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Barcelona

Multiscale Modelling of Dielectric Breakdown in Amorphous HfO_2

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APPLIED
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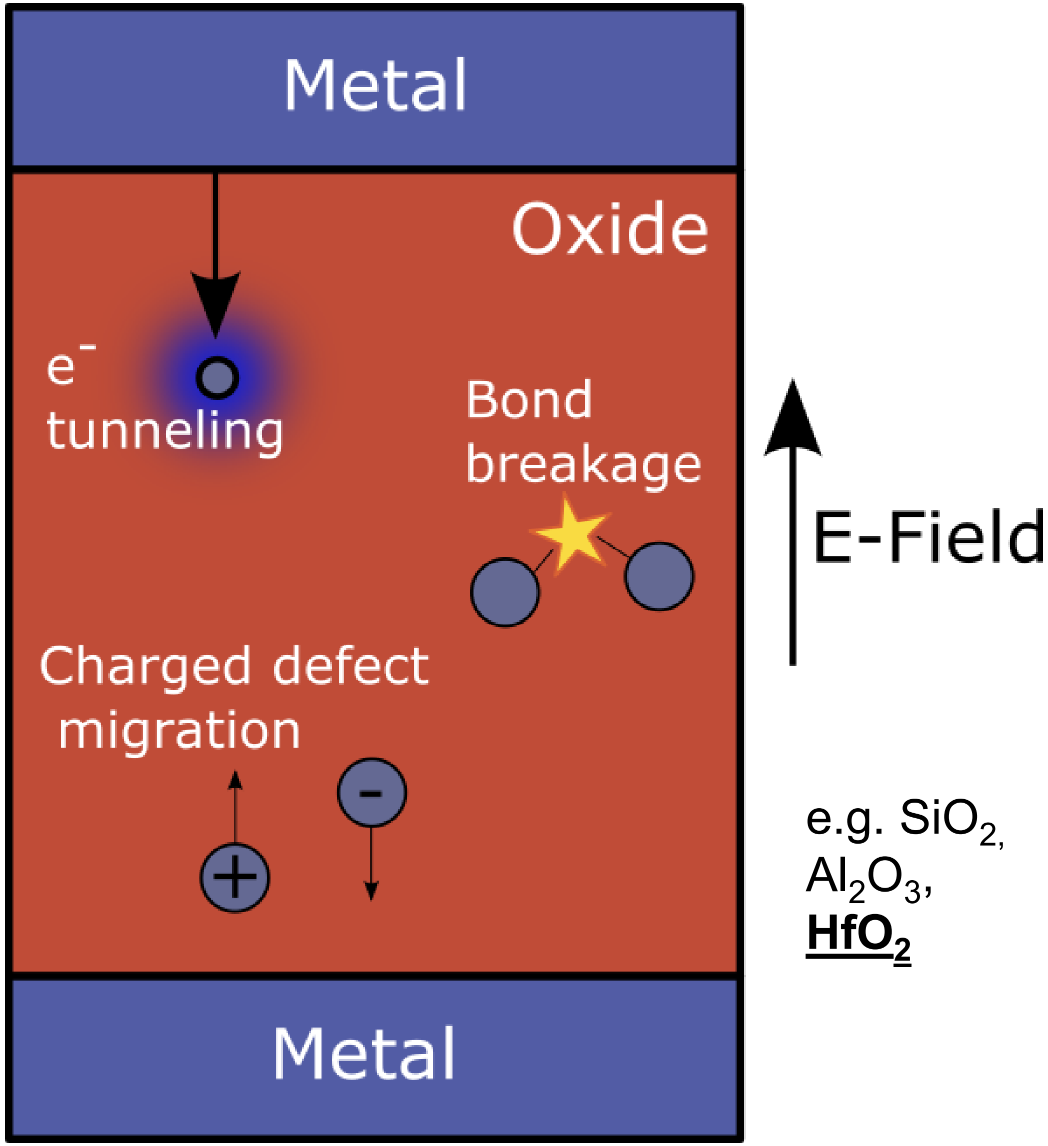
Metal-Insulator-Metal Stacks under Electrical Stress



e.g. SiO_2, Al_2O_3, **$\underline{HfO_2}$**

- The Metal-Oxide-Metal or (SC) stack is common to many nanoelectronic devices

- Application of E-Field leads to three phenomena (in bulk):
  1. **Charging** due to tunneling into defects

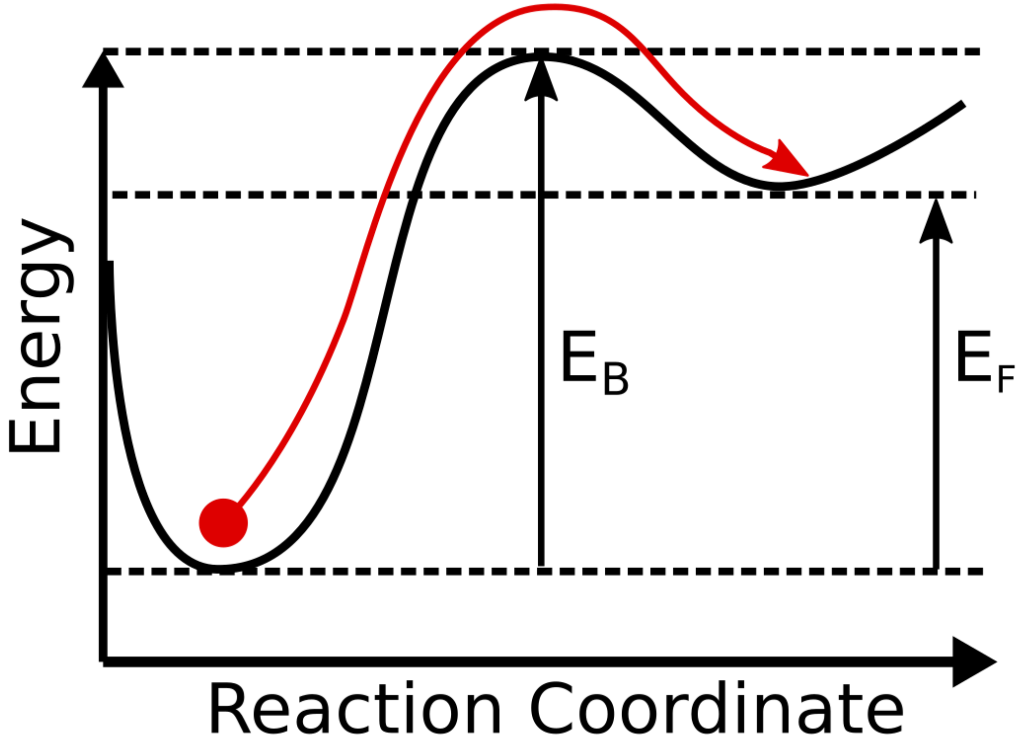
  2. Defect generation (**<u>Oxide degradation)</u>**
     - <u>Related to charging (process 1)</u>
     - <u>Breakdown related to O Vacancy generation</u>

  3. Migration of charged species/defects
     - Charged interstitial and vacancy defects drift under E-Field Effect

El-Sayed, Al-Moatasem, et al. "Effect of electric field on migration of defects in oxides: Vacancies and interstitials in bulk MgO." *Physical Review B* 98.6 (2018): 064102.

Action of E-Field

- For "things to happen" (defect migration, defect generation) we must overcome an energetic barrier (i.e. Activation energy):



Schematic of a general pathway

E_F = Formation Energy
E_B = Energy Barrier

- Formation energy can be positive or negative

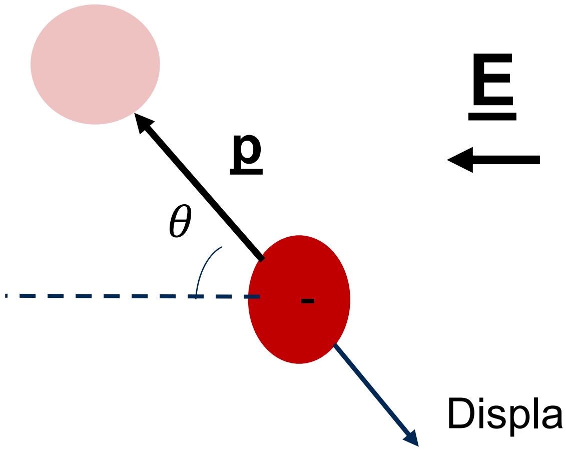
- Can **E**-field accelerate processes by reducing the energy barrier?

