Grain Focused Modeling and Simulation

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Overall Presentation Goals

Motivate the use of grain information in materials modeling and simulation

Using such information can provide results that cannot be provided by continuum approaches or by atomistic approaches (today).

Discuss some of our grain-focused M&S work

It is really an approach to nanoscale computations that sits between atomistic and continuum approaches.

Outline

- Motivate and define the use of grain-focused information in models
- Discuss our grain-focused modeling for 3D-ICs
- Discuss our efforts to model grain evolution
- Conclude

Grain Focused M&S

Grain structure impacts performance and reliability. . . .









Atomic representation of a PVD film; we are reaching the range of simulation volumes of interest, but not yet large enough to simulate test structures . . .





'Grain-continuum' representation of damascene structure, with schematic interface to atomistic codes. Large volumes very do-able – generated using process models...

A Grain-Focused Approach: PLENTE

(Parallel Levelset Environment for Nanoscale Topography Evolution)

- PLENTE is a robust 3D geometry tracker capable of representing and evolving complex systems.
- Interfaces with process simulators to track evolution.
- 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.

Initial, nucleated
substrateCoalesced
grain structureSingle grain pulled
from structureKinetically controlled, electroless deposition onto a
substrate with 5 nm rms roughness.

Bloomfield et al., *Phil. Mag.* 83(31-34), 3549-3568 (2003)
M.O. Bloomfield and T.S. Cale, in *Multiscale Materials Modeling in Structural Engineering*, Z.X. Guo, ed., Woodhead Publishing, 2007







PLENTE

A 3D Multiple-Material Evolution Code

(Parallel Levelset Environment for Nanoscale Topography Evolution)

- PLENTE is capable of representing and evolving complex systems, with features distinguished down to length scale of underlying volume mesh.
- PLENTE can take input from process models to simulate a variety of systems. *The physics are all in the process models*. This is analogous to deposition process simulators that requires users to input chemistry and process conditions.
- PLENTE has built in encapsulation and re-atomation abilities to convert discrete data from atomistic simulations to continuum representations and vice versa. By design, this is how it exxchanges information with atomistic codes.
- Near linear speed up across many CPUs (observed up to 64 processors, expected for many more.)

Hyper-Integration Approach at RPI



Key Challenges:

- Precise alignment of 200 mm wafers (≤ 1 μm accuracy)
- Thin glue-layer bonding at low temperature (≤ 400 °C)
- Precision thinning and leveling of top wafer (≤ 10 µm thick)
- Inter-wafer connection by highaspect-ratio (> 5:1) vias

• This process flow is designed to employ existing process technology and known-compatible materials as much as possible.

J.-Q. Lu et al., in *Proc. IEEE 2002 International Interconnect Technology Conference*, pages 78–80, IEEE, 2002.

Thermal Stresses in 3D ICs



- CTE mismatches is a reliability concern in 3D ICs. At RPI, we developed a BCB based approach.
- We studied induced stresses using COMSOL Multiphysics.
- We started by validating our modeling approach using published results for via chain test structures using SiCOH or SiLK as the dielectric.

R.G. Filippi, et al., 2004 IEEE IRPS Proc., IEEE, 2004, pp. 61 D. Edelstein, et al., 2004 IEEE IRPS Proc., IEEE, 2004, pp. 316

- J.-Q. Lu et al., in Proc. 2002 IITC, p. 78 (2002)
- J. Zhang et al., *Microelect. Eng.* 82, 534 (2005)
- J. Zhang et al., IEEE TSM 19(4), 437 (2006)

Continuum Calculation

• As a starting point, we assume that each of the materials in the system is continuous and use finite element methods to compute thermomechanical responses.



(Left) resulting von Mises stresses from -100K change in temperature for different size vias based on purely continuum assumptions of materials properties. (Right) trends in maximum von Mises stresses in copper for pictured structure, with changes in via geometry, using continuum approximations.

Elastic Anisotropy

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

Stress-Strain Relationship

 $\sigma_i = C_{ij} \varepsilon_j$

 $\sigma_i =$

 σ_{xx}

 $\sigma_{_{yy}}$

 σ_{zz}

 τ_{yz}

 τ_{xz}

 au_{xy}

Typically

- 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

C₂₂

C₃₃

C

Spherical Plot of the Directional Dependence of Young's Modulus



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

<100> $C_{11} = C_{22} = C_{33} = 168.4 \text{ GPa}$ <110> $C_{11} = C_{33} = 220.3 \text{ GPa}$: $C_{22} = 168.4 \text{ GPa}$ <111> $C_{11} = C_{22} = 220.3 \text{ GPa}$: $C_{33} = 237.6 \text{ GPa}$



Grain-Continuum Calculations

- Use PLENTE to simulate the development of grain structure using a simple electrodeposition model.
- Create an unstructured, body-fitted mesh in PLENTE and import into Comsol Multiphysics along with anisotropic materials information.
- Solve the thermomechanical FEM problem with Comsol.
- The presence of "grains" creates stress concentrations, significant increases in maximum stress/strains.



