Simulation of Nanoscale Interconnects

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ESSDERC/ ESSCIRC Workshop “Process Variations from Equipment Effects to Circuit and Design Impacts”

September 3, 2018, Dresden, Germany

Outline

- Introduction
- Copper Conductivity
  - Electron Scattering Mechanisms
    - Electron-Electron
    - Surface Roughness
    - Grain Boundary
- Electromigration Reliability
- Conclusions and Outlook

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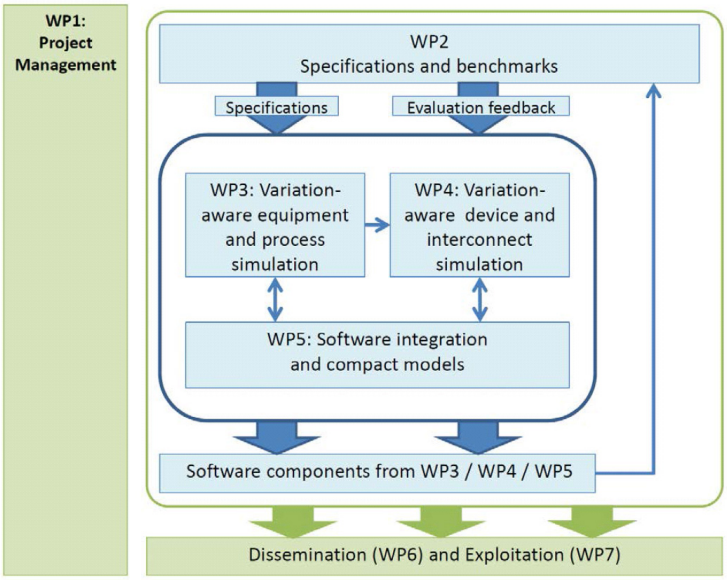
Introduction – Goals and Strategy

- Copper-based metallization in use at least down to 7nm node
  - Nanoscale Cu behavior is influenced by grain size and surface roughness
- Simulations of nano-interconnects lack a connection between modeling the individual interfaces and the continuum simulation of the entire interconnect
  - True for both conductivity and electromigration reliability
- Our goal is to provide simulations to
  - Better understand electron and atom movement inside nanoscale Cu
    - Using Monte Carlo simulations
  - Provide simplified simulation options, while avoiding complex meshes
    - Using spatial parameters in FEM framework

Introduction – Project Context

- This work fits into WP4, dealing with variation-aware interconnect simulations
- The goal is to provide a link between grain boundary/ surface roughness and continuum simulations
- Primarily concentrating on copper conductivity and electromigration reliability



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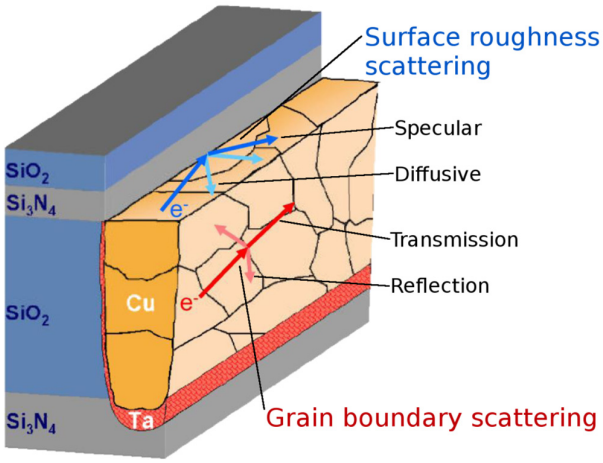
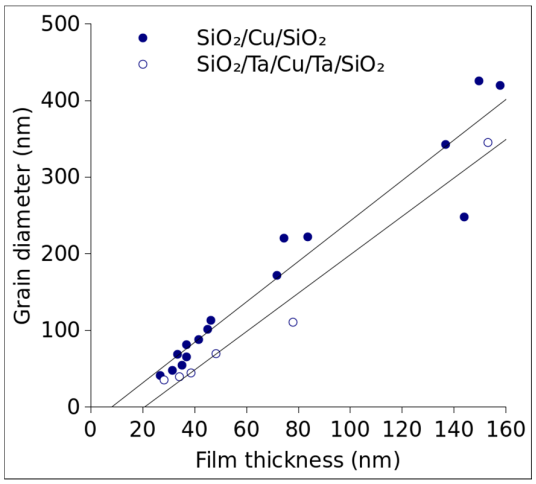
Copper Conductivity

- Cu interconnect scaling results in reduced dimensions
  - Surface roughness and grain boundary play an increasing role



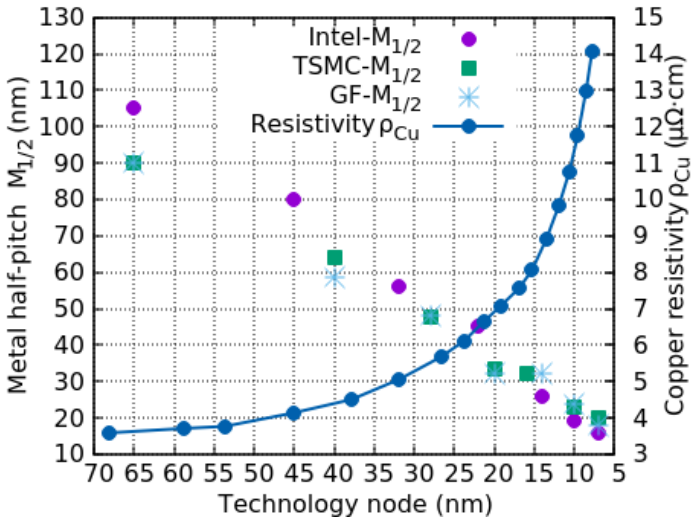
G. Schindler, Sematech workshop on Cu resistivity (2005)



