Virtual Processing of Nanostructured Materials

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Acknowledgments

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Process Evolution

Overall Presentation Goal

Introduce/motivate grain focused models – as distinct from:

traditional continuum models

and

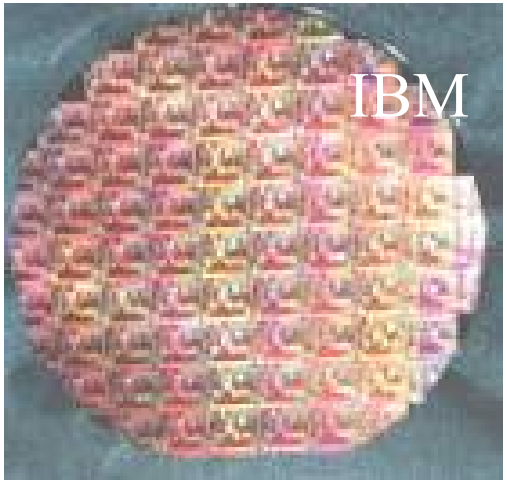
atomistic models.

Outline

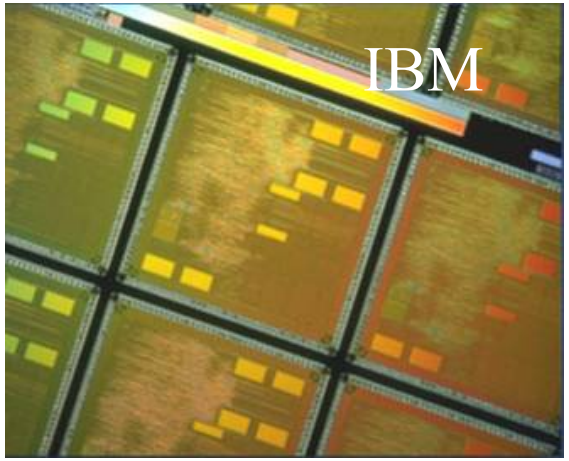
- A Grain-Focus
- ‘Grain-focused’ modeling of Cu interconnects:
  - PLENTE (a general 3D evolution simulation environment)
  - Annealing
  - Stress induced evolution
- Conclusions
- Future work

Some Scales in ICs

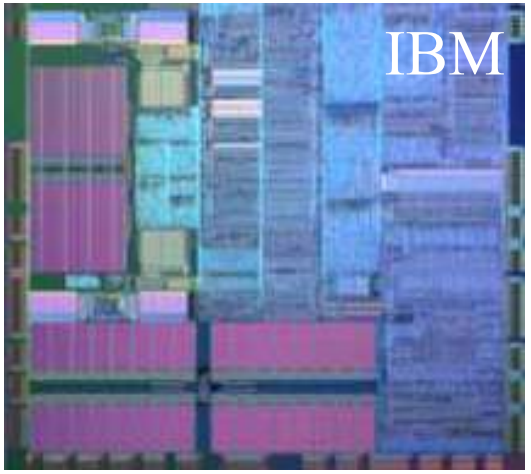
Wafer



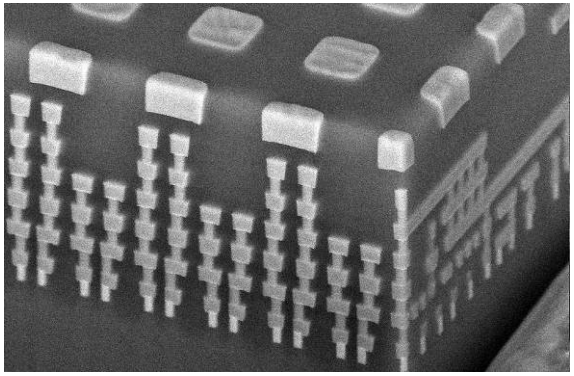
Chip



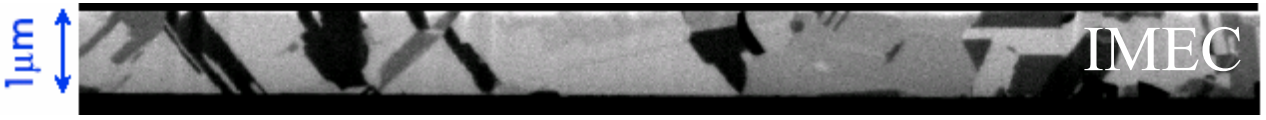
Pattern

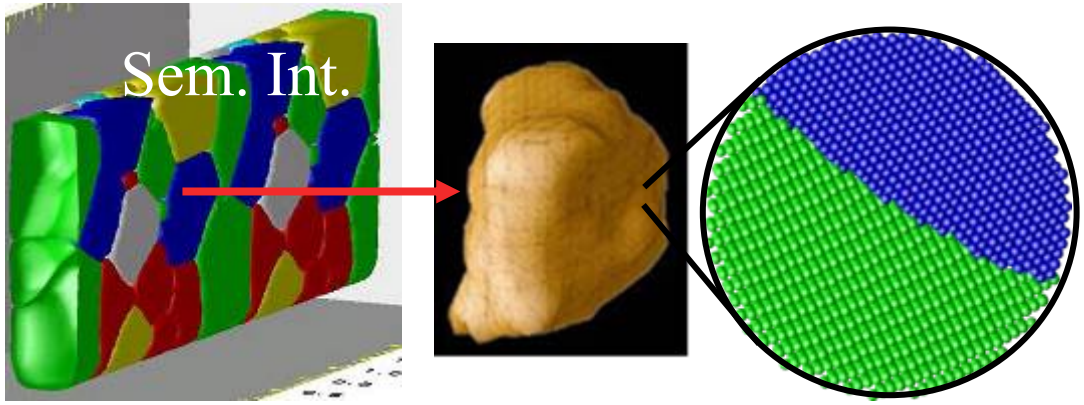


Interconnect



Grain

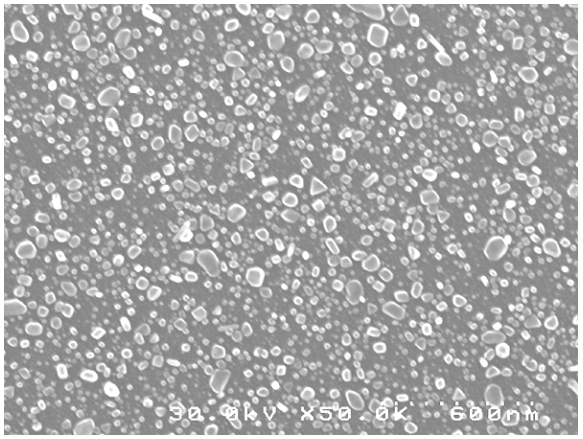




Grains: Al CVD Islands

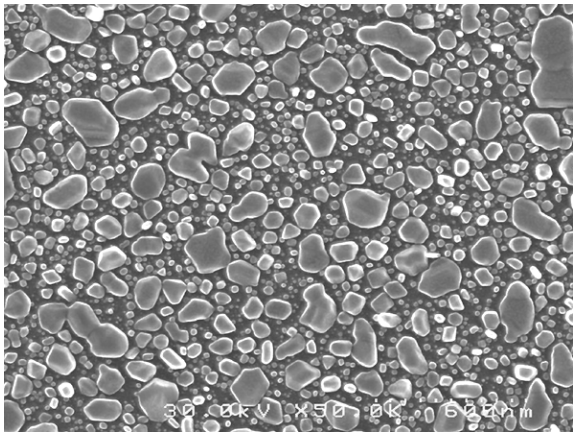
CVD Al on TiN, 265°C, 2 torr Dimethyl aluminum hydride (DMAH) and hydrogen

2 seconds

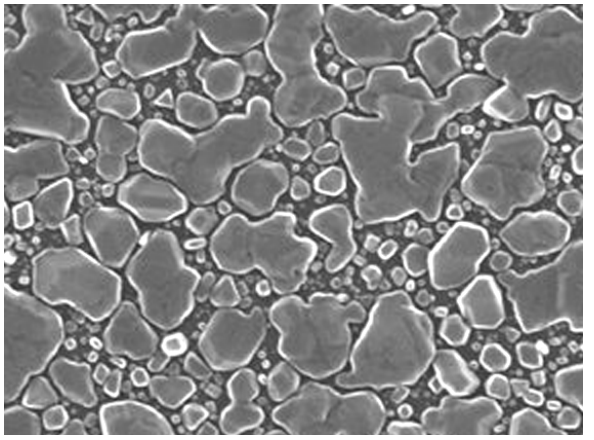


600 nm

5 seconds

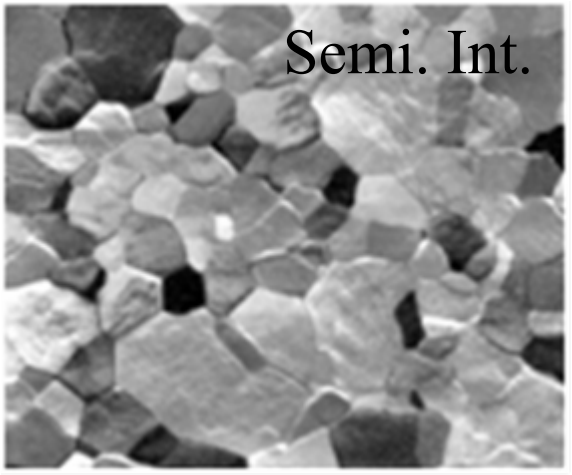


15 seconds



Grains: Continuous Film

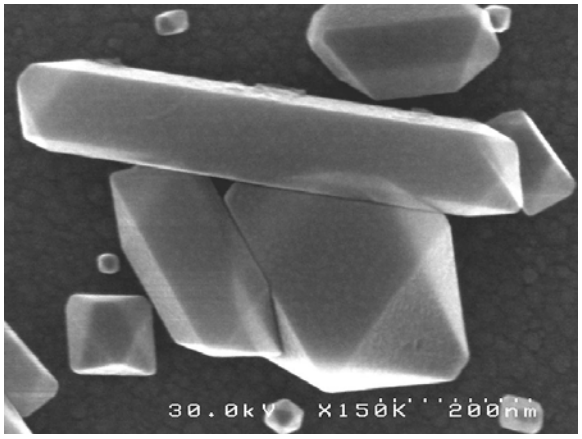
Continuous Al film, as might exist after a few minutes of CVD.