Action of E-Field

E-field can affect barrier heights in two ways:

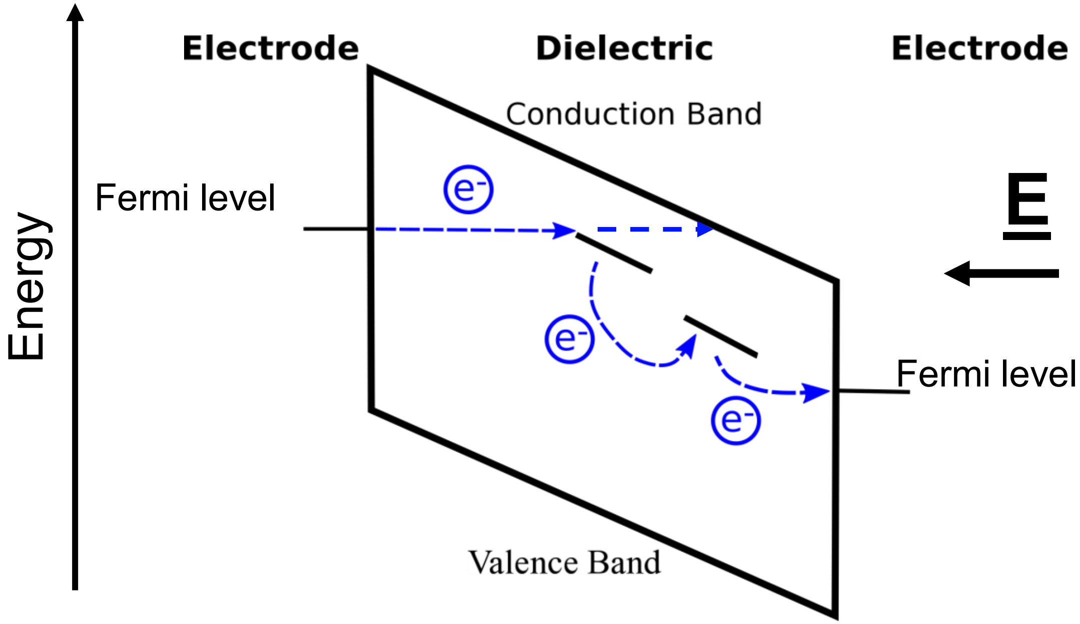
1- “Direct” Effect: Displacement of oxygen ion creates dipole which interacts with **E** field.

$$U = -\boldsymbol{E} \cdot \boldsymbol{p}$$



Effect depends on orientation of E field w.r.t. dipole

2- Electron Injection: **E** field can realign relative energy of electrode Fermi level and trap states



Charging leads to ‘bond weakening’

Methodology–Density Functional Theory Calculations

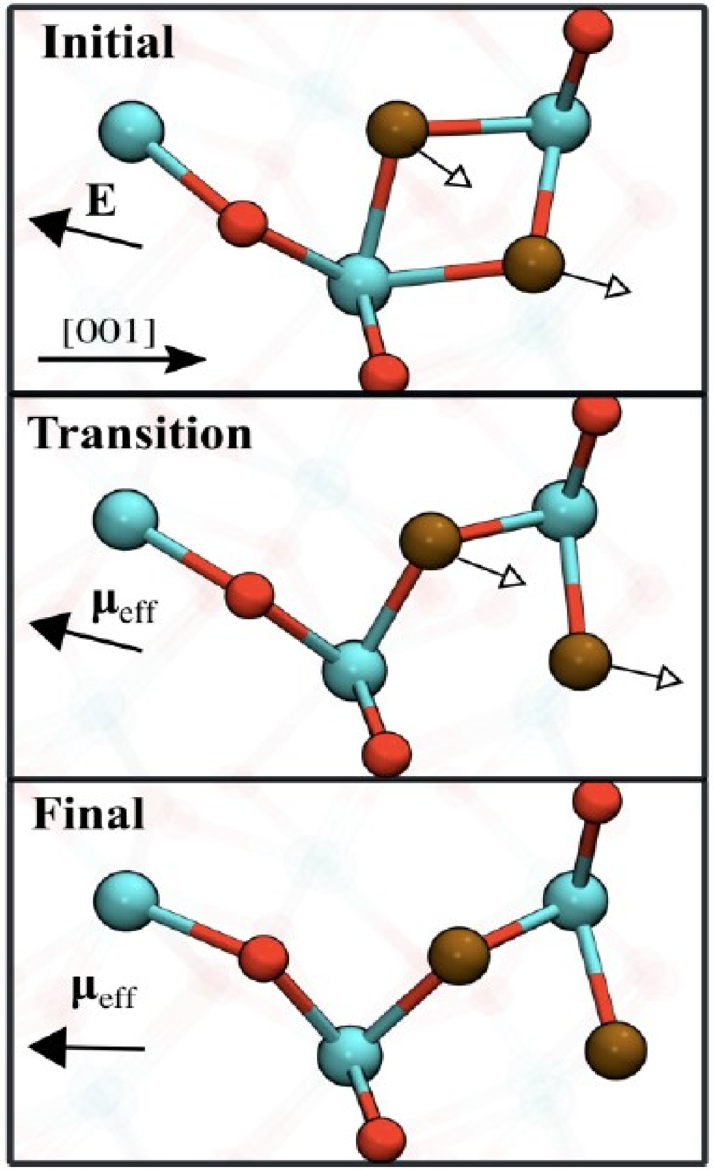
- Calculation of defects and defect processes use density functional theory (DFT)

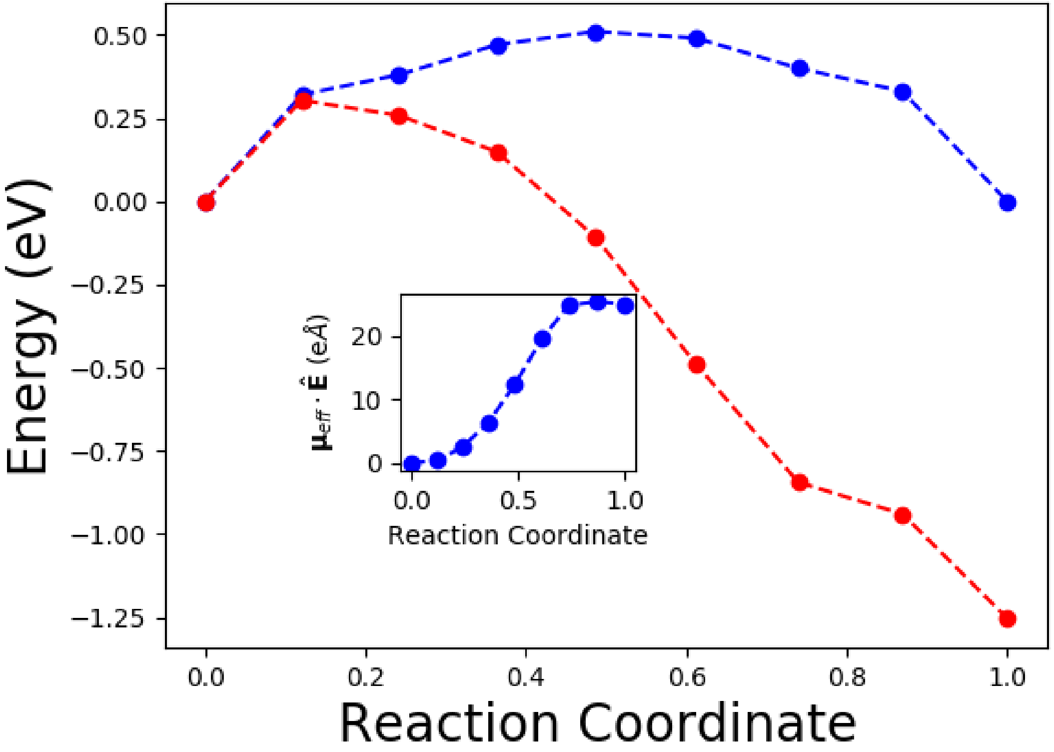
- Software: CP2K

- XC Functional: PBE0-TC-LRC. This is a variant of the hybrid PBE0 functional.
  - **Hybrid functionals contain non-local exchange, which improves accuracy of localized states associated with defects**.

- Electric field interaction with charged particles calculated using the modern theory of polarization. (”Berry phase approach”, see Resta, Raffaele et al *Physics of Ferroelectrics*. 2007. 31-68.)