T. Sun, PhD Dissertation, U of Central Florida (2009)

Electron Scattering in Metals

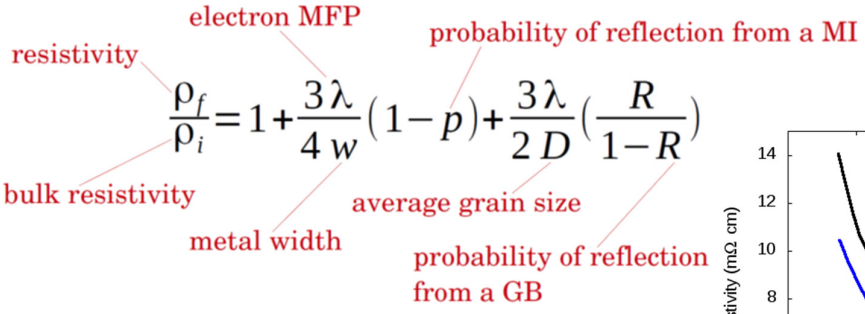
- Cu interconnect scaling results in reduced dimensions
  - Surface roughness and grain boundary play an increasing role



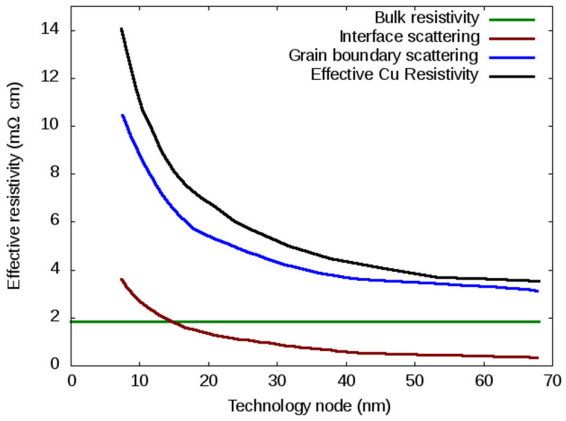
L. Filipovic et al., SISPAD (2017)

Electron Scattering in Metals

- The effects of the granular microstructure on resistivity is modeled by



J.S. Clarke et al., VLSI Symposium (2014)



Electron Scattering in Metals

- Classical macroscopic model for electron transport
  - Scattering events are independent of each other
  - Calculate each event separately, then sum to give total probability
- Microscopic models for electron transport
  - Physical semiconductor models have matured over many decades
  - Modern physical models of transport in metals is far from mature
- Use lessons learned from semiconductor transport (heavily doped)
  - Semiconductor: Moving electrons occupy states above conduction band
  - Metals: Moving electrons in a half-occupied band near the Fermi energy

Equilibrium Electron Statistics I

- Quantum state of an electron is characterized by the quantum number k and energy $\epsilon(k)$
- Equilibrium electron statistics center around the Fermi-Dirac distribution:

$$f(k) = f(\epsilon(k)) = \frac{1}{e^{\frac{\epsilon(k)-\zeta}{k_B T}} + 1}$$

- ζ is the chemical potential, which is a large positive quantity for a many-particle system

Equilibrium Electron Statistics II

- Given the Pauli exclusion principle, the average number of electrons N can be determined as a sum of probabilities of given states to be occupied

$$N = 2\sum_k f(\epsilon(k)) = \frac{2V}{(2\pi)^3}\int d^3k f(\epsilon(k)) = \int_0^\infty d\epsilon 2g(\epsilon)f(\epsilon)$$

where k- states are discrete and 2 accounts for the Pauli exclusion principle

- A single state per volume of Fermi sphere $\frac{V}{(2\pi)^3}$
- Given 3D parabolic energy dispersion, the density of states is

$$g(\epsilon) = V\frac{\sqrt{2}m^{3/2}}{\pi^2\hbar^3}\sqrt{\epsilon}$$

Equilibrium Electron Statistics III

- Normalizing with $\xi = \zeta/k_BT$ and $x = \epsilon/k_BT$ we obtain the ½ Fermi integral

$$n = \frac{\sqrt{2}(mk_BT)^{3/2}}{\pi^2\hbar^3}\int_0^\infty dx \frac{\sqrt{x}}{e^{x-\xi}+1}$$

- And the Fermi energy is obtained

$$e_F = \frac{\hbar^2}{2m^*}(k_F)^2$$

Equilibrium Electron Statistics IV

- Relevant copper properties for electron statistics:

Parameter	Symbol	Value
Density	ρ	8.960 g/cm^3
Atomic mass	m_a	63.546 kg/mole
Permittivity	ε	8.85419 x 10^{-12} F/m
Effective mass	m^*	1.0 m_e = 911 x 10^{-31} kg

- Total electron density and the Fermi energy are then solved to give

$$n_e = \frac{N_A \times \rho}{m_a} = 8.49 \times 10^{28}\mathrm{m}^{-3} \qquad e_F = \frac{\hbar^2 k_F^2}{2m^*} = 7.0\mathrm{eV}$$

Equilibrium Electron Statistics V

- In semiconductors the bottom of the conduction band is above the chemical potential and serves as the origin of the energy
- In metals the number of *free* electrons taking part in conduction are those within a thin energy band around the Fermi energy

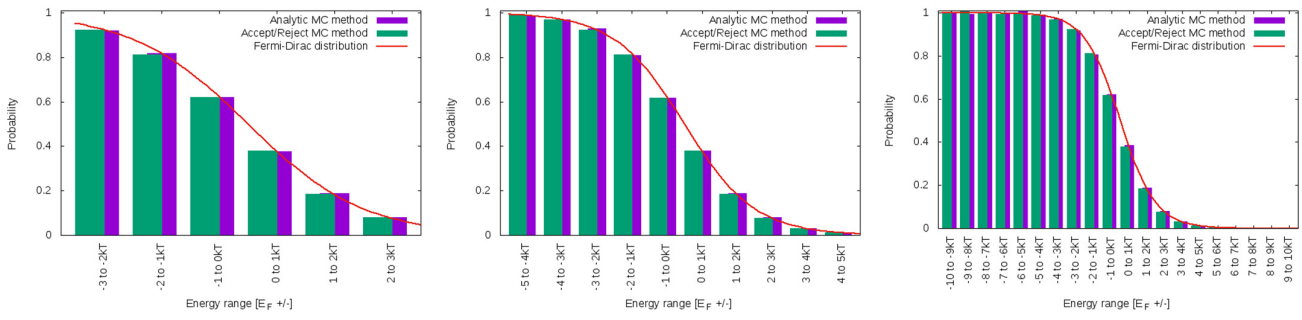
$$n_C = \int_{e_F - e_n}^{e_F + e_n} \frac{(2m^* e)^{1/2}}{8\hbar^3 \pi^2} \times \frac{de}{\exp\left(\frac{e - e_F}{k_B T}\right) + 1}$$

- Generated electron energies are assigned within the range $[e_F - e_n : e_F + e_n]$ according to the FD distribution

Equilibrium Electron Statistics VI

- We used two MC techniques to solve the previous equation and generate the conducting electrons and their energies.

