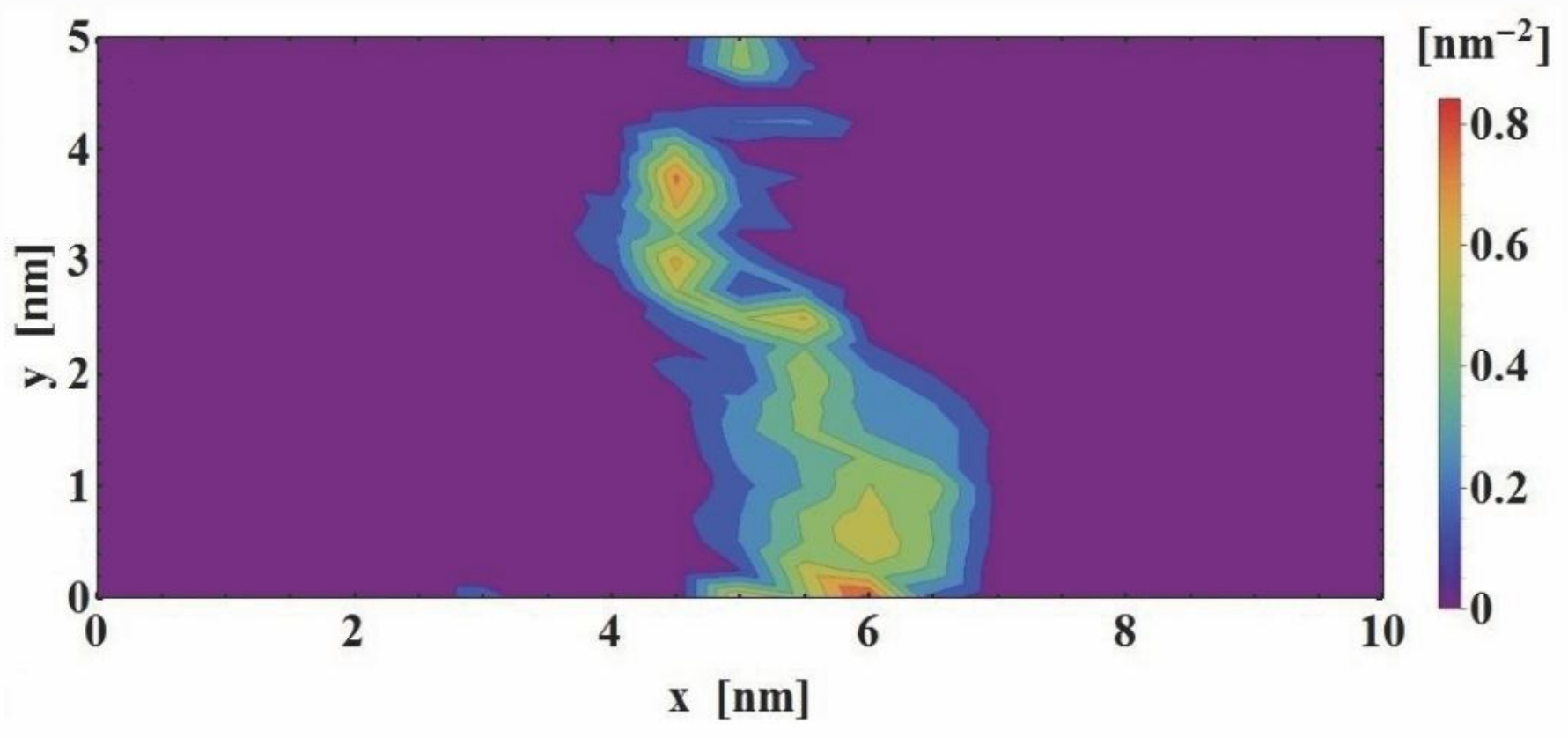


Figure 3: simulation results of OV concentration within the RSL depicting a ruptured CF.

Conclusions

Local heat contributions at the beginning of the forming stage create "hot spots" in the random high agglomeration defect areas. The temperature increase is due to concentration of electrons passing through the HSs resulting in liberated energy by phonon emission. The contribution of these small currents at each step is accumulated and a temperature gradient is thus generated between the HS and the heat sinks. These localized high temperature surges lead to increased generation and hopping of species in a positive feedback thus providing a 'seed' out of which the CF evolves.