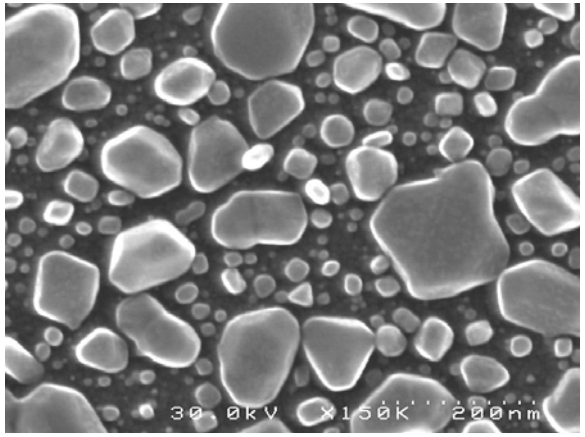
Grains: Al CVD Nuclei

Al nucleates differently on different surfaces; the properties of the resulting films are also different; e.g., roughness and nanovoiding.

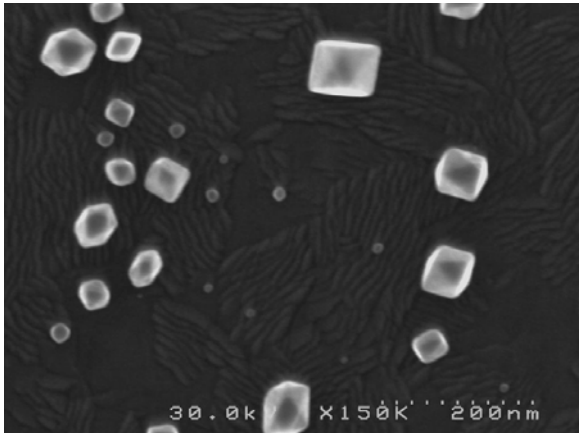
200 nm



TaN, 265 °C



TiN, 265 °C



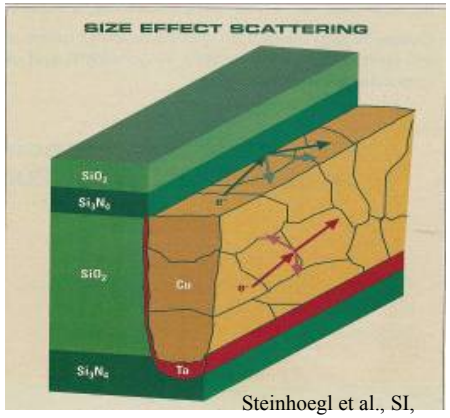
Ti-W, 265 °C

Dimethyl aluminum hydride (DMAH) and hydrogen

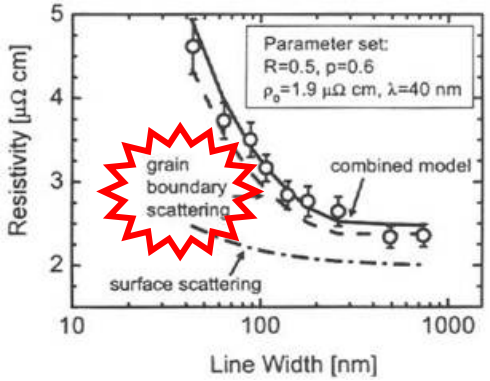
Some Drivers for Grain-Focused Models

Grains-focused models seem like a natural place to start looking at:

Grain boundary scattering

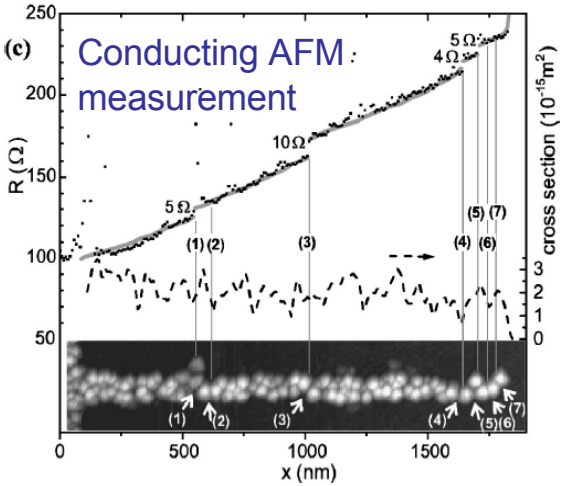


Steinhoegl et al., SI, 2005



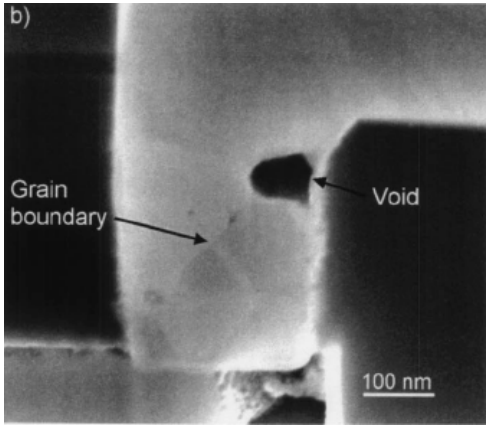
Data are for 230 nm high lines, see Steinhoegl *et al.* from SISPAD 2003, p 29. for details.

Resistivity jumps in small lines



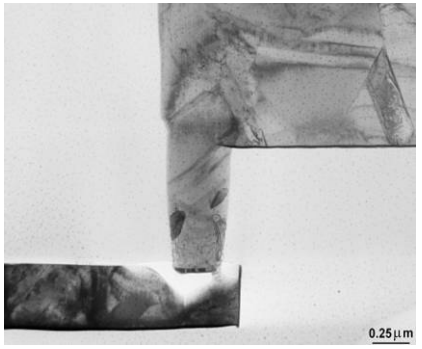
Bietsch and Michel, *Appl. Phys. Let.* **80,** p. 3346 (2002).

Current and stress induced voiding



G. Schneider *et al., J. Vac. Sci. Technol. B* **20**(6), 3089 (2002).

Thermal and mechanical performance. . .

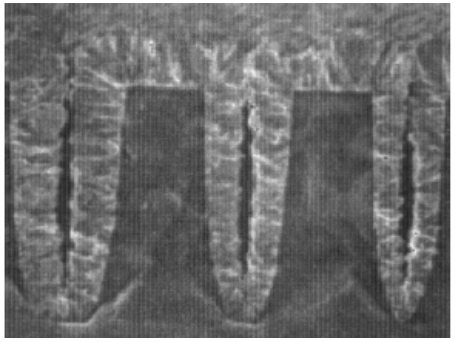


Source: Valeriy Sukharev, LSI

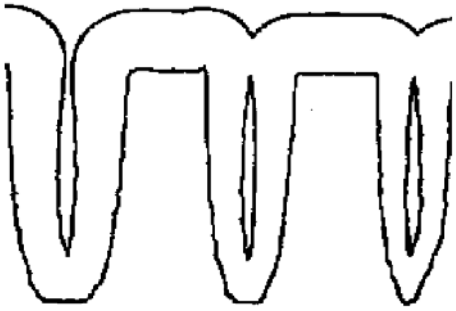
Continuum Film Models

Predictive capabilities of models that use continuum representations of films can be good, but some properties cannot be predicted; e.g., those that depend upon microstructure, such as resistivity and anisotropic mechanical properties.