Migration of Charged Ions





Blue Line = Zero applied field

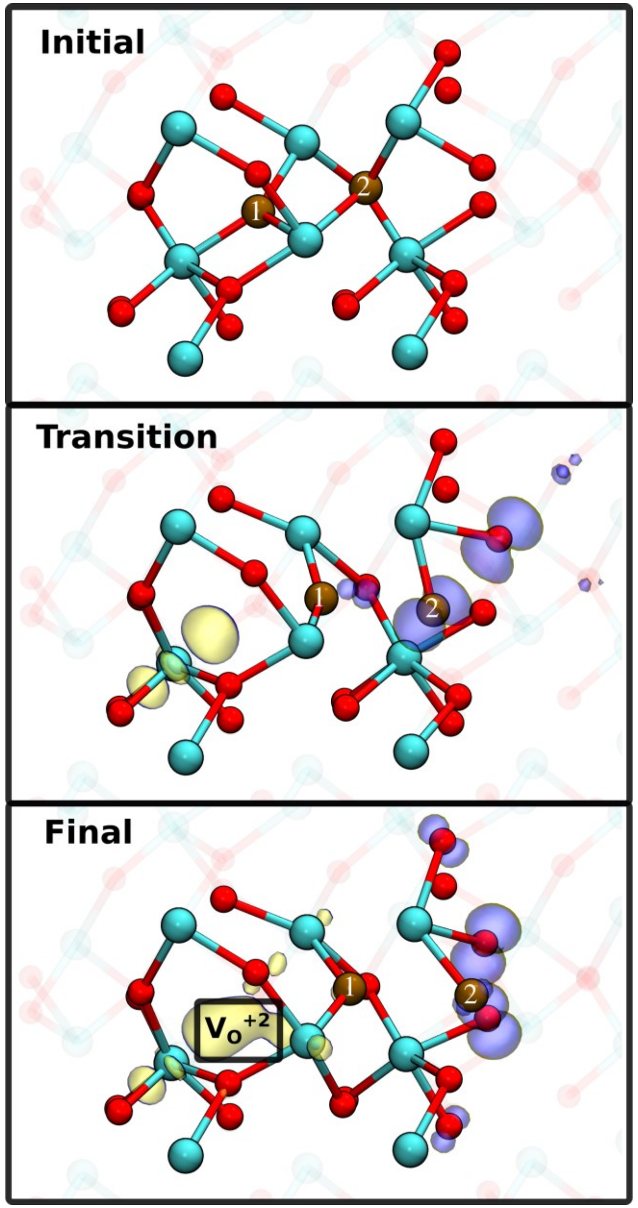
Red Line = 0.5 Vnm^{-1} applied field

- O_I^{-2} defect moves by interstitialcy mechanism
- Field free barrier is only 0.5 eV
- E-Field reduction leads to 0.25 eV barrier height at 0.5 Vnm^{-1}

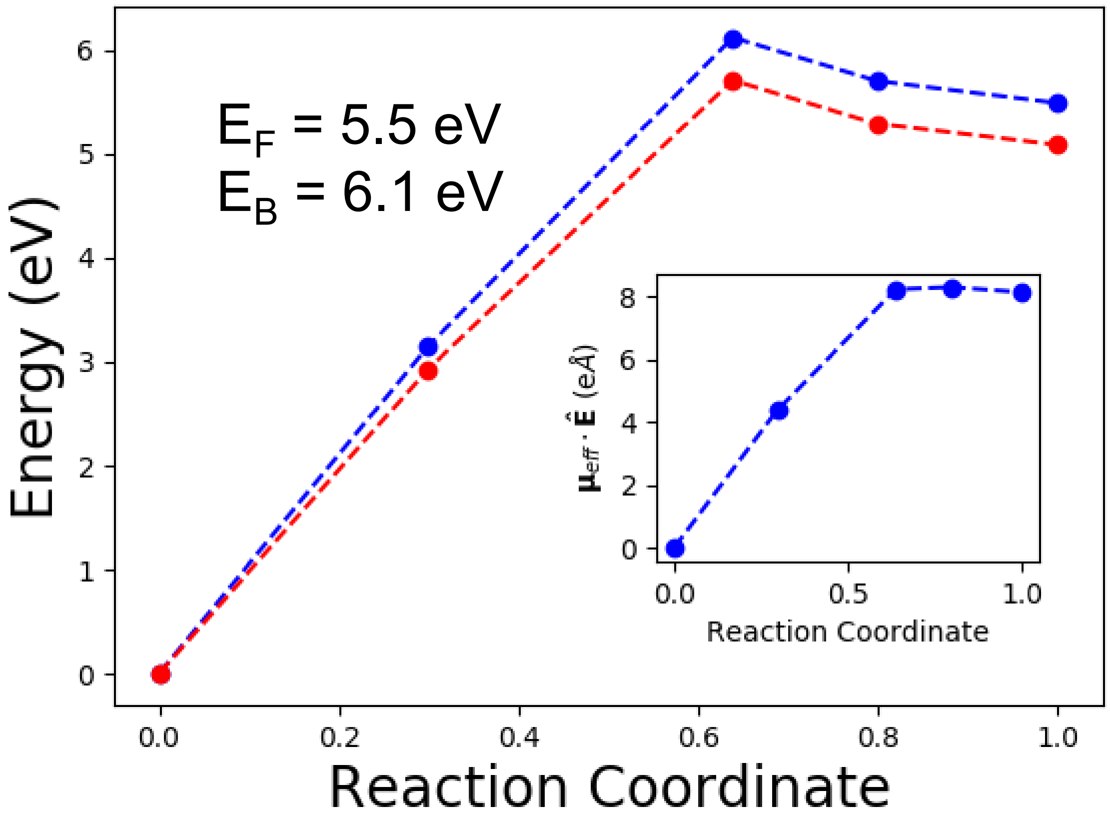
Strand, Jack W., et al. "Effect of electric field on defect generation and migration in HfO_2." *Physical Review B* 102.1 (2020): 014106

O Vacancy Generation

Reaction pathway:



Perfect Crystal $\rightarrow V_O^{+2} + O_I^{-2}$



Blue Line = Zero applied Field

Red Line = 0.5 Vnm^{-1} applied Field

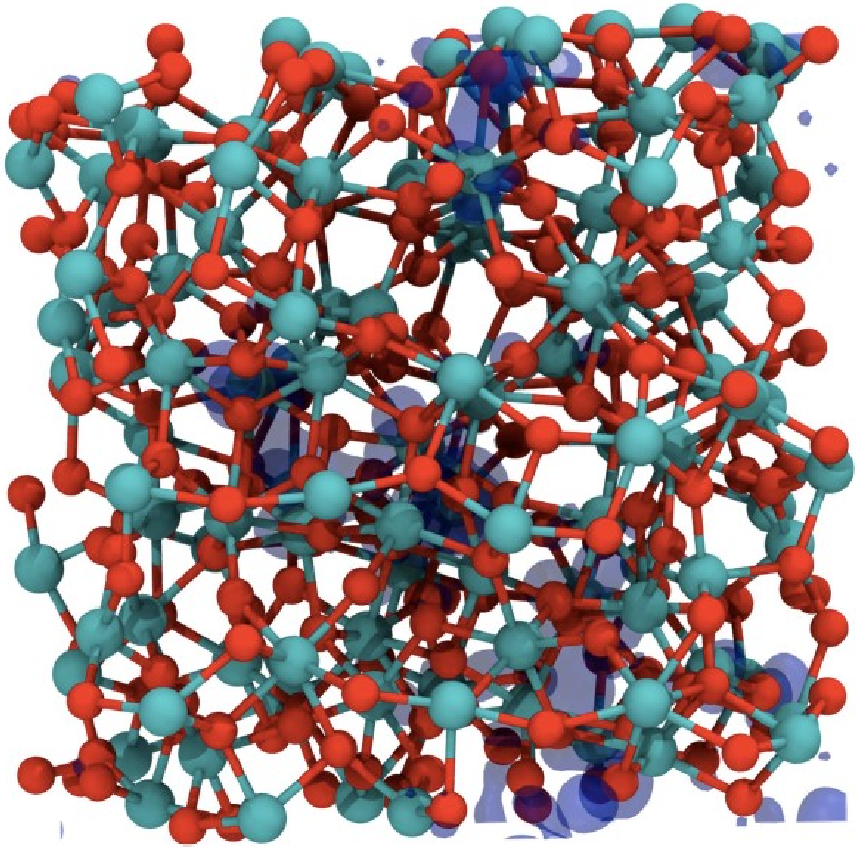
- Barrier height reduction is very small relative to activation energy
- 5 eV activation energy far too high for room T effects
- Direct effect of **E**-field not strong enough to induce vacancy production.