$\epsilon_n = 3k_BT$ $\epsilon_n = 5k_BT$ $\epsilon_n = 10k_BT$



Improved simulation accuracy
Increased simulation time and effort

Scattering Mechanisms: Electron-Electron

- Electron-electron scattering depends on the electron density, applied field, energy, etc.
- It does not significantly increase at reduced dimensions
- In our simulator EE scattering is applied using a scattering time τ_{ee}, calculated using the classical definition of the conductivity baseline:

$$\sigma = \frac{q^2 n_e \tau_{ee}}{m^*} \qquad or \qquad \rho = \frac{m^*}{q^2 n_e \tau_{ee}}$$

- With a bulk resistivity of 1.7 x 10^{-8} Ωm the scattering time is τ_{ee} = 2.64 x 10^{-14} s

Scattering Mechanisms: Surface Roughness I

- Heuristic models associate to specular scattering, where the incident and reflected angels are equal
- Roughness results in randomization of the reflected angle of the scattered electron
- We set a parameter γ which determines the ratio between the specular and random scattering events

$0 \leq \gamma(r_\Phi) \leq 1$, where $\Phi(r_\Phi) = 0$ defines the surface of the boundary

Scattering Mechanisms: Surface Roughness II

- Comprehensive models account for stochastic properties of the roughness, based on the Fermi Golden Rule
- Probability *S* is given for a transition *per unit time* from an initial state $|k\rangle$ defined by quantum numbers k and energy E_k, to a state k' under the action of a perturbing Hamiltonian H':

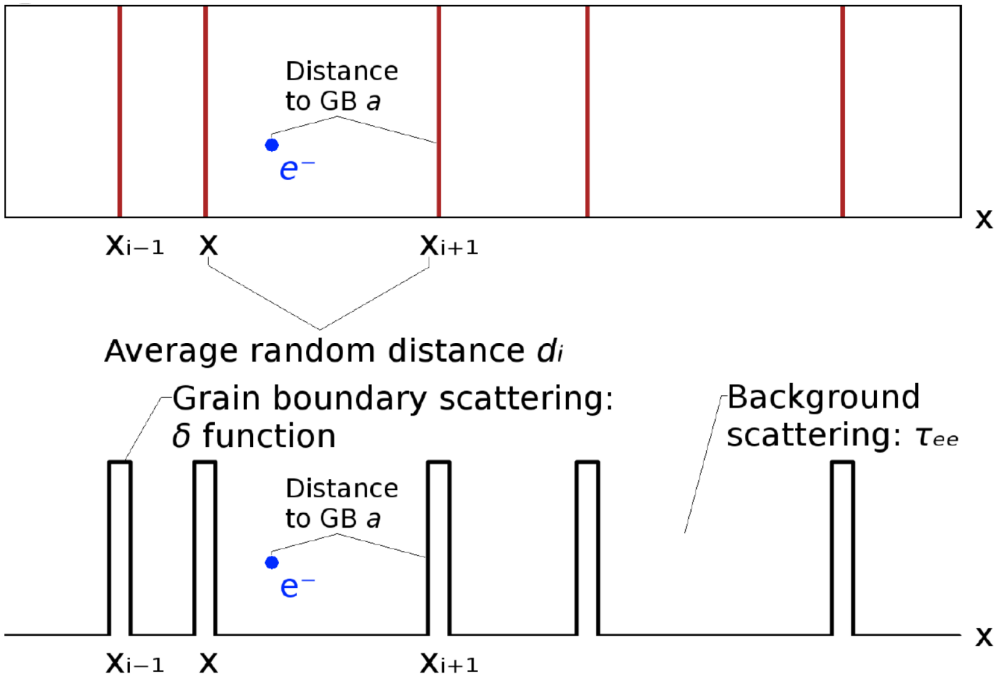
$$S(\mathbf{k}, \mathbf{k}') = \frac{2\pi}{\hbar} \left| \langle \mathbf{k}' | H' | \mathbf{k} \rangle \right|^2 \delta(E_{\mathbf{k}'} - E_{\mathbf{k}})$$

- Here the δ function accounts for the energy conservation of the interaction with the surface roughness potential H'

Scattering Mechanisms: Grain Boundaries

- An electron, interacting with a grain boundary has a probability of reflection *R* or transmission *(1 - R)*
- A combination of specular and diffusive reflection represents the physical reflection from a grain boundary
- Electron energy loss during reflection or transmission should also be included

Scattering Mechanisms: Grain Boundaries



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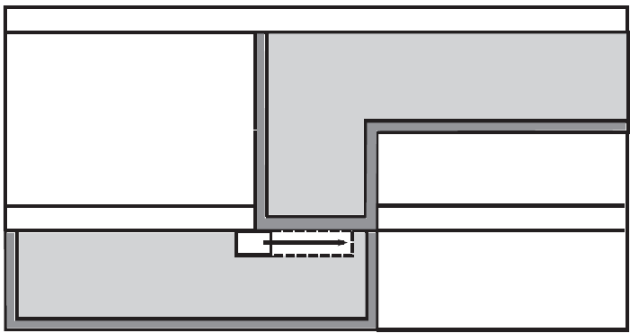
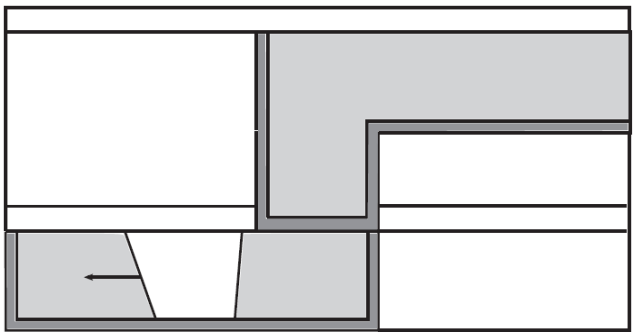
Electromigration in Copper: Failure Modes