Topography (CVD)



A set of trenches after tungsten CVD



EVOLVE simulation

Can predict

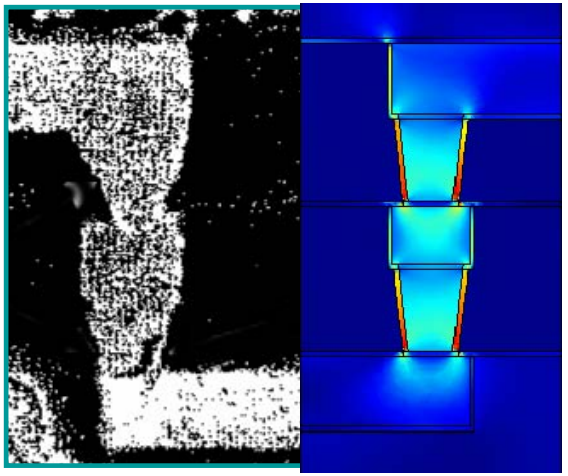
- Topography
- Composition

Do not predict

- Texture
- Grain size
- Microstructural defects

Cale *et al*., Proc. AMC, MRS, 1992, pp. 101
Cale *et al*., ***Thin Solid Films*** **365(2)**, 152 (2000)

Thermomechanical



Thermally induced stress in Cu interconnect

- Use average materials parameters
- No information on anisotropy
- Successfully used to explain some issues; e.g., mechanical stability

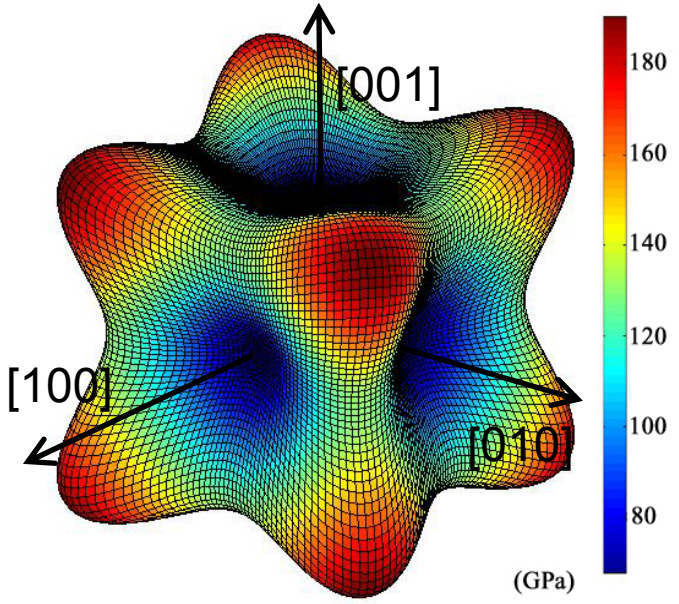
Edelstein *et al., 42nd Rel. Phy. Symp*., 2004, p.316.
Zhang *et al*., *Microelect. Eng.* **82**, 534 (2005).

Elastic Anisotropy

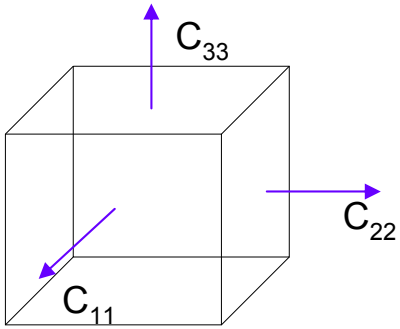
The elastic characteristics of single crystal Cu change significantly with orientation.

- The [111] direction is 2.9 times stronger than the [100] direction.
- Young's Modulus along [100] = 66.6 GPa
- Young's Modulus along [111] = 191.2 GPa

Spherical Plot of the Directional Dependence of Young's Modulus



Stress-Strain Relationship



$$\sigma_i = C_{ij}\varepsilon_j$$

$$\sigma_i = \begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \tau_{xy} \\ \tau_{yz} \\ \tau_{xz} \end{bmatrix}$$

Comsol

$$C_{ijkl}^{<100>} = \begin{bmatrix} 168.4 & 121.4 & 121.4 & 0 & 0 & 0 \\ & 168.4 & 121.4 & 0 & 0 & 0 \\ & & 168.4 & 0 & 0 & 0 \\ & & \textit{sym.} & 75.4 & 0 & 0 \\ & & & & 75.4 & 0 \\ & & & & & 75.4 \end{bmatrix}$$

Components of the Stiffness Matrix for Cu oriented (along Z axis):

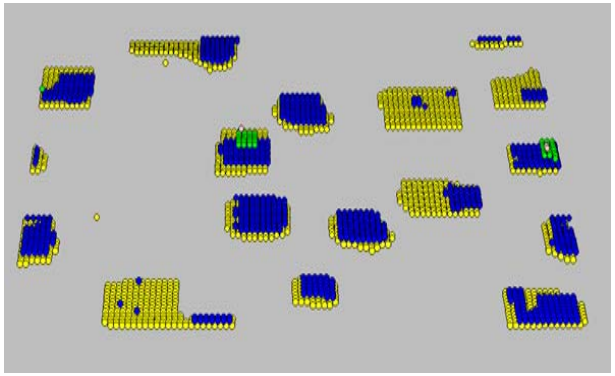
<100> $C_{11} = C_{22} = C_{33} = 168.4$ GPa

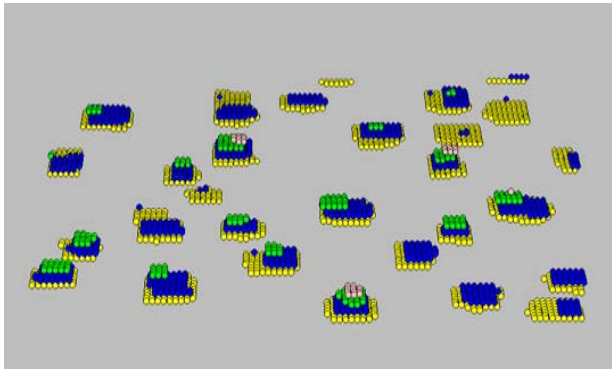
<110> $C_{11} = C_{33} = 220.3$ GPa: $C_{22} = 168.4$ GPa

<111> $C_{11} = C_{22} = 220.3$ GPa: $C_{33} = 237.6$ GPa

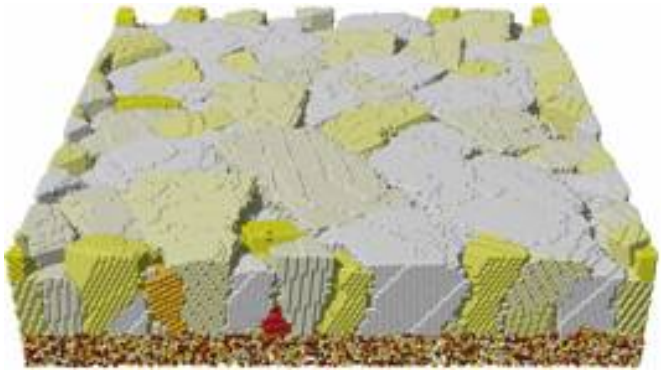
G. Simmons and H. Wang, *Single crystal elastic constants and calculated aggregate properties: a handbook*, M.I.T. Press, Cambridge, MA, 1971.

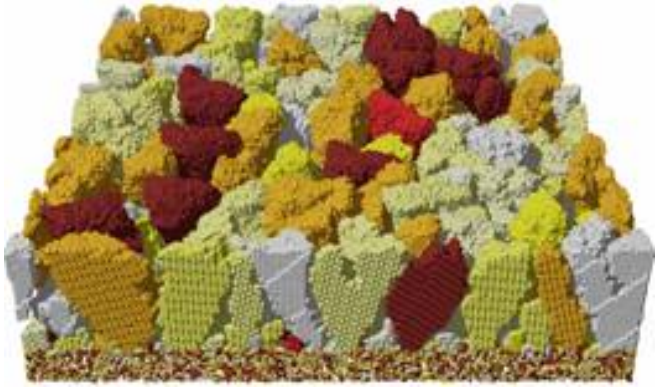
Atomistic Models





Adams, Cale @ ASU
(Mid-90s)





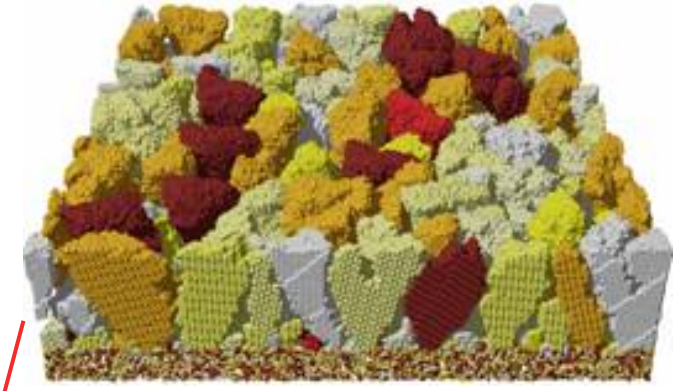
Huang, Zhou @ RPI
(J. Comp.-Aided Design, 2005)

Discrete models for nucleation and early stages of growth, or for small structures; cannot reasonably cover the volumes needed; e.g., for reliability work.