Strand, Jack W., et al. "Effect of electric field on defect generation and migration in HfO_2." *Physical Review B* 102.1 (2020): 014106

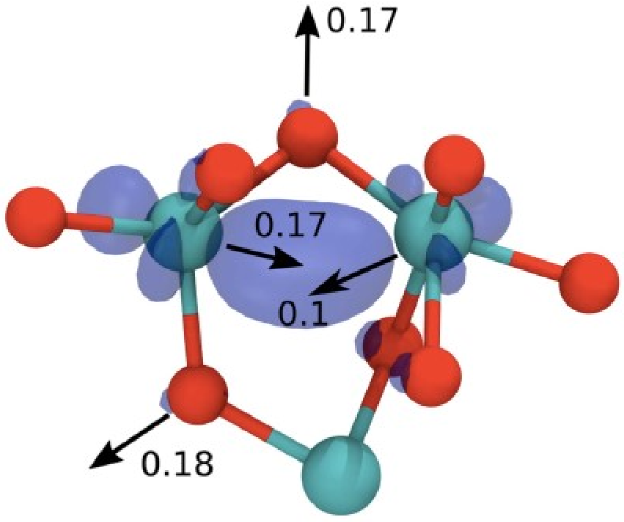
Intrinsic Electron Traps in amporphous HfO_2

Previous work shows that crystal and amorphous HfO_2 can self-trap electrons.

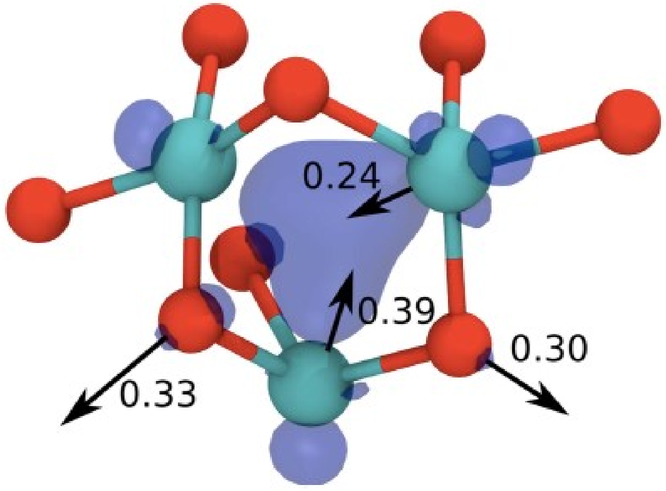
Intrinsic Deep Trap states exist in amorphous HfO_2 due to disorder!



Part-localized state in a-HfO_2



e^- trap in HfO_2



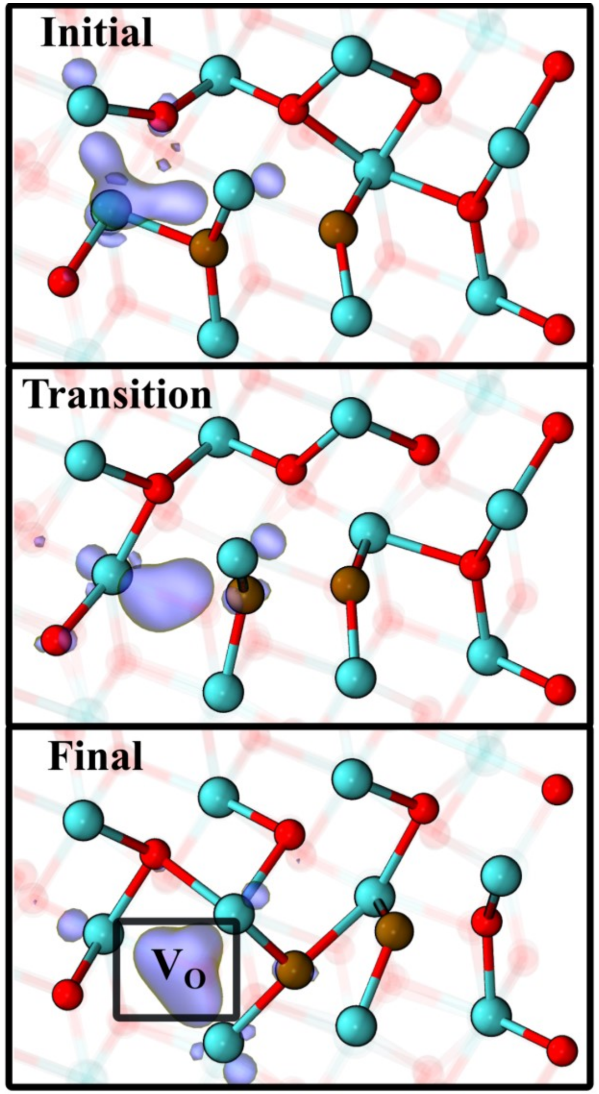
Double e^- trap in HfO_2

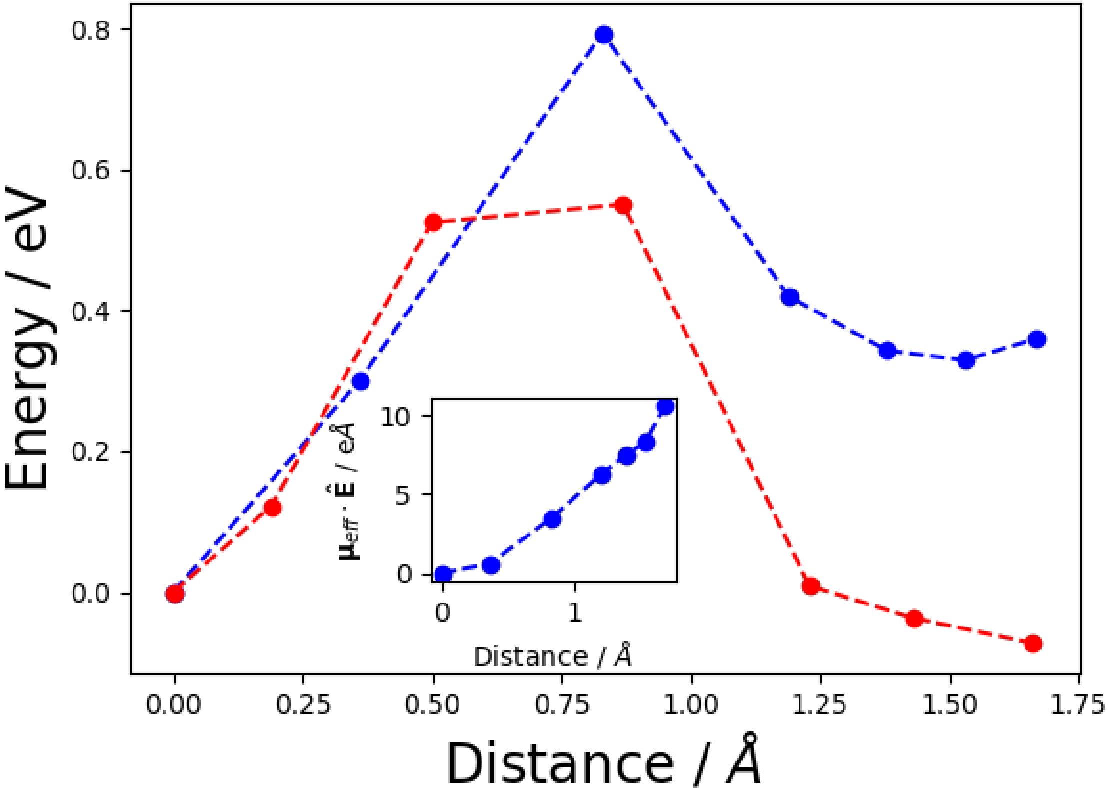
- Strand, Jack, et al. "Intrinsic electron trapping in amorphous oxide." *Nanotechnology* 29.12 (2018): 125703.
- Strand, Jack, et al. "Intrinsic charge trapping in amorphous oxide films: status and challenges." *Journal of Physics: Condensed Matter* 30.23 (2018): 233001.

Vacancy Generation from e^- Trap

Start from $2e^-$ trap:

$$2e^- \rightarrow V_O^0 + O_I^{-2}$$





Blue Line = Zero applied field (e^- trap effect only)

