Simulation of Nanoscale Interconnects

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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

Electron Scattering in Metals

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

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

\[
\frac{\rho_f}{\rho_i} = 1 + \frac{3\lambda}{4w} (1-p) + \frac{3\lambda}{2D} \left( \frac{R}{1-R} \right)
\]

- Probability of reflection from a MI
- Bulk resistivity
- Average grain size
- Metal width
- Probability of reflection from a GB

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:
  \[ f(k) = f(\epsilon(k)) = \frac{1}{e^{\frac{\epsilon(k) - \zeta}{k_B T}} + 1} \]
- $\zeta$ 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
  \[ g(\epsilon) = V \frac{\sqrt{2m^3/2}}{\pi^2 \hbar^3} \sqrt{\epsilon} \]
Equilibrium Electron Statistics III

- Normalizing with $\xi = \zeta/k_B T$ and $x = \epsilon/k_B T$ we obtain the $\frac{1}{2}$ Fermi integral

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

- 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:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density</td>
<td>$\rho$</td>
<td>8.960 g/cm$^3$</td>
</tr>
<tr>
<td>Atomic mass</td>
<td>$m_a$</td>
<td>63.546 kg/mole</td>
</tr>
<tr>
<td>Permittivity</td>
<td>$\varepsilon$</td>
<td>8.85419 x 10^{-12} F/m</td>
</tr>
<tr>
<td>Effective mass</td>
<td>$m^*$</td>
<td>1.0 $m_e = 911 \times 10^{-31}$ kg</td>
</tr>
</tbody>
</table>

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

$$n_e = \frac{N_A \times \rho}{m_a} = 8.49 \times 10^{28} \text{ m}^{-3}$$

$$e_F = \frac{\hbar^2 k_F^2}{2m^*} = 7.0 \text{ eV}$$
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.

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

- 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.

<table>
<thead>
<tr>
<th>(\epsilon_n)</th>
<th>3(k_BT)</th>
<th>5(k_BT)</th>
<th>10(k_BT)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Probability</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- 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 $\tau_{ee}$, calculated using the classical definition of the conductivity baseline:

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

- With a bulk resistivity of $1.7 \times 10^{-8} \ \Omega m$ the scattering time is $\tau_{ee} = 2.64 \times 10^{-14} \ s$

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 $\gamma$ which determines the ratio between the specular and random scattering events

$$0 \leq \gamma(\Phi) \leq 1, \ \text{where } \Phi(r_\Phi) = 0 \ \text{defines the surface of the boundary}$$
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 $H'$:

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

- Here the $\delta$ 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


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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

\[
\nabla \cdot \left[ \rho m c_p \frac{\partial T}{\partial t} \right] = 0
\]

\[
\nabla \cdot \left[ \rho m c_p \frac{\partial T}{\partial t} \right] = -\hat{q} + \frac{Q}{kT} \left( \nabla T + \frac{\omega}{\omega_T} \nabla \sigma \right)
\]

\[
G = \frac{\partial C_{v,T}}{\partial t} = \frac{1}{\tau} \left[ C_{v,eq} - C_{v,T} (1 + \frac{\omega}{\omega_T} C_v) \right]
\]

\[
\frac{\partial \epsilon_{ij}^m}{\partial t} = \frac{1}{3} \left[ 1 - f \right] \Omega \nabla \cdot \vec{J}_v
\]

\[
\frac{\partial \epsilon_{ij}^{pa}}{\partial t} = \frac{1}{3} f \Omega G
\]

\[
\epsilon_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)
\]

\[
\sigma = \sigma : (\epsilon - \epsilon^p)
\]
Electromigration in Copper: Model II

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

<table>
<thead>
<tr>
<th>Parameter</th>
<th>(E_a) (eV)</th>
<th>(D_{v0}) (cm(^2)/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grain</td>
<td>0.89</td>
<td>0.52</td>
</tr>
<tr>
<td>GB</td>
<td>0.7</td>
<td>52</td>
</tr>
<tr>
<td>MI</td>
<td>0.5</td>
<td>520</td>
</tr>
</tbody>
</table>


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

Electromigration in Copper: Modeling Approach II

- Developed approach:
  - Grain tessellation (Neper)
  - Geometry
  - Boundary thickness $d_{gb}$
  - Grid resolution $d_g$
  - Grid dependent parameter assignment
  - Electromigration simulation (COMSOL)
  - EM-induced stress & Vacancy accumulation
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

Electromigration in Copper: Parameter Assignment I

Geometry
- Boundary thickness $d_{gb}$
- Grid resolution $d_i$

Advance to next grid point $(x_i, y_j)$
- Find grain $G_k$ which has grid point $(x_i, y_j)$
  - Find nearest edge $E_k$ to point $(x_i, y_j)$ in $G_k$
    - Find distance $d_k$ from $(x_i, y_j)$ to edge $E_k$

$L. Filipovic et al., SISPAD (2018)$
Electromigration in Copper: Parameter Assignment II

The effects of microstructure are immediately evident!

Electromigration in Copper: Simulation Results I

- Current density variation when 1MA/cm² is applied (bulk vs microstructure):

The effects of microstructure are immediately evident!
Electromigration in Copper: Simulation Results I

- Vacancy concentration at 0.1ms when 1MA/cm² at 300°C is applied (bulk vs microstructure):

  Normalized vacancy concentration ($C_v/C_{v0} - 1$)

  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/cm² 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

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