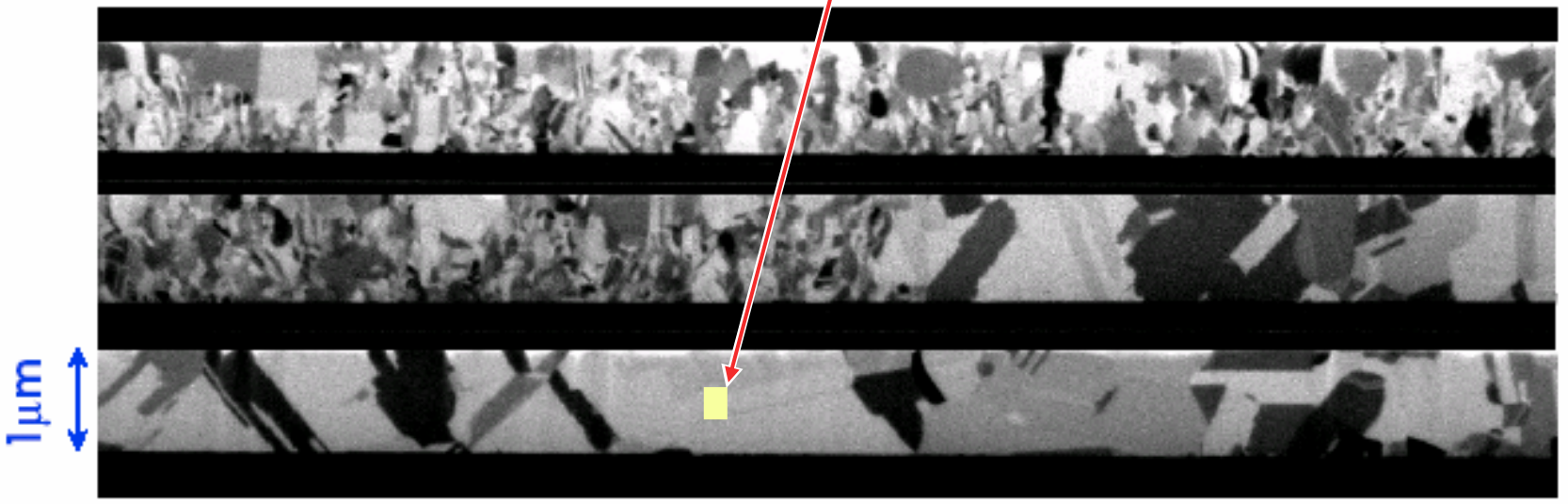
Atomistic Models

Atomistic simulations are not yet able to deal (reasonably) with volumes needed for many engineering analyses.

In particular, we cannot yet study the thermal and mechanical responses of interconnects.



Huang, Zhou @ RPI
(J. Comp.-Aided Design, 2005)

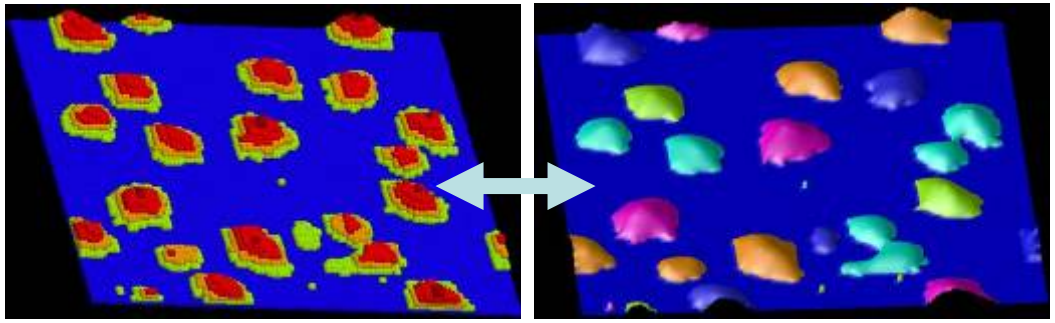


IMEC via D. Merricks, Ferro 3/4/03

‘Grain-Continuum’ Model: PLENTE

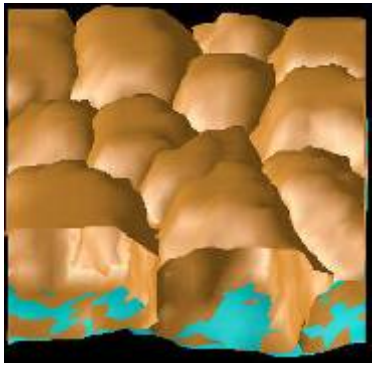
(**P**arallel **L**evelset **E**nvironment for **N**anoscale **T**opography **E**volution)

- PLENTE is a robust 3D geometry tracker capable of representing and evolving complex systems.
- Interfaces with process simulators to track evolution; *all physics are in these codes*.
- PLENTE has built-in encapsulation abilities to convert discrete data from atomistic simulations to continuum representations
- Can recover atomic scale information for property predictions via “re-atomation” procedures.

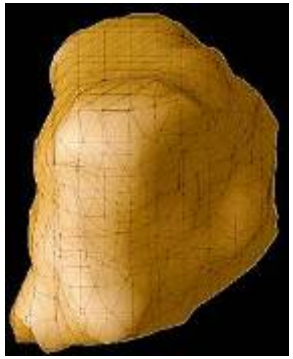


Nucleated substrate – atomistic representation

Nucleated substrate – GC representation



Coalesced grain structure – GC representation



Single grain pulled from structure

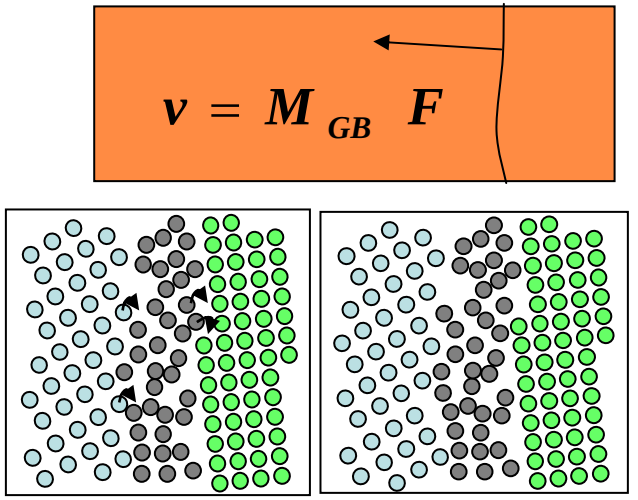
Kinetically controlled, electroless deposition onto a substrate with 5 nm rms roughness.

Bloomfield et al., *Phil. Mag.* **83**(31-34), 3549-3568 (2003)

Grain Boundary Motion

M_{GB} – Grain Boundary Mobility

A measure of how easy atoms transition from one grain to another.



Potential Forces on Grain Boundary

- Curvature
- Changes in surface or interface energies
- Strain Energy Density
- Vacancy migration

Approximation for High Angle Grain Boundaries ⇨ $$M_{GB} = \frac{b\upsilon\ \Omega}{kT}\exp\left(-\frac{Q}{kT}\right)$$

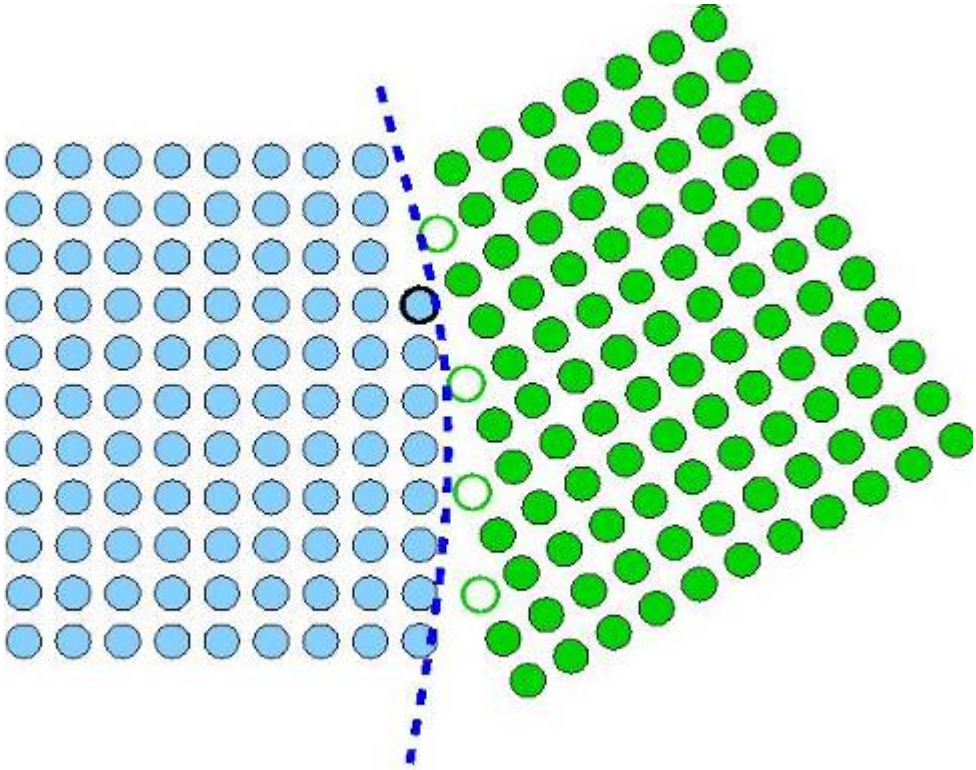
B. Schonfelder, G. Gottstein, and L. S. Shvindlerman, *Acta Mat.* **53**(6)**,** 1597-609 (2005).