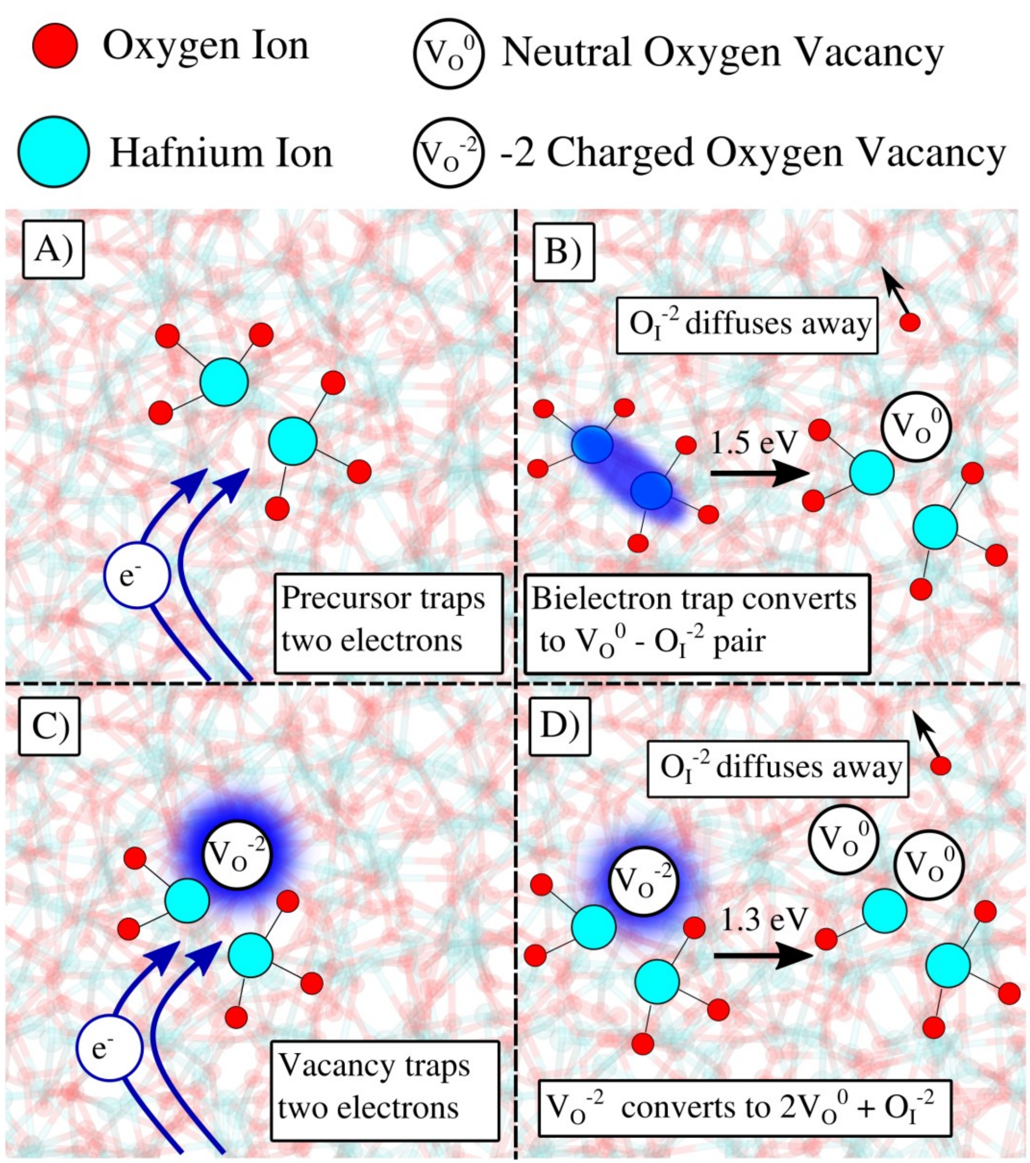
Red Line = 0.5 Vnm^{-1} applied field (e^- trap effect + $-\boldsymbol{E} \cdot \boldsymbol{p}$ effect)

- Defect generation near 2- charged trap has barrier height of 0.8 eV.
- Electron injection effect leads to 5 eV barrier height reduction!
- Direct effect of E-Field responsible for further ~0.5 eV reduction.

Strand, Jack W., et al. "Effect of electric field on defect generation and migration in HfO_2." *Physical Review B* 102.1 (2020): 014106

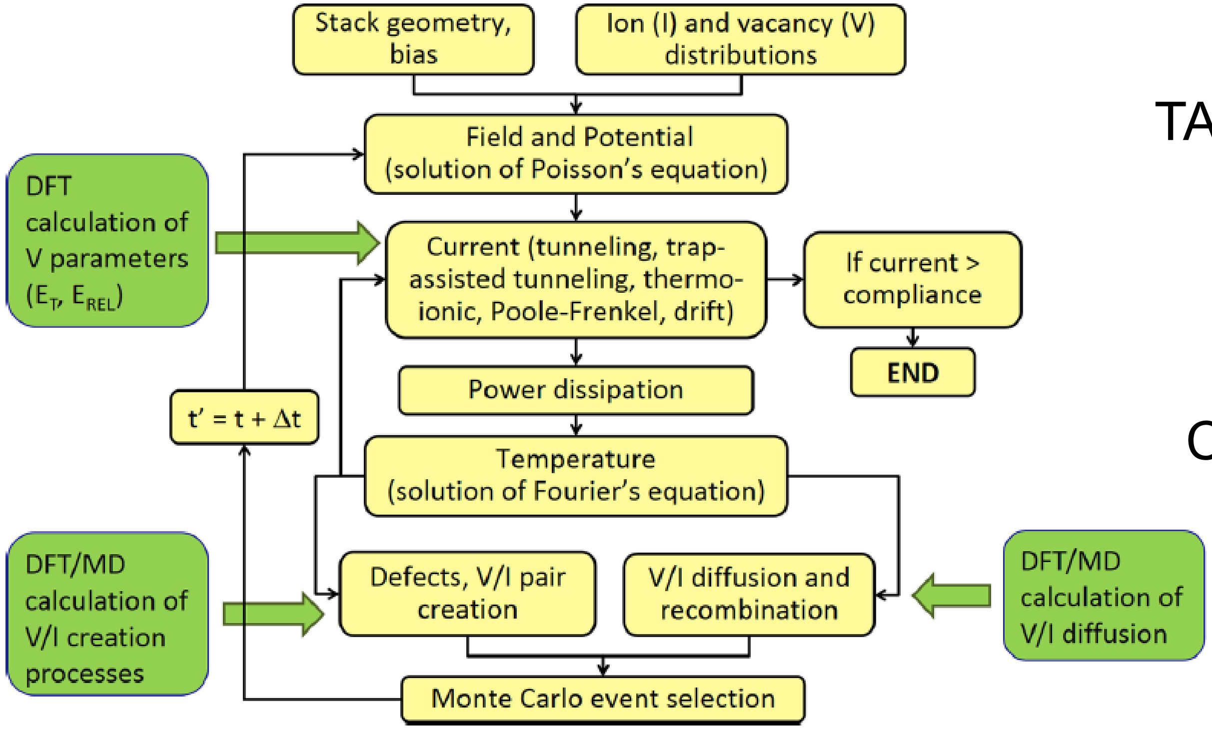
A model for breakdown

- Trapping of electrons can generate oxygen vacancies
- Oxygen Vacancies can also trap electrons, and generate more vacancies by the same mechanism
- These reactions combined provide a mechanism for degradation of the oxide under electrical field stress



Multiscale Modelling

Ginestra^{TM} :



Stack geometry, bias

Ion (I) and vacancy (V) distributions

Field and Potential (solution of Poisson's equation)

DFT calculation of V parameters (E_T, E_{REL})

Current (tunneling, trap-assisted tunneling, thermo-ionic, Poole-Frenkel, drift)

If current > compliance

END

Power dissipation

t' = t + Δt

Temperature (solution of Fourier's equation)

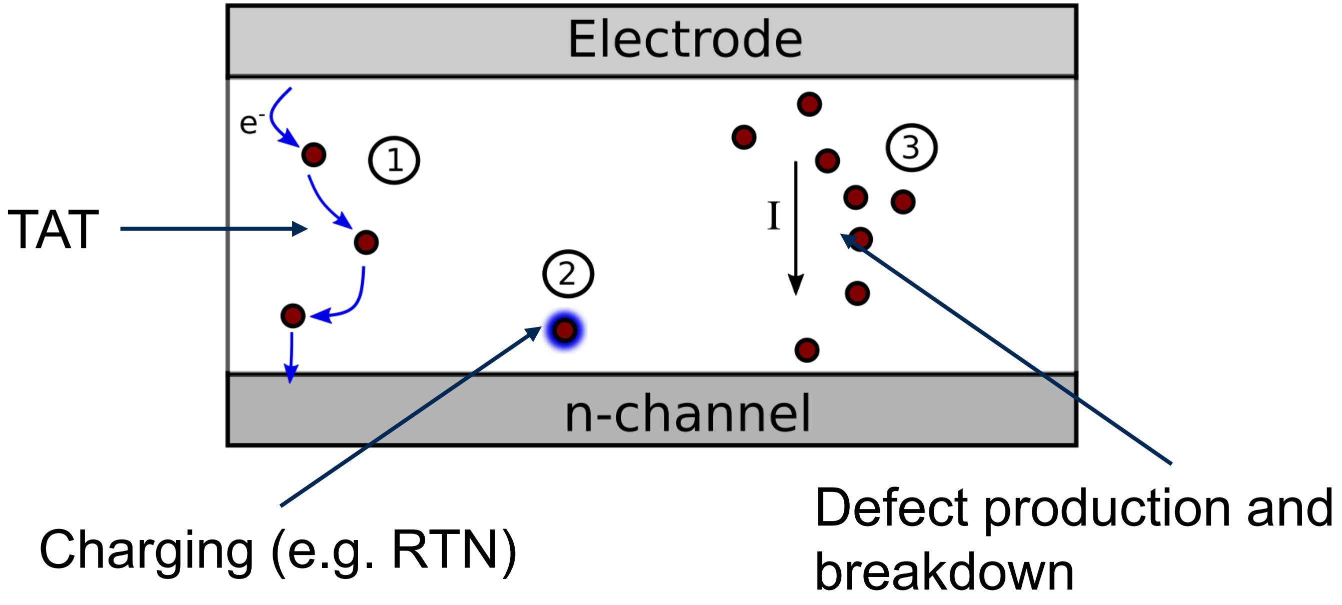
DFT/MD calculation of V/I creation processes