- Time to failure due to electromigration is a combination of two failure modes:





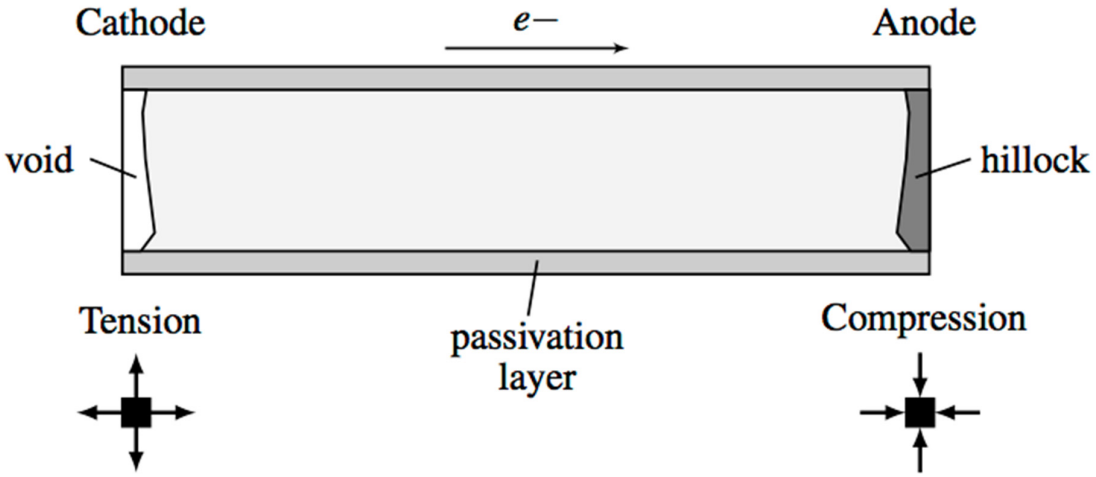
Early failure mode:
- E-field causes movement of ions
- Ion transport forms vacancy/hillock
- Vacancy and hillock induce stress
- Critical stress causes crack/failure

Late failure mode:
- Critical stress causes void nucleation
- Nucleated void grows to relieve stress
- Void growth increases line resistance
- Fails at critical resistance/open circuit

R.L. de Orio et al., Microelectron. Rel. (2011)

Electromigration in Copper: Early Failure Mode

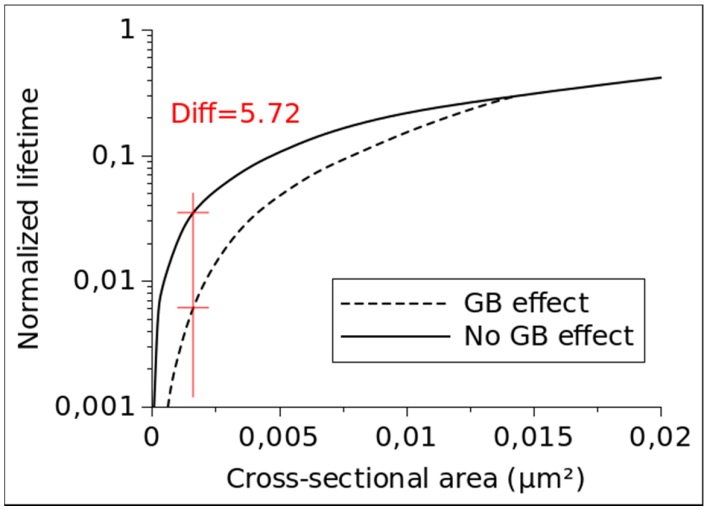
- Early failure mode is a combination of
  - Vacancy transport (anode to cathode) forming voids/hillocks
  - Resulting tensile (cathode) and compressive (anode) stress



Electromigration in Copper: Scaling

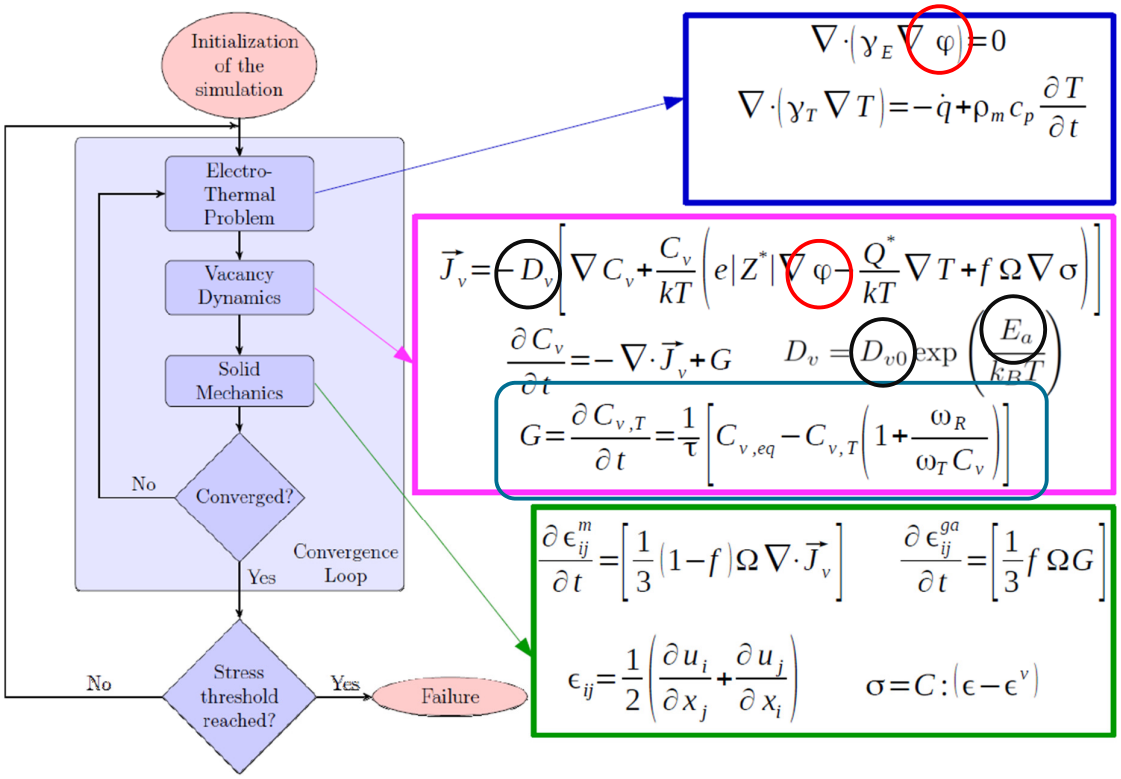
- Shrinking dimensions result in increased current densities
- Experiments show increased grain boundaries reduce expected lifetimes