Hybrid Grain-Continuum (HGC)

- Retaining grain structure throughout an entire 3D-IC structure is not feasible for parameter studies.
- We mostly care about the stresses in the areas for concern determined by continuum simulations.
- Use continuum simulations to determine regions of interest, then employ explicit grain representations in that region only.



D.N. Bentz, *et al.*, in <u>Advanced Metallization Conference (AMC) 2006</u>, MRS, 2007, pp. 275-80. M.O. Bloomfield, et al., in *2007 IEEE IRPS*, IEEE, 2007, pp. 644-5.

Efficient HGC Splitting



Von Mises stresses for different division of structure into GC and continuum. Arrow indicates the position of boundary coupling between regions.

Continuum vs. HGC: DoE Results

Continuum

HGC



Used PLENTE/COMSOL as a testbed, and developed DoE models. Similar trends are seen in the continuum and HGC results. HGC results show that the maximum stresses can be considerably higher.

Microstructure Evolution

- Grain structures can be important in property and performance simulations.
- Grain structures can also evolve in time.
 - Example: recrystallization of electrodeposited copper films
 - Example: electromigration of grain boundaries in electrical interconnects
- We want to track microstructural evolution to predict changes in properties over time.

Grain Boundary Motion

M_{GB} – Grain Boundary Mobility

(Velocity of the interface in response to a driving force)

Potential Forces on Grain Boundary

- Curvature
- Differences in surface or interface energies
- Jumps in strain energy density

Grain boundary mobility measures how easy atoms transition from one grain to another (Depends on grain boundary type)

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

Approximation for high angle grain boundaries $\longrightarrow M_{GB} = \frac{b \upsilon \Omega}{kT} \exp\left(-\frac{Q}{kT}\right)$

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



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 \rightarrow more adatoms
 - Concave \rightarrow 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.



GC Annealing M&S using PLENTE



- Start with capped Damascene line "grown" via electrolesslike 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.



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.

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

Strain Energy-Driven Grain Motion

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





$$v = M \Delta u_{\varepsilon}$$
$$= M_{GB} \frac{(\sigma_{+}\varepsilon_{+} - \sigma_{-}\varepsilon_{-})}{2} \hat{n}_{+to-}$$

- $\sigma_{\scriptscriptstyle +}, \ \epsilon_{\scriptscriptstyle +} \text{Stress and stain on positive side} \\ \text{of boundary}$
- 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

We compute the thermo-mechanical response in carefully constructed polycrystalline films.

- Polycrystalline film is represented as collections of distinct interacting continua each are assigned uniform, material and orientation-dependent parameters
- Here we study regular hexagonal grains on a silica layer sitting on a silicon wafer.
- We impose a temperature change from 525 K to 425 K.







Anisotropic Elasticity

in a Polycrystalline Film

- <111> textured film has uniform stress of 262 MPa.
- For comparison, an 'isotropic' Cu film has uniform spherical stress (average of non-shear stresses) of 178 MPa.
- Spherical stresses in <100> grain range from 150 MPa to 300 MPa







Young's modulus

Grain Boundary Motion

Strain Energy Release

- Calculate strain energy from the stress computed by Comsol Multiphysics.
- Compute GB velocities
- Move in PLENTE; cycle to model large motions





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 SiO₂ 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.
- View of embedded line

- 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 0.1 J/cm³.
- Maximum strain energy differences between grains 0.15 J/cm³.

View along line showing cell and texture convention



GB Motion in a Cu Interconnect



Evolution: 8.6 hours

Embedding oxide not shown

Back to 3D-ICs

- Strain energy density in 3D-IC via shows effects of grain structure.
- Areas of high and low strain energy can be seen.
- Quantifying jumps in strain energy at grain boundaries is difficult "by eye".



Initial GBM in a 3D-IC via



A) section of 3D-IC via where it passes through BCB layer (dark lines),B) spherical stresses from grain structured calculation projected on structureD) structure evolved for 25 hours at 425K, dark lines show initial positions of GBs at Cu interfaces with surrounding materials.

Summary

- Grain-focused models can give different results than simulations using continuum approximations.
 - It is important to capture the microstructural details.
 - It is a nanoscale focus that sits between atomistic and continuum.
- PLENTE provides a 3D, multiple material geometry tracking tool; e.g., for forming and evolving polycrystalline microstructures.
- PLENTE interfaces with other software that provide models of transport and reaction; i.e., process and microstructure models.
- Much more information on grains is needed to make detailed predictions of grain structure.
 - Engineering models can provide guidance.
 - By analogy, 'we' develop and improve processes w/o detailed knowledge of their physics and chemistry; i.e., using engineering models.

Thank You!

Questions?