Defects, V/I pair creation

V/I diffusion and recombination

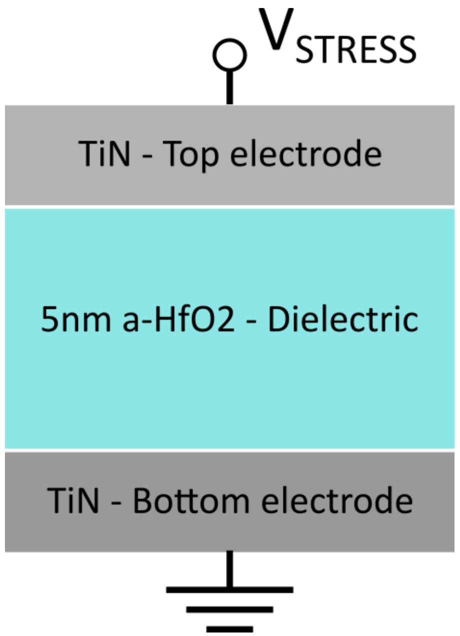
DFT/MD calculation of V/I diffusion

Monte Carlo event selection



Charging (e.g. RTN)

Defect production and breakdown



TiN - Top electrode

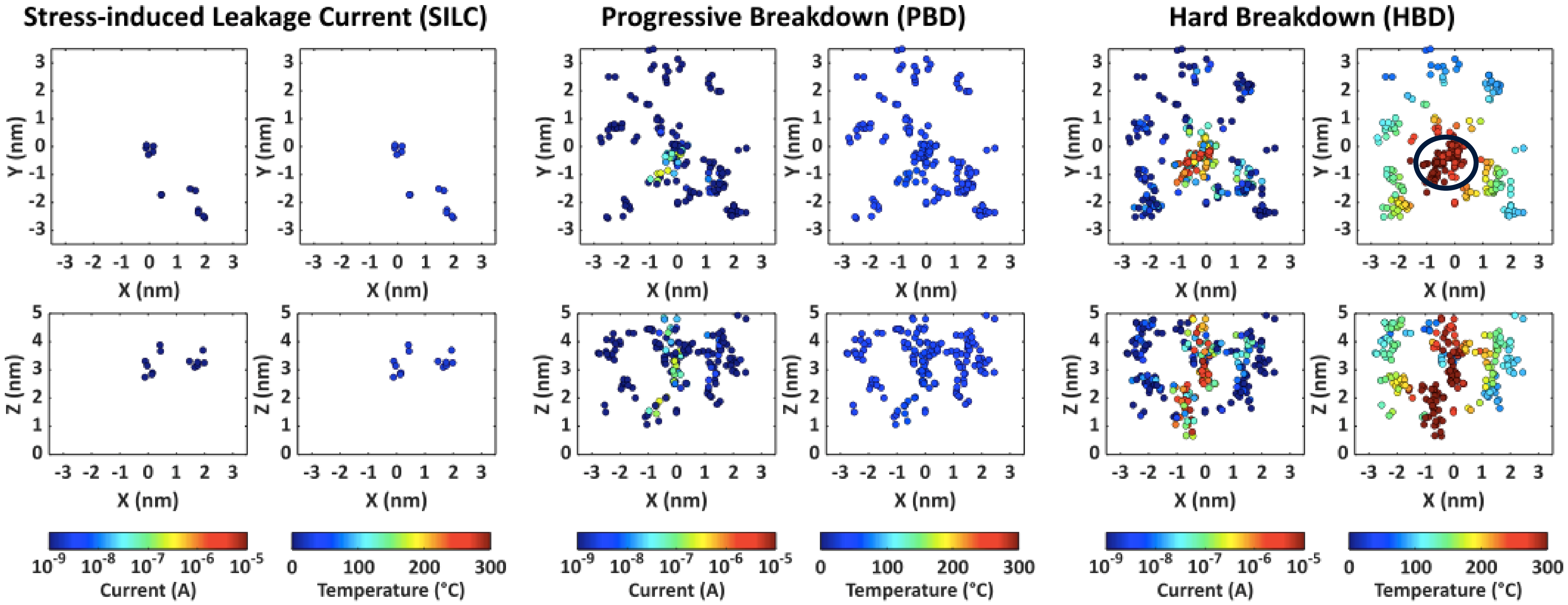
5nm a-HfO2 - Dielectric

TiN - Bottom electrode

- Simulated device has area of <u>7nmx7nm</u>
- Initial vacancy calculation ~1x10^{19} cm^{-3}
- Statistical sample of 20 devices

- Formation energy, barrier heights et cetera can parameterize multiscale models
- Simulate defect generation and TAT current in a MIM device

Distribution of defects and temperature



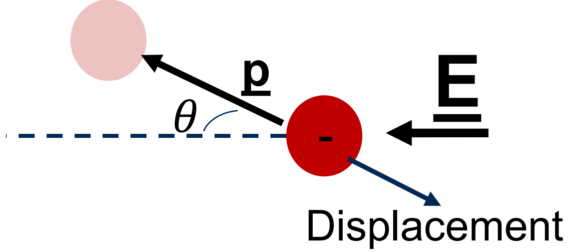
- Up until hard breakdown, defect are generated relatively uniformly
- At hard breakdown, a hot spot develops where the temperature and the number of defects is very large.

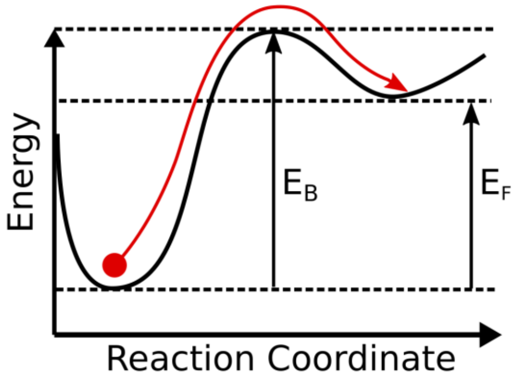
Conclusions

Field-Dipole Interaction

Charge defect reaction have typical barrier reduction of ~ 0.5 to 1 eV

$$U = -\boldsymbol{E} \cdot \boldsymbol{p}$$



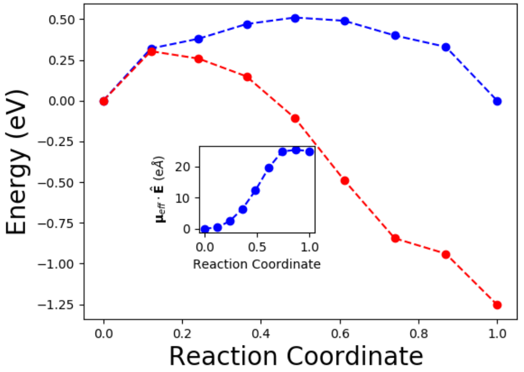


Migration of Charged Defects

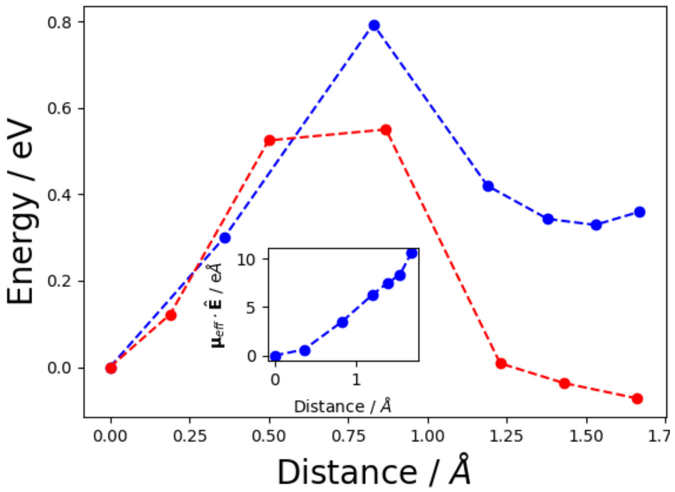
Migration of charged defects can be rapidly accelerated using an E-Field