D. A. Porter and K. E. Easterling, *Phase Transformations in Metals and Alloys*, 2nd ed. (CRC Press, 1992)

D. Turnbull, *Trans. Amer. Inst. Mining Eng.*, 661 (1951)

Curvature-Driven Grain Coarsening

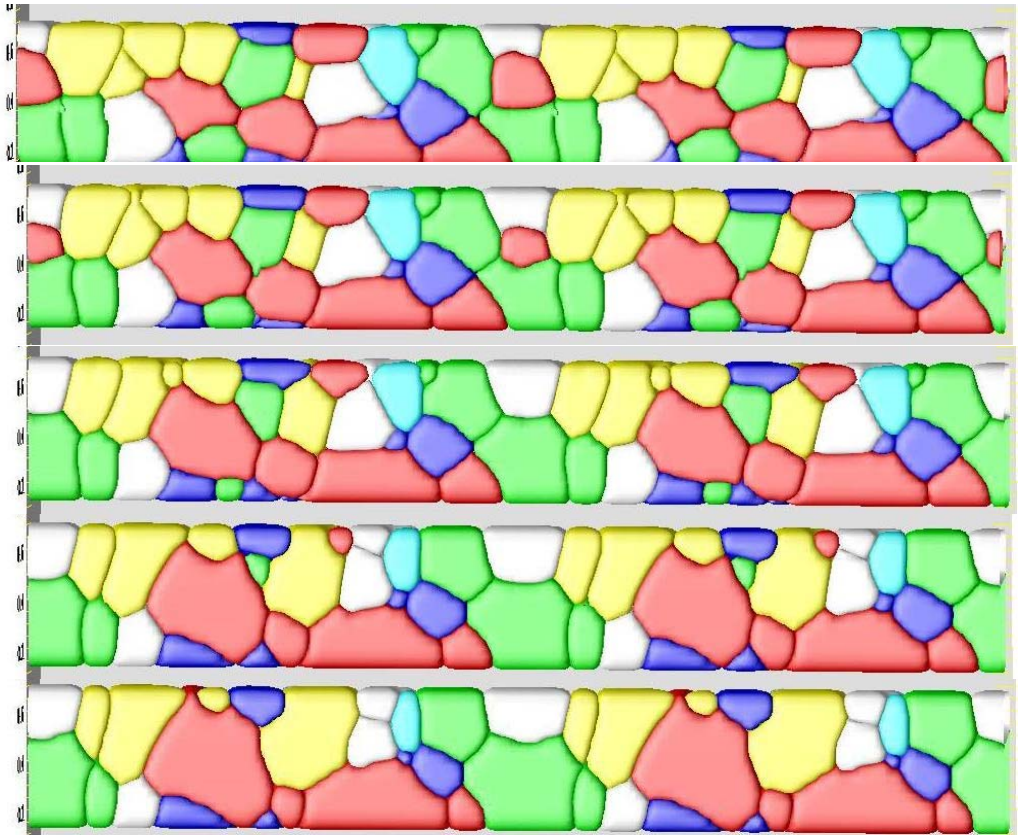
- The concentration of adatoms on a grain surface is a function of its curvature [Mullins et al., 1951]. So is the concentration of empty lattice sites with high coordination.
  - Convex → more adatoms
  - Concave → more sites
- Atoms tend to move to increase their coordination number, *i.e.*, from convex→concave.
- This gives Gibbs-Thompson-like motion, with migration rate a function of a GB mobility, GB energy density, and local curvature.

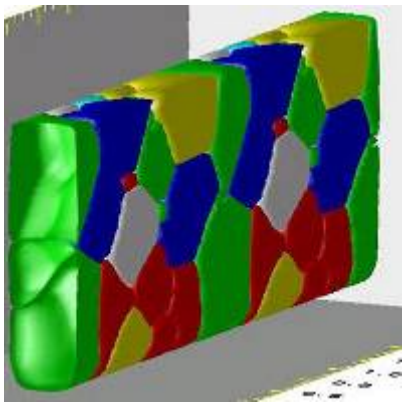


$$v = M\gamma\kappa = \gamma\kappa M_0 \exp\left(-\frac{Q}{kT}\right)$$

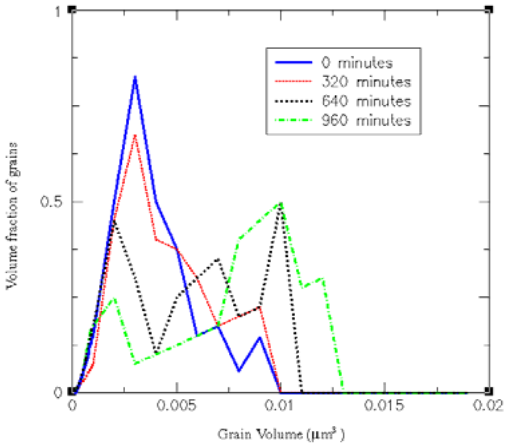
$$M = \frac{b\upsilon\Omega}{kT}\exp\left(-\frac{\Delta G}{kT}\right)$$

GC Annealing M&S using PLENTE





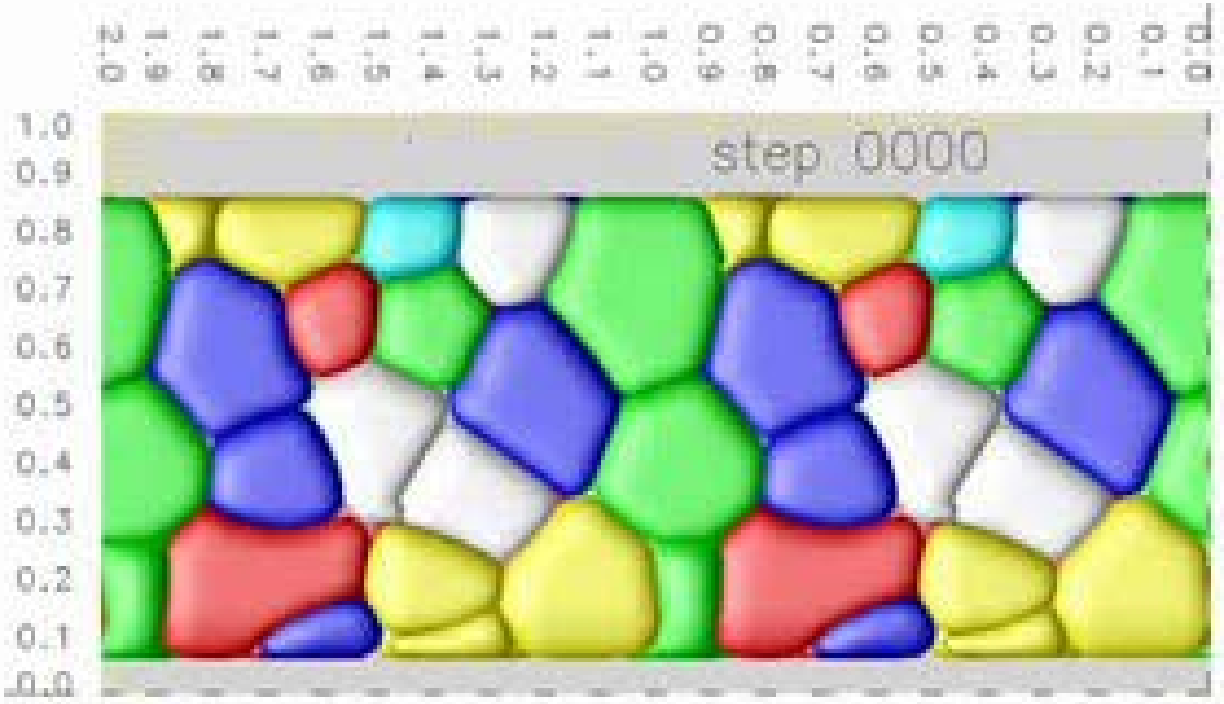
Example starting (post-CMP) Cu line
(corresponding to experimental work at IMEC and IBM)