An electromigration model must include the effects of material interfaces and grain boundaries

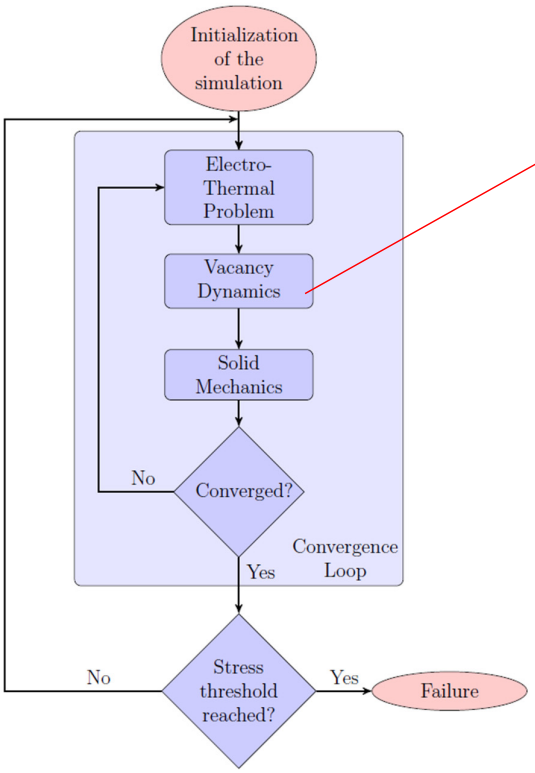


L. Filipovic et al., SISPAD (2017)

Electromigration in Copper: Model I



Electromigration in Copper: Model II



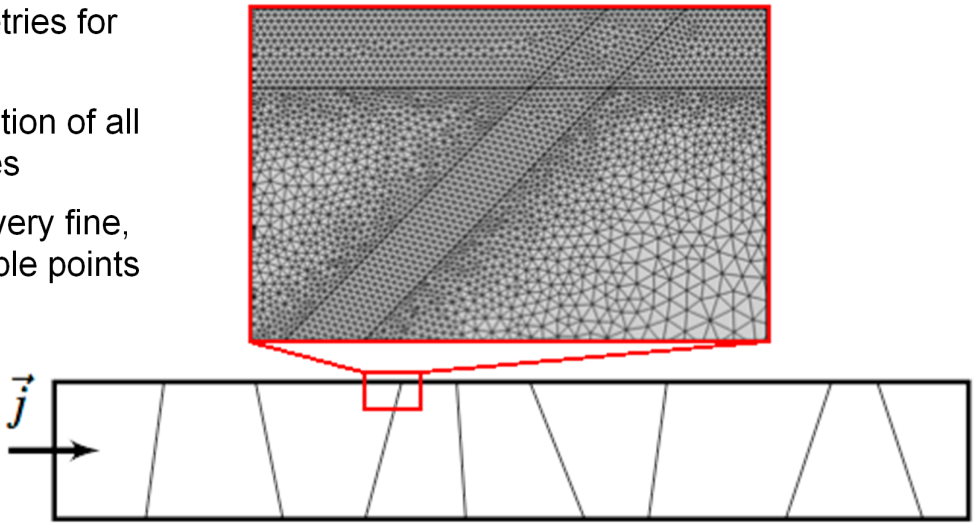
$$D_v = D_{v0}\exp\left(\frac{E_a}{k_B T}\right)$$

Parameter	E_a (eV)	D_{v0} (cm²/s)
Grain	0.89	0.52
GB	0.7	52
MI	0.5	520

R.L. de Orio et al., Microelectron. Rel. (2011)

Electromigration in Copper: SOA

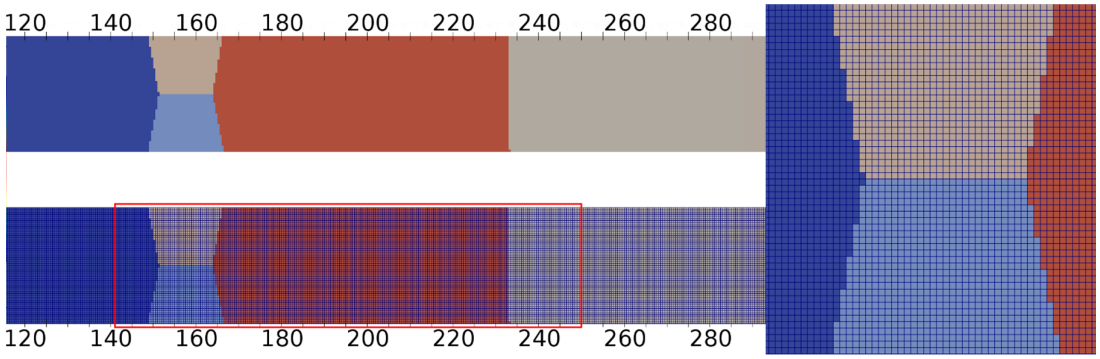
- Microstructure treated using predefined geometries for GB and MI
  - Must know location of all grain boundaries
  - Mesh must be very fine, especially at triple points