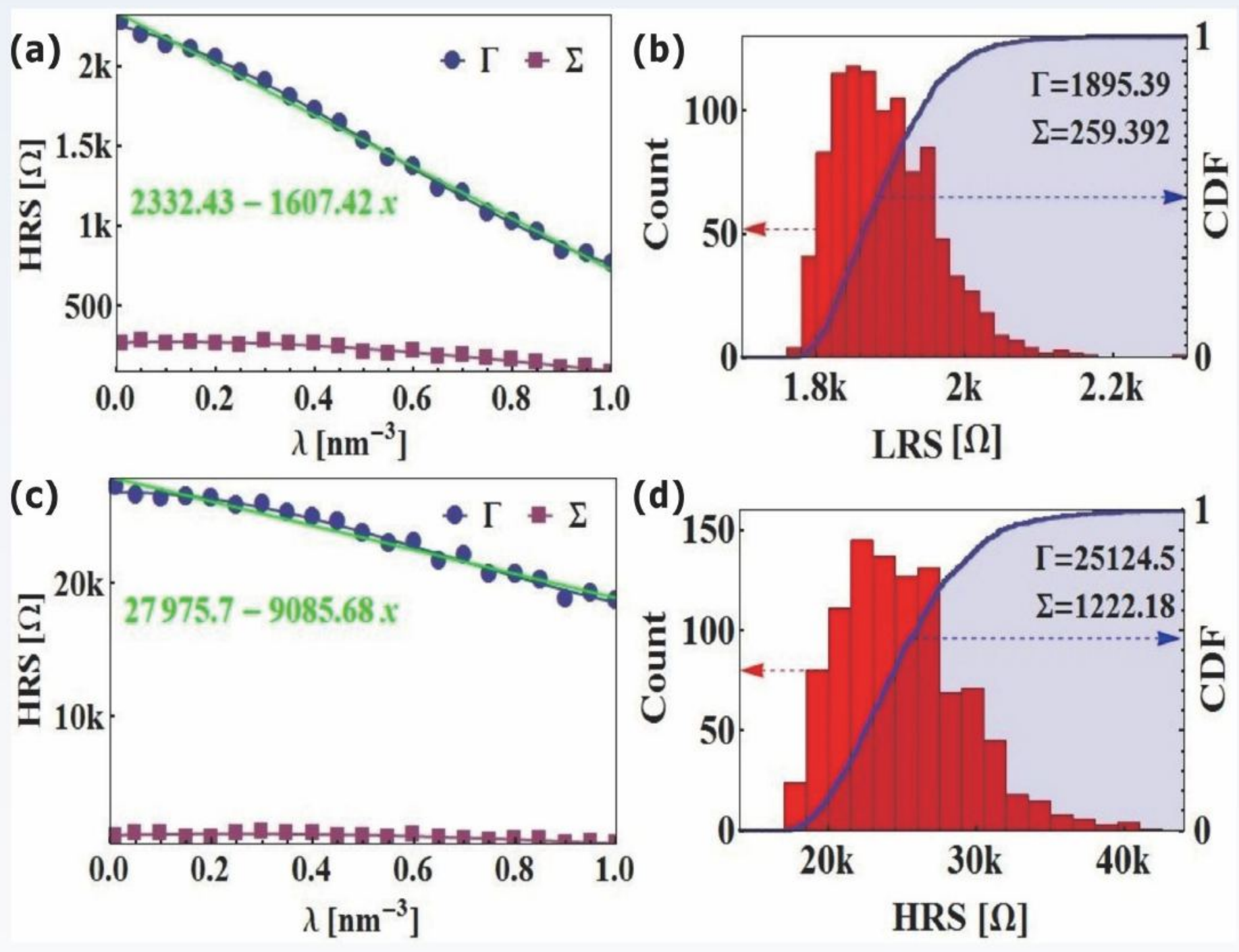


Figure 4: Statistical analysis of CF resistance. LRS: (a) mean value Γ and variance Σ for λ sweep (b) Histogram plot and CDF for λ=0.3 nm^{-3} ; HRS: (c) mean value Γ and variance Σ for λ sweep (d) Histogram plot and CDF for λ=0.3 nm^{-3}.

References

D. Berco and T. Y. Tseng, "A comprehensive study of bipolar operation in resistive switching memory devices", Journal of Computational Electronics, August 2015.