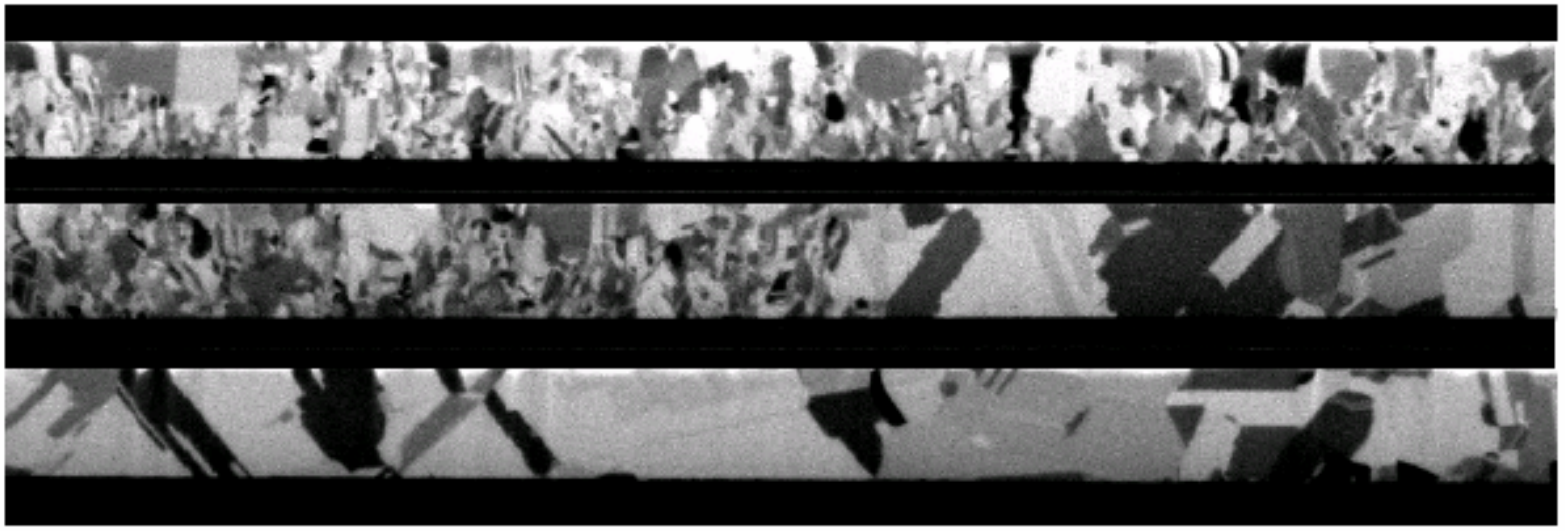


Grain size distributions at various times, corresponding to a decrease in resistance.

- Start with capped Damascene line "grown" via electroless-like process model, has log-normal grain size distribution.
- Use literature values and estimated input parameters for Cu.
- Significant coarsening; number of grains reduced by factor ~2 after 30 hours@360 K.
- Grain size distribution becomes bi-modal, as in experiments with Cu [Zielinski *et al.*, 1994].
- Right order for magnitude for Cu low-temp annealing times.

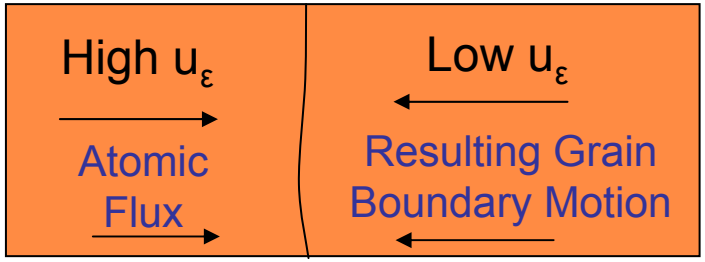
M.O. Bloomfield et al. *Phil., Mag.* 83, 3549(2003); *Microelectr. Eng.* 76, 195 (2004); SISPAD, 2003, p. 19


step 0000
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0


1μm

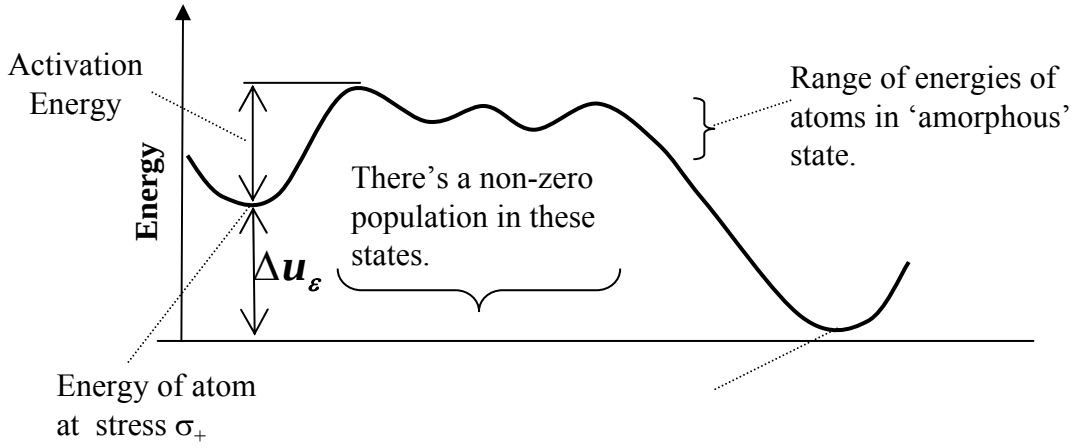
Strain Energy-Driven Grain Motion

- Strain energy differences across GBs give rise to a driving force for GB motion.
- Atomic motion across a GB moves it in opposite direction.
- Strain energy differences can be due to discontinuous mechanical properties across the GB, e.g., due to different orientations.



$$\boldsymbol{v} = \boldsymbol{M}\,\Delta\boldsymbol{u}_{\boldsymbol{\varepsilon}}$$

$$= \boldsymbol{M}_{\boldsymbol{GB}}\,\frac{(\boldsymbol{\sigma}_{+}\boldsymbol{\varepsilon}_{+} - \boldsymbol{\sigma}_{-}\boldsymbol{\varepsilon}_{-})}{2}\,\hat{\boldsymbol{n}}_{+\boldsymbol{to}-}$$



σ_+, ε_+ – Stress and stain on positive side of boundary

σ_-, ε_- – Stress and stain on negative side of boundary

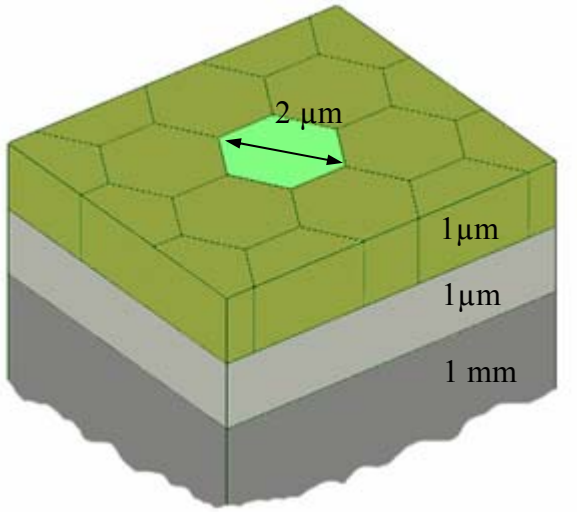
n – Unit vector pointing from positive side to negative side

R. Carel, C.V. Frost, and H.J. Thompson, *Acta Mater*. **44(**6), 2419 (1996).

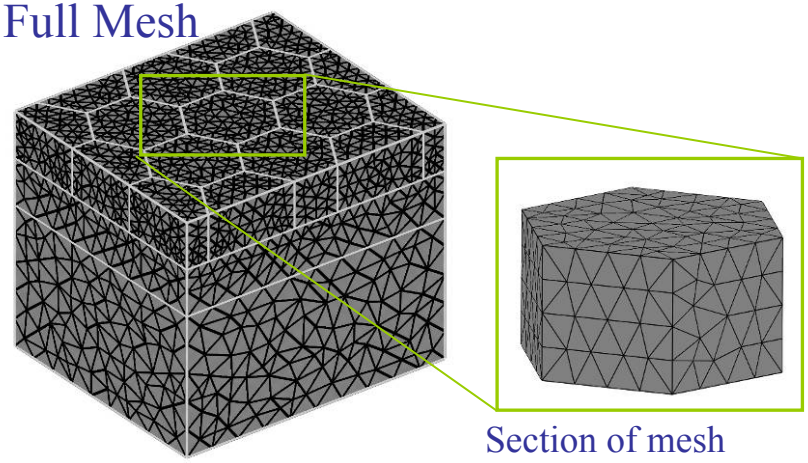
Anisotropic Elasticity
in Idealized Polycrystalline Films

Insight using thermo-mechanical responses in carefully constructed polycrystalline films.

- Polycrystalline film is represented as collections of distinct interacting continua each are assigned uniform, material and orientation-dependent parameters (Grain-continuum or GC)
- Here we study regular hexagonal grains on a silica layer sitting on a silicon wafer.
- The temperature shifts from 525 K to 425 K.