M. Rovitto, *PhD Dissertation* TU Wien (2016)

Electromigration in Copper: Modeling Approach I

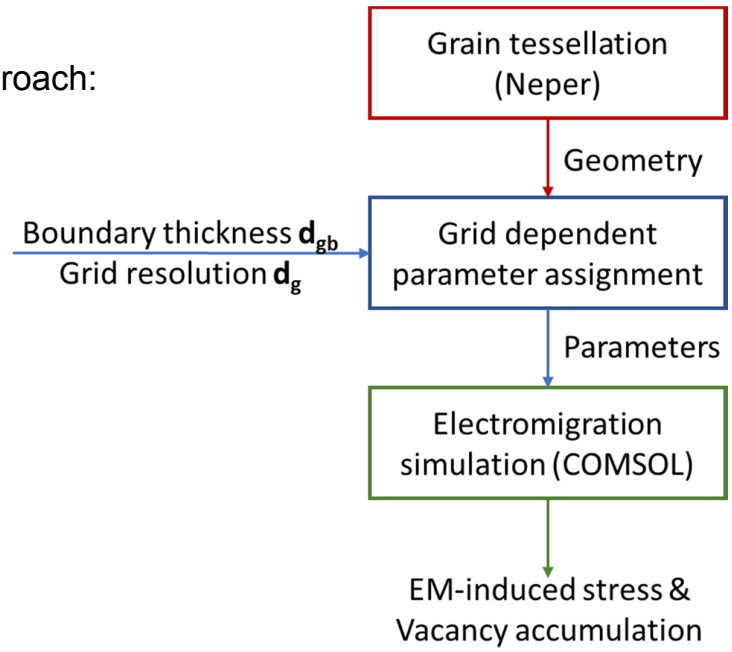
- Developed approach:
  - Treat microstructure using a spatial material parameter to define GBs, MIs, and Cu grains, applied to:
    - Conductivity, Vacancy diffusivity, Effective valence Z*
    - Apply the vacancy generation/annihilation term at GB/MIs



L. Filipovic et al., SISPAD (2018)

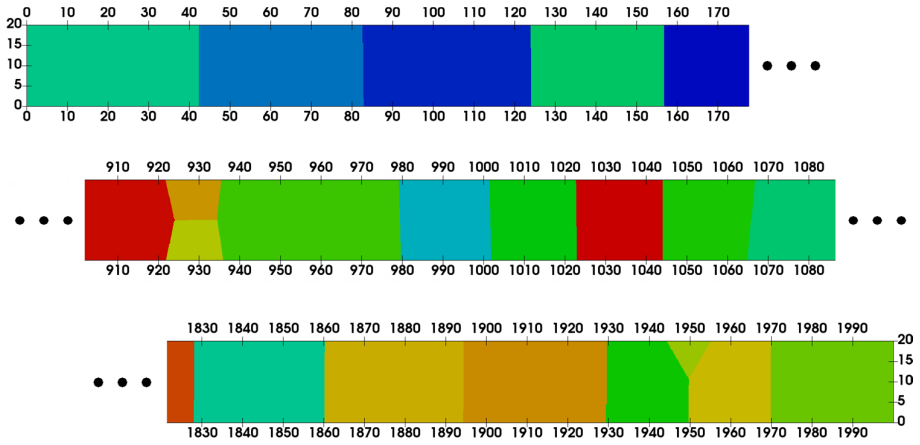
Electromigration in Copper: Modeling Approach II

- Developed approach:



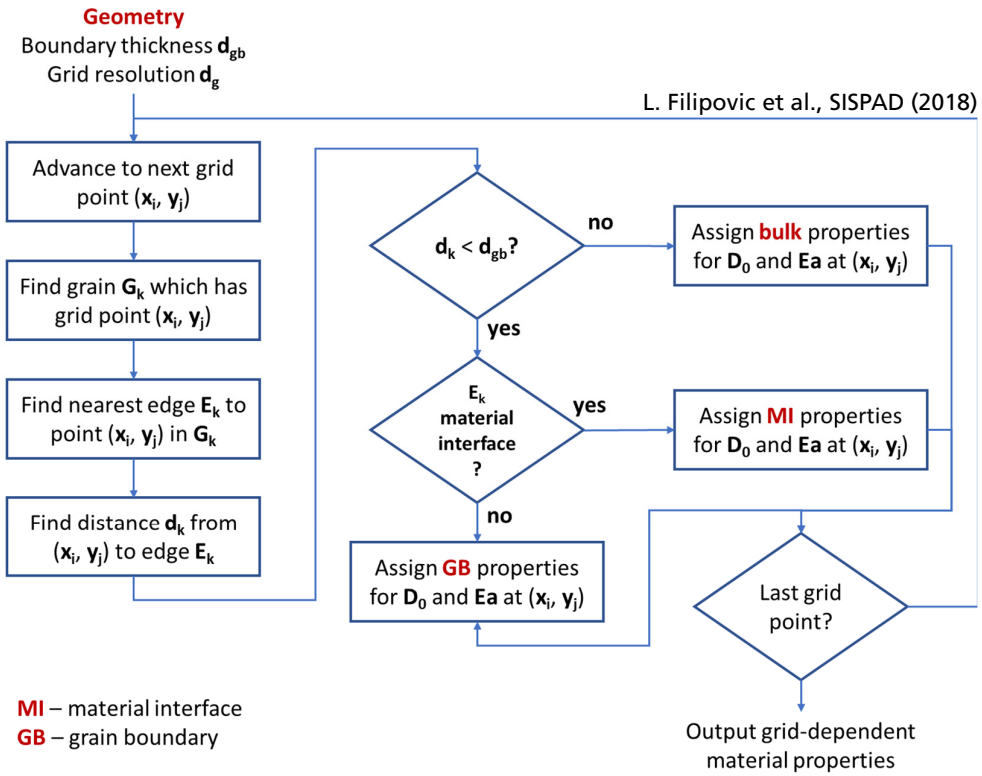
Electromigration in Copper: Grain Tessellation

- Grain tessellation
  - Using an average grain size, set total number of grains (seeds)
  - Randomly place seeds in the copper line and grow until filled