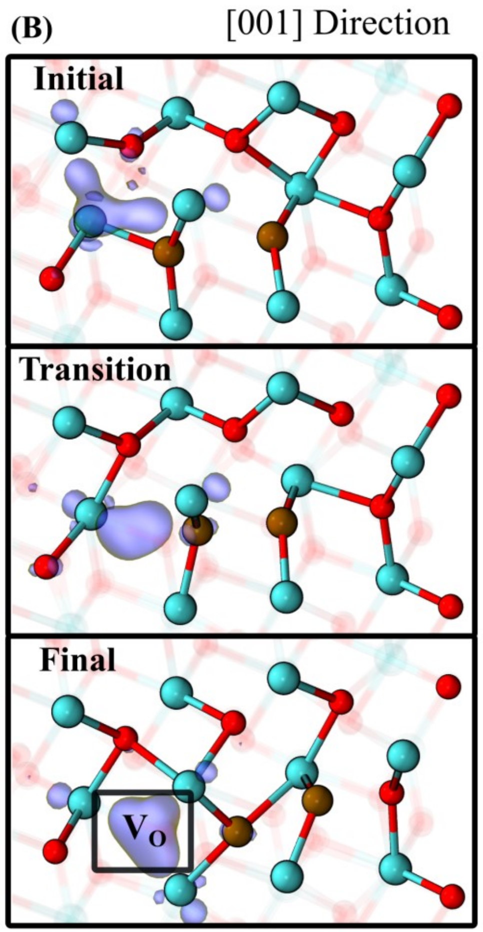
- Only affected by Field-Dipole interaction

→Barrier reduction ~ 0.5 eV



Electron Injection into localized states





Injection of carriers into trap states can reduce defect generation barrier heights by ~ 5 eV.

Defect production leads to oxide degradation.

Any Questions?

Acknowledgments:

- Prof. Alex Shluger
- Prof. Luca Larcher
- Dr. David Gao
- Dr. Al-Moatasem El-Sayed
- Dr. Moloud Kaviani
- Dr. Andrea Padovani
- Dr. Paolo La Torraca

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Relevant Publications

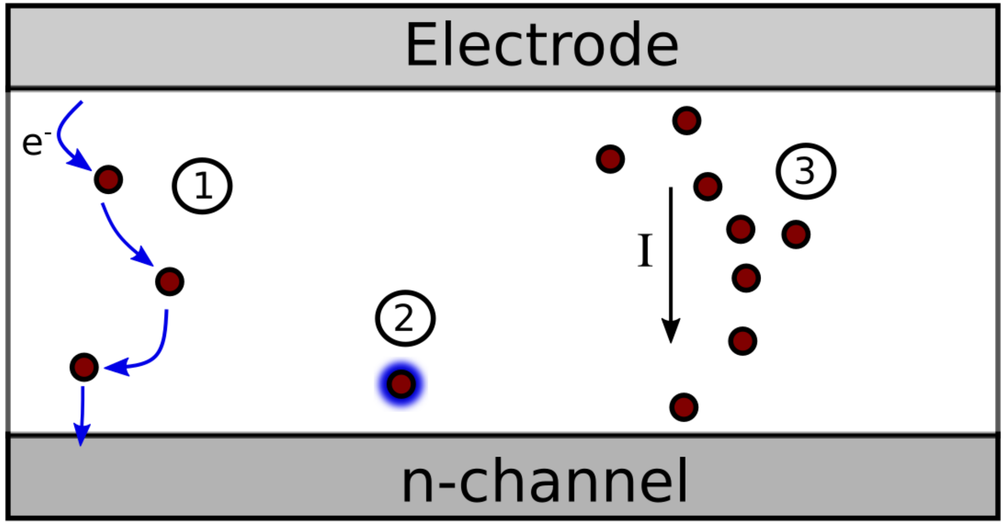
- Strand, Jack, et al. "Dielectric breakdown in HfO_2 dielectrics: Using multiscale modeling to identify the critical physical processes involved in oxide degradation." *Journal of Applied Physics* 131.23 (2022): 234501.
- Strand, Jack W., et al. "Effect of electric field on defect generation and migration in HfO_2." *Physical Review B* 102.1 (2020): 014106.
- Padovani, A., et al. "A microscopic mechanism of dielectric breakdown in SiO_2 films: An insight from multi-scale modeling." *Journal of Applied physics* 121.15 (2017): 155101.
- Gao, David Z., Al-Moatasem El-Sayed, and Alexander L. Shluger. "A mechanism for Frenkel defect creation in amorphous SiO_2 facilitated by electron injection." *Nanotechnology* 27.50 (2016): 505207.

Extra Slides…

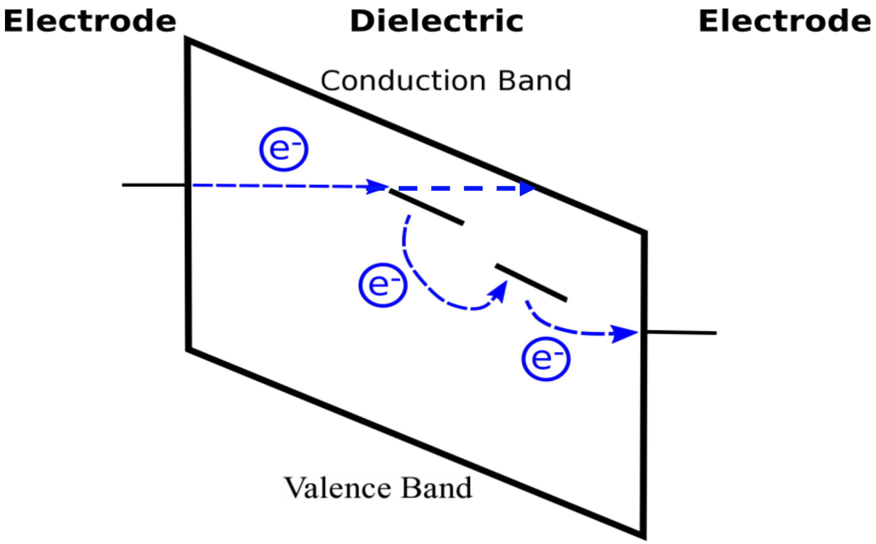
Practical Consequences of Electrical Stress

Charging, bond breakage and migration lead to three main consequences:

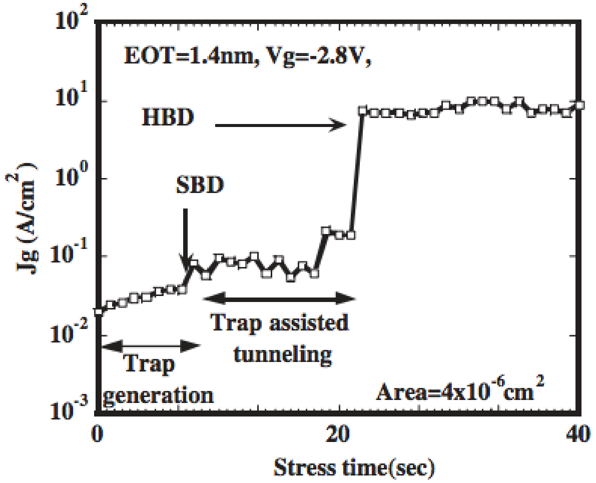
1. Trap Assisted Tunneling (SILC)
2. Charging and de-charging of defects (RTN, threshold voltage shift)
3. Buildup of defect population and current (dielectric breakdown)



Trap Assisted Tunneling

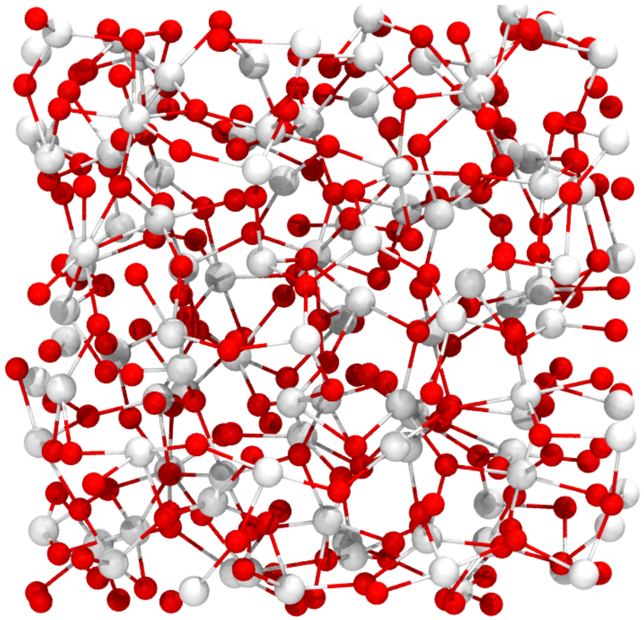


Dielectric Breakdown



Kim et al Microelectronics Reliability 44(2) 2004

Amorphous HfO_2 Models



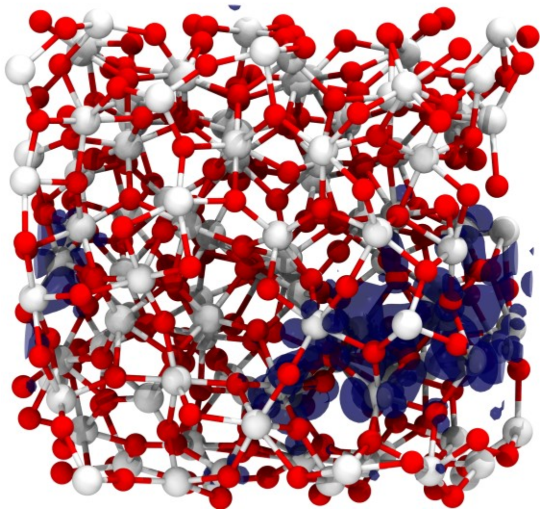
Geometric Structure:

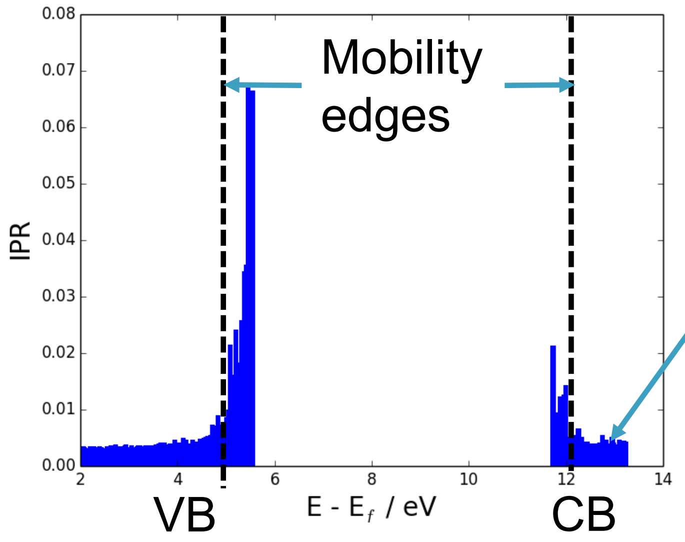
Type	CN	96	324	768	1500	6144
Hf	5	8.1[11.6]	9.6[14.1]	9.0	9.7	8.2
	6	47.6[48.7]	65.6[60.9]	78.1	75.5	75.3
	7	44.3[39.7]	24.8[25.0]	12.9	14.8	16.5
O	2	6.4[10.5]	6.0[10.9]	6.1	6.6	5.8
	3	69.2[65.0]	83.1[71.0]	85.9	84.3	84.2
	4	24.4[24.5]	10.9[18.1]	8.0	9.1	10.0

- Average density = 9.6 g cm^{-3}
- Undercoordinated Hf ions
- Extended bond lengths

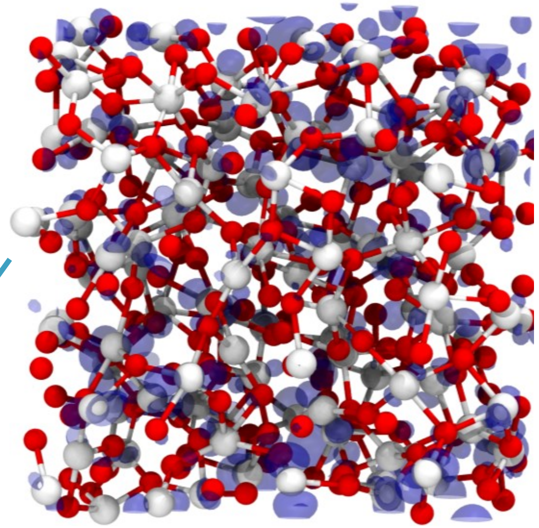
Electronic Structure:

CBM State





Deep CB state



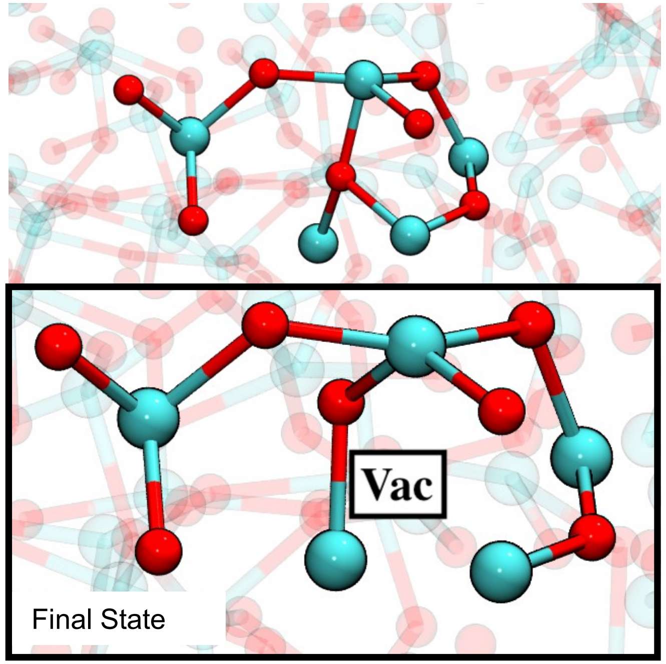
$$\mathrm{IPR}(\psi_n) = \frac{\sum_i^N c_{ni}^4}{(\sum_i^N c_{ni}^2)^2}.$$

Large IPR = localized state
Small IPR = Delocalised state

Defect Generation in Amorphous Oxide

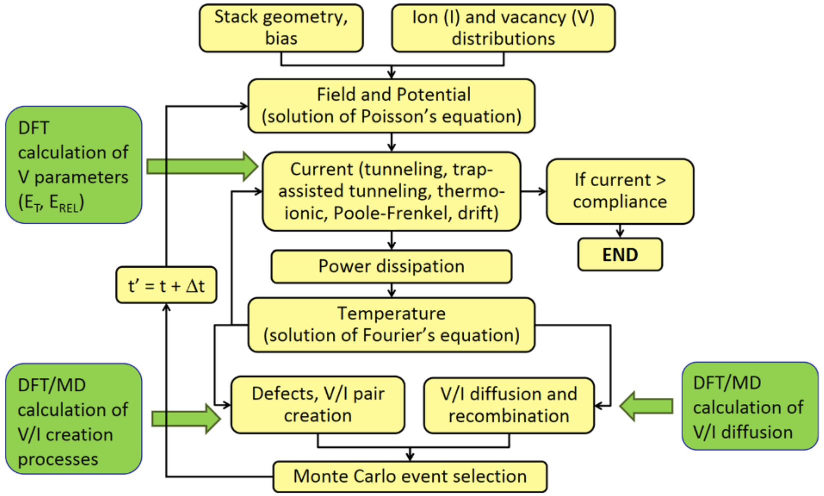
Same reaction mechanism to crystal:

$$2e^- \rightarrow V_O^0 + O_I^{-2}$$



Spread of activation energy heights: 1.1 to 3 eV

Multiscale modelling using Ginestra^{TM} show how trap-based model explains degradation:



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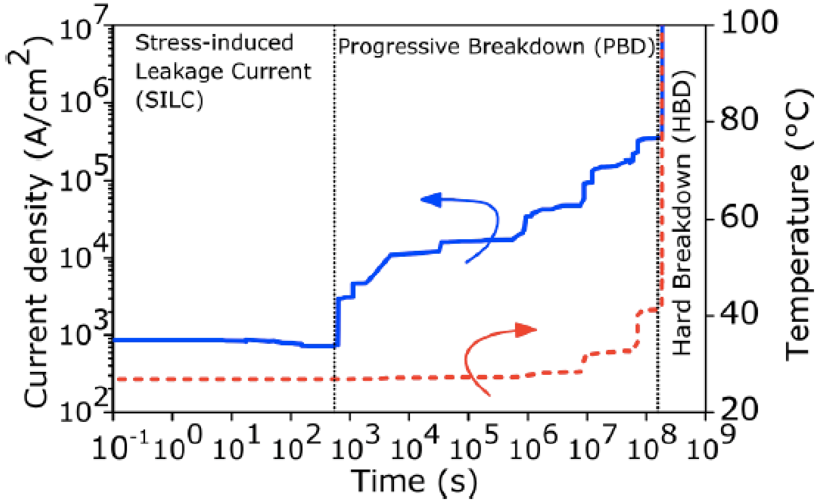

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