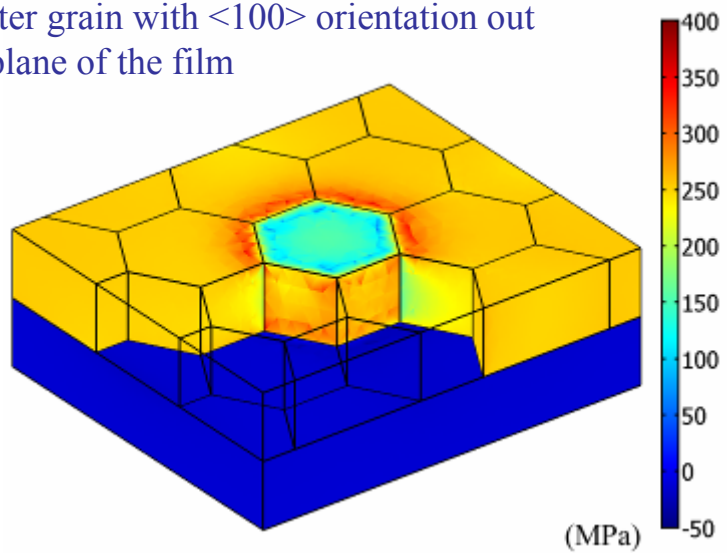


Full Mesh



Section of mesh displaying a single grain

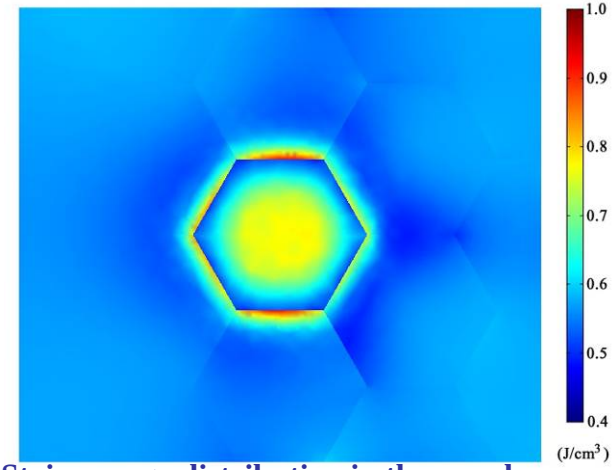
Fiber textured <111> grains surround a center grain with <100> orientation out of plane of the film



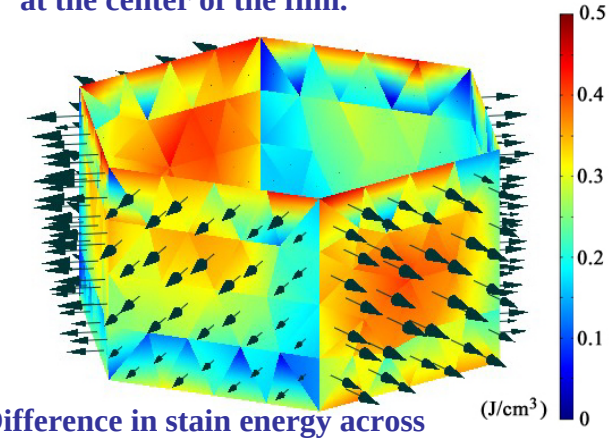
Grain Boundary Motion

Strain Energy Release

- Calculate strain energies from the stresses computed by Comsol Multiphysics.
- Compute GB velocities – the <100> grain grows.
- Move in PLENTE; cycle to model large motions

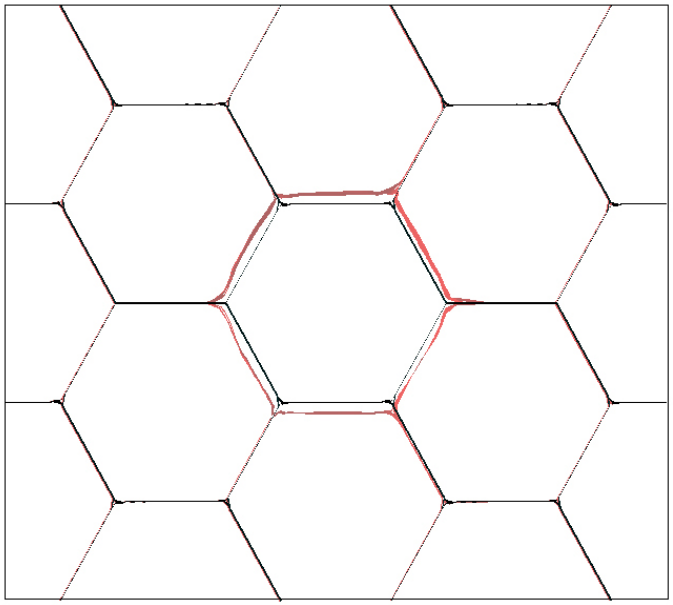


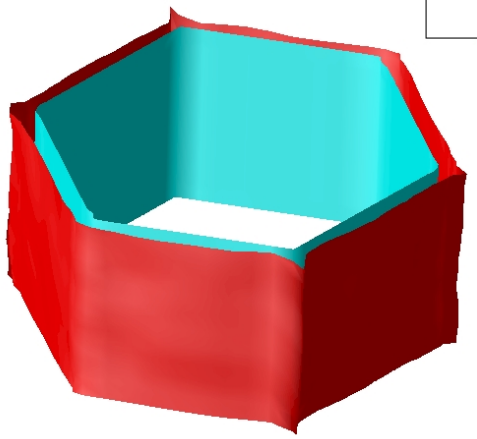
Stain energy distribution in the x-y plane at the center of the film.



Difference in stain energy across grain boundary for <100> grain.

(right) Top view of the level set grain boundaries in PLENTE before (in black) and after 12.5 hours at 425K (in red). (speeds on the order of 10 nm/hour)





(left) Close up of central <100> grain after simulated atom-mediated.

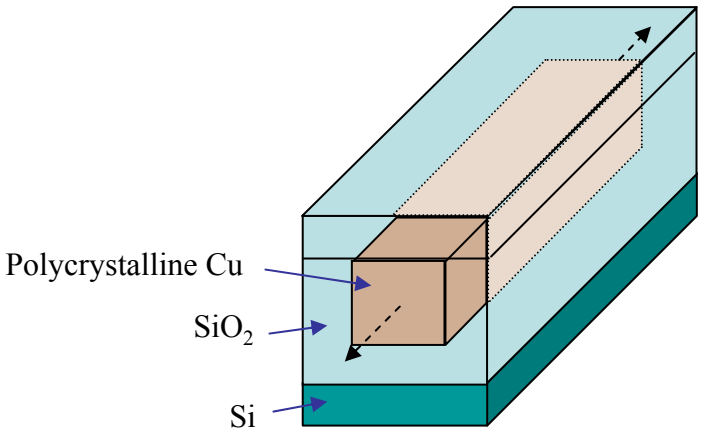
Velocities calculated using materials parameters from:

M. O. Bloomfield and T. S. Cale, *Microelec. Eng.* **76,** 195 (2004).

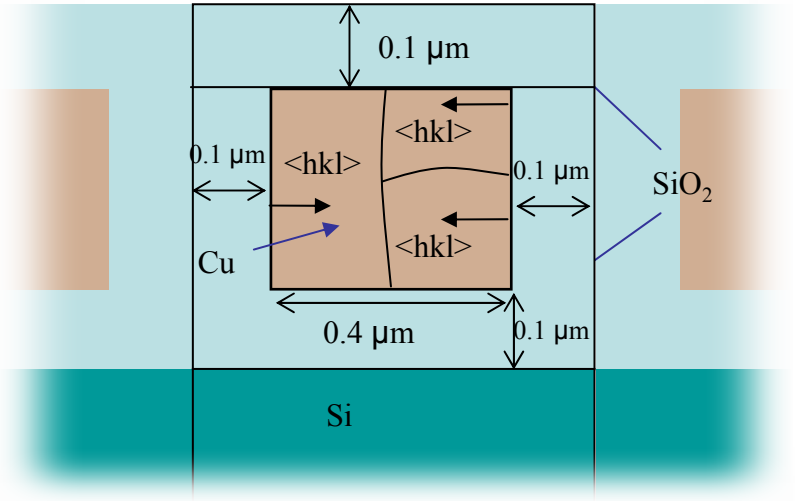
GB Motion in a Cu Interconnect

- 1 x 0.4 x 0.4 micron segment of a long polycrystalline Cu line, embedded in SiO_2 deposited on a Si substrate.
- Initial construction is by an isotropic deposition model, with nucleation on sidewalls and bottom of damascene trench.
- We assign a texture relative to sidewalls. All <111> grains except one anomalous <100> grain.
- 525 K to 425 K, perfect adhesion between phases, and the strain energies are calculated throughout the structure.
- Strain energy density in Cu ranges from 0.4 to 1 J/cm^3.
- Maximum strain energy differences between grains 0.15 J/cm^3.