L. Filipovic et al., SISPAD (2018)

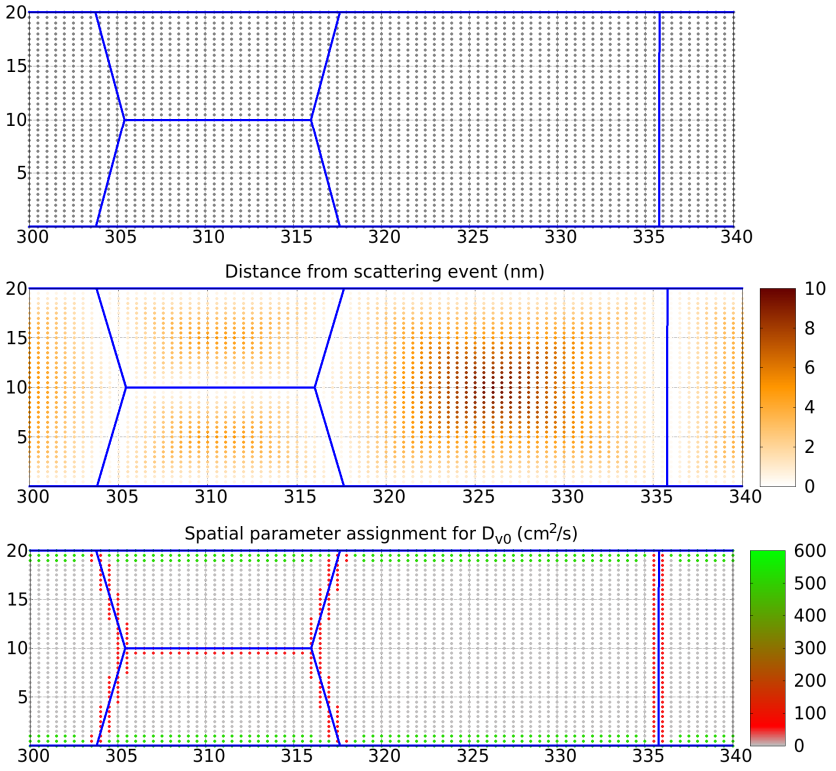
Electromigration in Copper: Parameter Assignment I

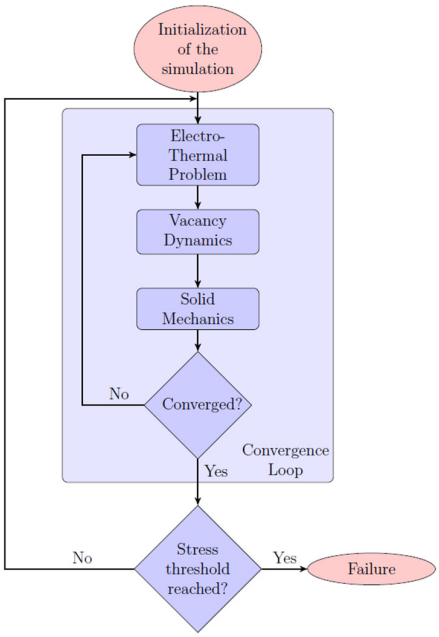


L. Filipovic et al., SISPAD (2018)

MI – material interface
GB – grain boundary

Electromigration in Copper: Parameter Assignment II

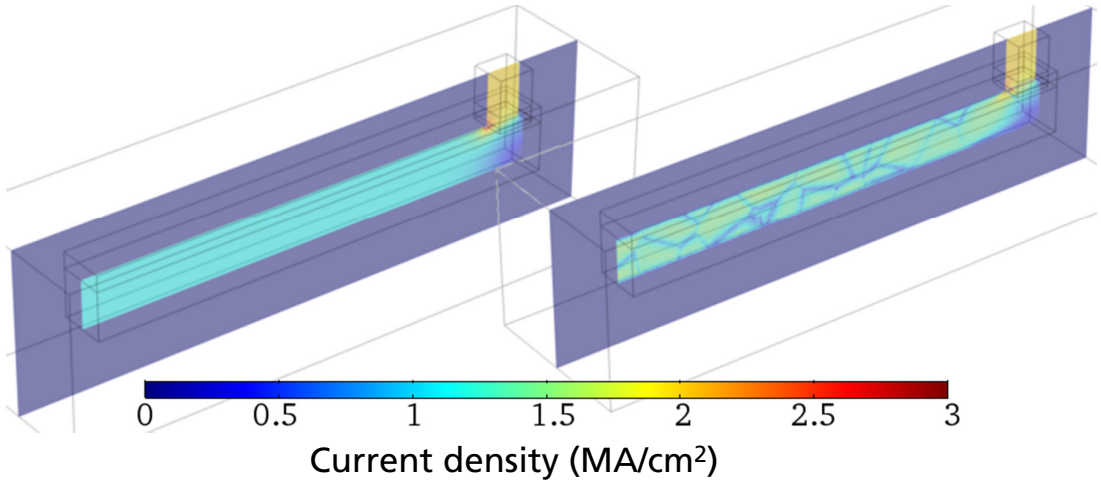




L. Filipovic et al., SISPAD (2018)

Electromigration in Copper: Simulation Results I

- Current density variation when 1MA/cm^2 is applied (bulk vs microstructure):

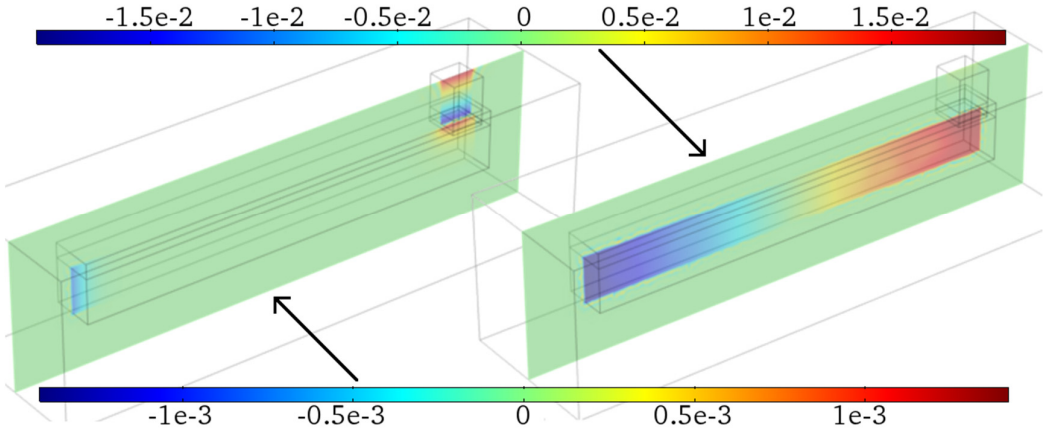


The effects of microstructure are immediately evident!