View of embedded line

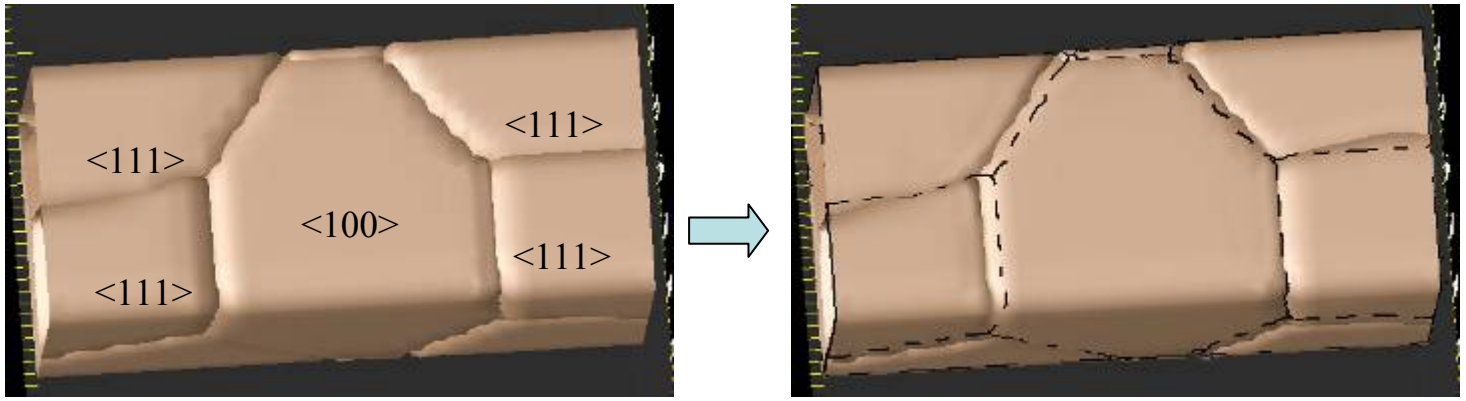


View along line showing cell and texture convention

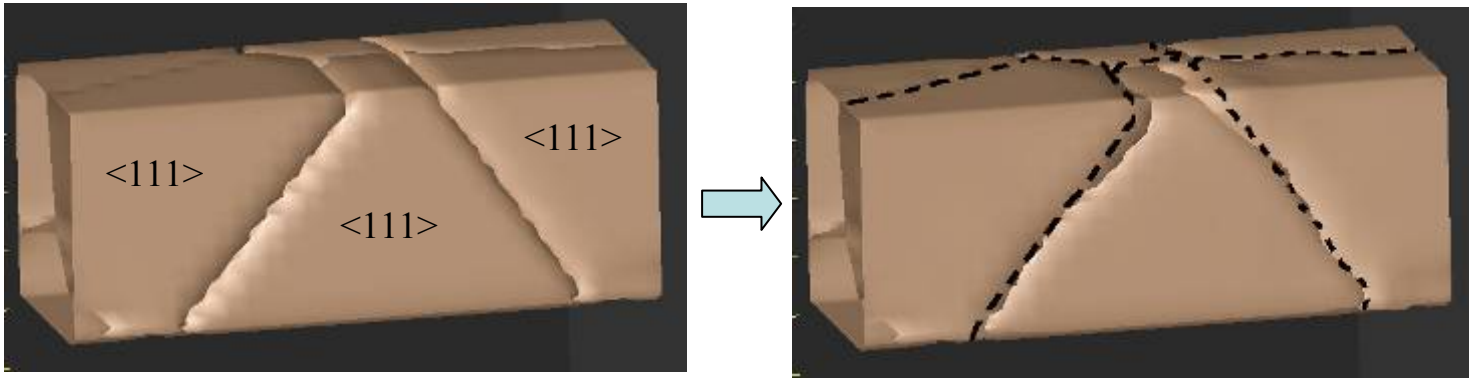


GB Motion in a Cu Interconnect

Front side



Back side



Evolution: 8.6 hours

Embedding oxide not shown

Concept of 3D grain evolution is proven – but is very taxing.

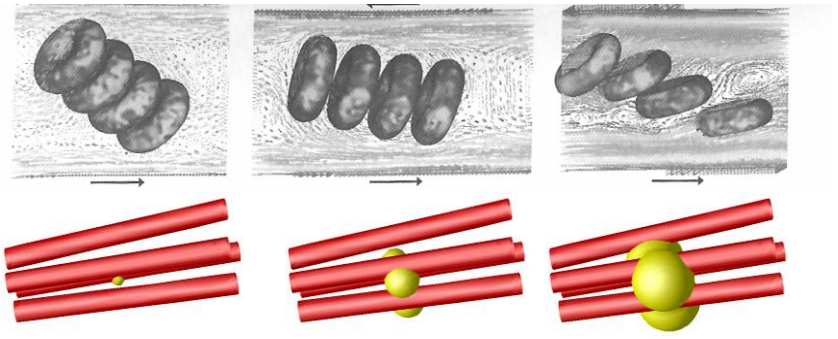
Conclusions

- Advanced models are not all atoms! Grain-focused models can be an important bridge between continuum and atomistic models
  - Can deal with large enough systems to help interpret experimental results from test structures
  - Can incorporate atomistic information (more work needed in this area)
- Grain-Focused modeling is a new field
  - A lot of opportunities for improving our ability to predict reliability, both in terms of data and in terms of materials science in the models.

Ongoing/Future Work

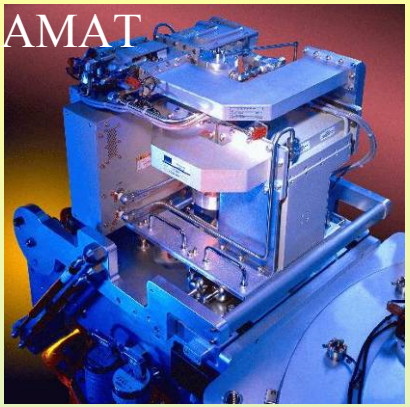
Integrate Grain-focused approach with atomistic approaches to improve grain boundary models.

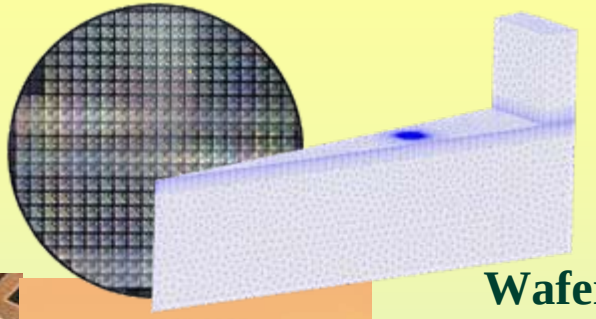
- Macroscopic microstructural changes due to a variety of imposed forces during product fabrication and usage. (ICs to date.)
- Other application areas - Similar, but 'less general' models than PLENTE have been used in:
  - Structural materials
  - Multi-phase flow
  - Tumor growth
  - . . .



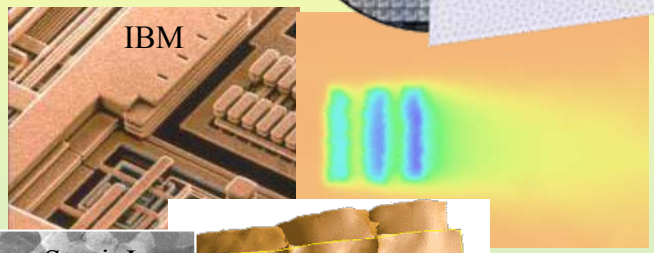
Virtual Wafer Fab

Enterprise ($)
Fab – VFW
Module – e.g., pattern transfer

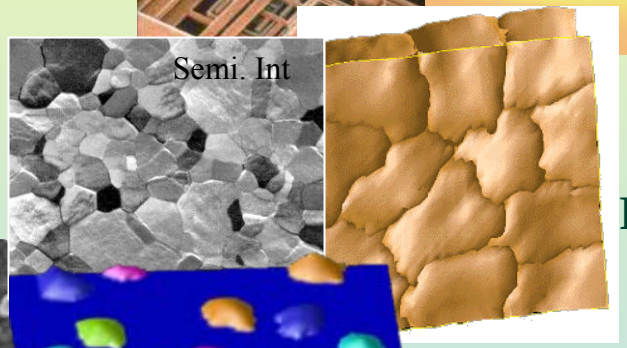




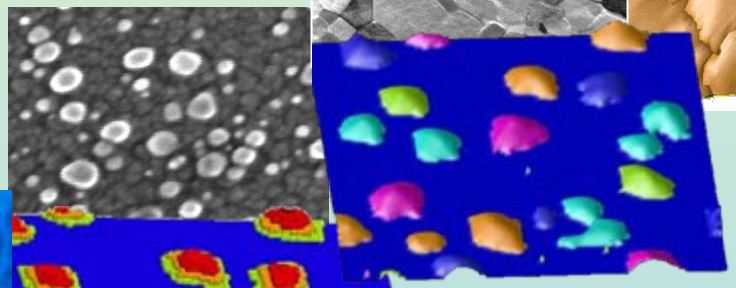
Wafer/ Equipment



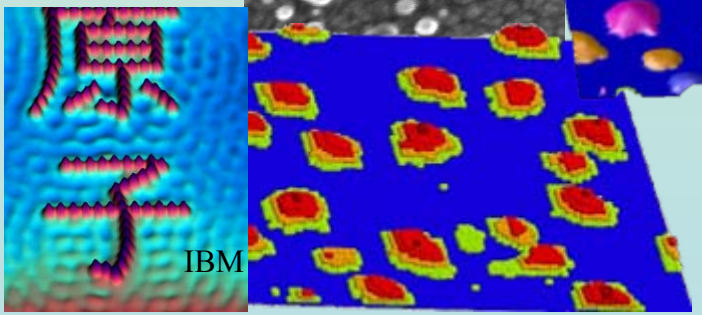
Pattern/Chip



Film/Interconnect



Island/Grain



Atomic/Discrete

Thanks!