L. Filipovic et al., SISPAD (2017)

Electromigration in Copper: Simulation Results I

- Vacancy concentration at 0.1ms when 1MA/cm^2 at 300°C is applied (bulk vs microstructure):

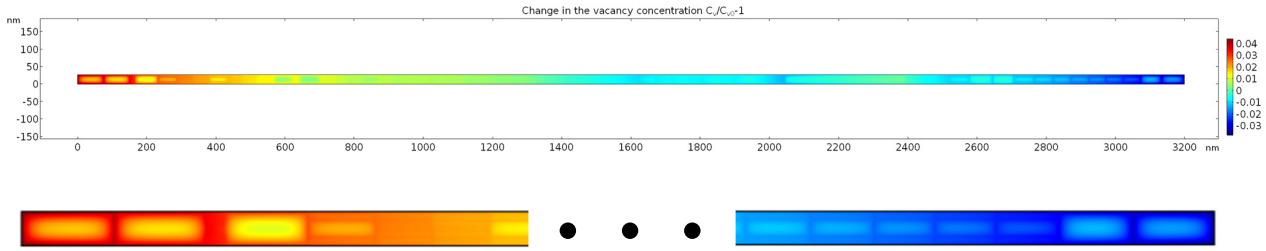


Vacancies accumulate much faster due to the GBs and MIs

L. Filipovic et al., SISPAD (2017)

Electromigration in Copper: Simulation Results I

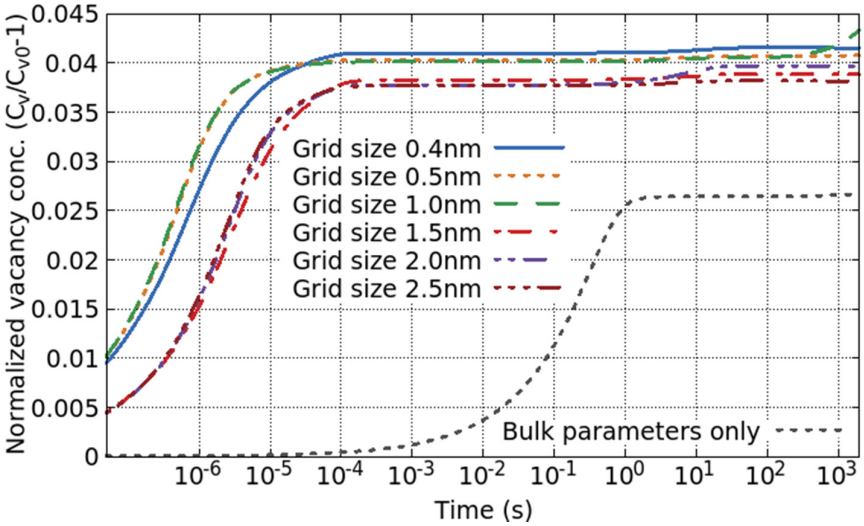
- Electromigration simulations using different mesh resolutions were performed
  - Geometry: 2000 x 20nm, grain size 25nm
  - Electromigration setup: 1MA/cm^2 current density applied at 300°C
  - Vacancy concentration at onset of electromigration:



L. Filipovic et al., SISPAD (2018)

Electromigration in Copper: Simulation Results II

- Electromigration simulations using different mesh resolutions were performed

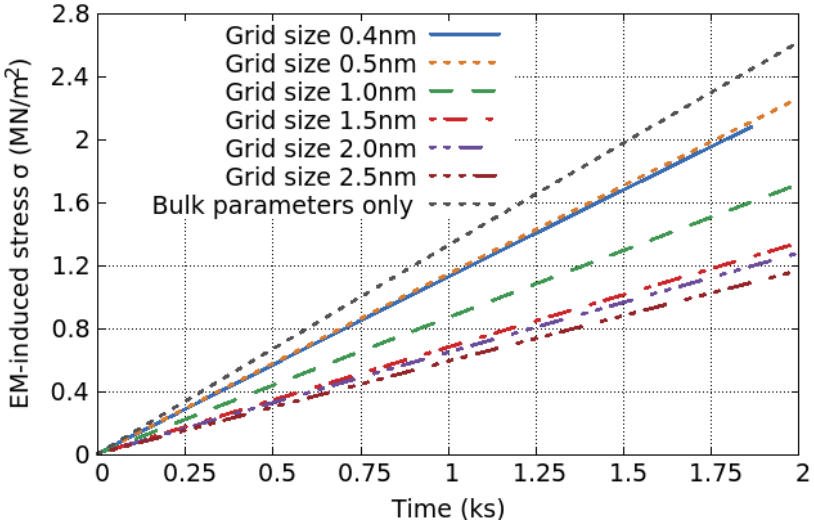


- Even coarse grids show reasonable results for the vacancy concentration
- Bulk parameters underestimate the time at which EM effects initiate

L. Filipovic et al., SISPAD (2018)

Electromigration in Copper: Simulation Results III

- Electromigration simulations using different mesh resolutions were performed



- Underestimated stress values with increasing grid size

L. Filipovic et al., SISPAD (2018)

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Conclusions and Outlook

- As interconnects shrink grain boundaries and material interfaces play increasing roles in copper conductivities and reliability
- A Monte Carlo model was developed to include electron scattering mechanisms in metal lines
  - Model is based on semiconductor knowledge developed over decades
  - Will be implemented and released in an open simulator from TU Wien
- The effect of microstructure on interconnect lifetime is examined
  - Treat grain boundaries and material interfaces as parameters
  - Introduced spatial parameters within a finite element framework
    - Conductivity, atom diffusivity, activation energy …
  - Model will enable variation to be introduced to complex EM simulations