Grain-Focused Modeling of Thin Films

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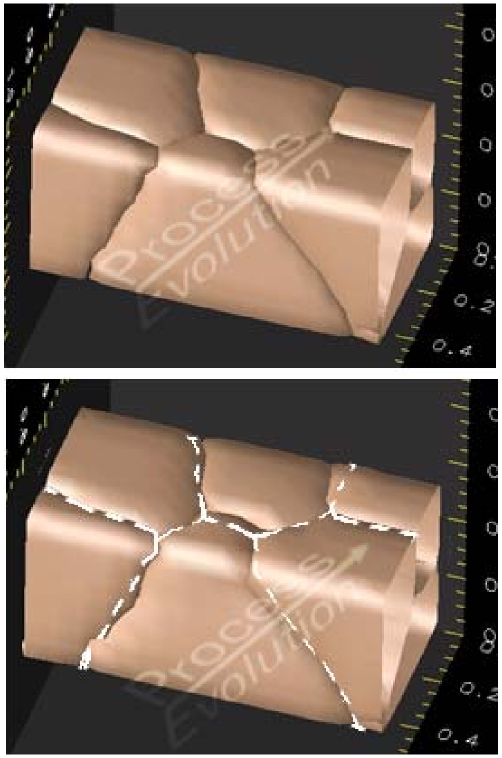
- Our modeling and simulation efforts target the increasing need to represent microstructure during thin film process and materials simulations:
  - The formation and evolution of microstructured films
  - The properties and performance of microstructured films
- Our efforts focus on thin film applications in microelectronics, and are extendable to other application domains.



3D Grain boundary motion in a Cu line, due to differences in strain energy in the grains. Anisotropic elastic properties play an important role. The white lines indicate grain boundary motion.

The Grain-Focused Paradigm

- Roughly speaking, thin film process simulations represent solids as being either ‘continuum’ or ‘discrete’.
  - Continuum simulations represent films as continua, and generally produce films with no internal microstructure. This approach excels in determining thin film topography evolution.
  - Discrete simulations represent solids as made up of small particles; atoms or groups of atoms. This approach excels at determining parameters directly based on atomistic motion, assuming atomic resolution.
- The Grain-Focused approach involves treating grains as continua, but making each grain a distinct entity.
  - Excels at capturing the grain structure and/or other microstructural details; e.g., pore networks, phase separated materials, etc.
  - There is no particle size to build in a scale limit, so the approach is easily applied to films of many scales, from tens of nanometers to macroscopic, as determined by the size of the microstructure.

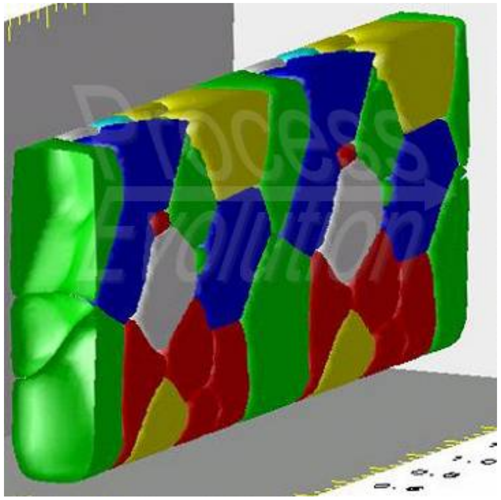
A Grain-Focused Approach: PLENTE

PLENTE is the **P**arallel **L**evel-set **E**nvironment for **N**anoscale **T**opography **E**volution [1].

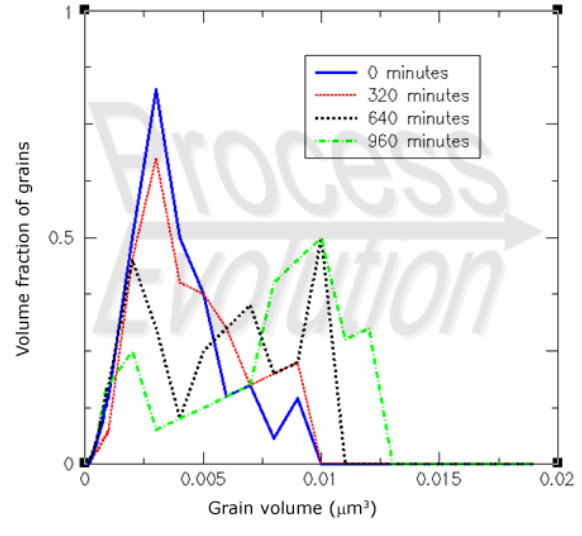
- –Is a framework for the grain-focused approach, in the form of a robust 3D geometry tracking code, capable of representing and evolving complex systems with many distinct materials or grains.
- –Interfaces with process simulators to track evolution.
- –Based on methods commonly used in computer vision and image analysis.
- –Has built-in encapsulation abilities to convert discrete data from atomistic simulations to continuum representations
- –Can distribute the computational load across many processors, with almost linear speed-up (tested for up to 60 processors).

Curvature Driven Grain Evolution [2,3]

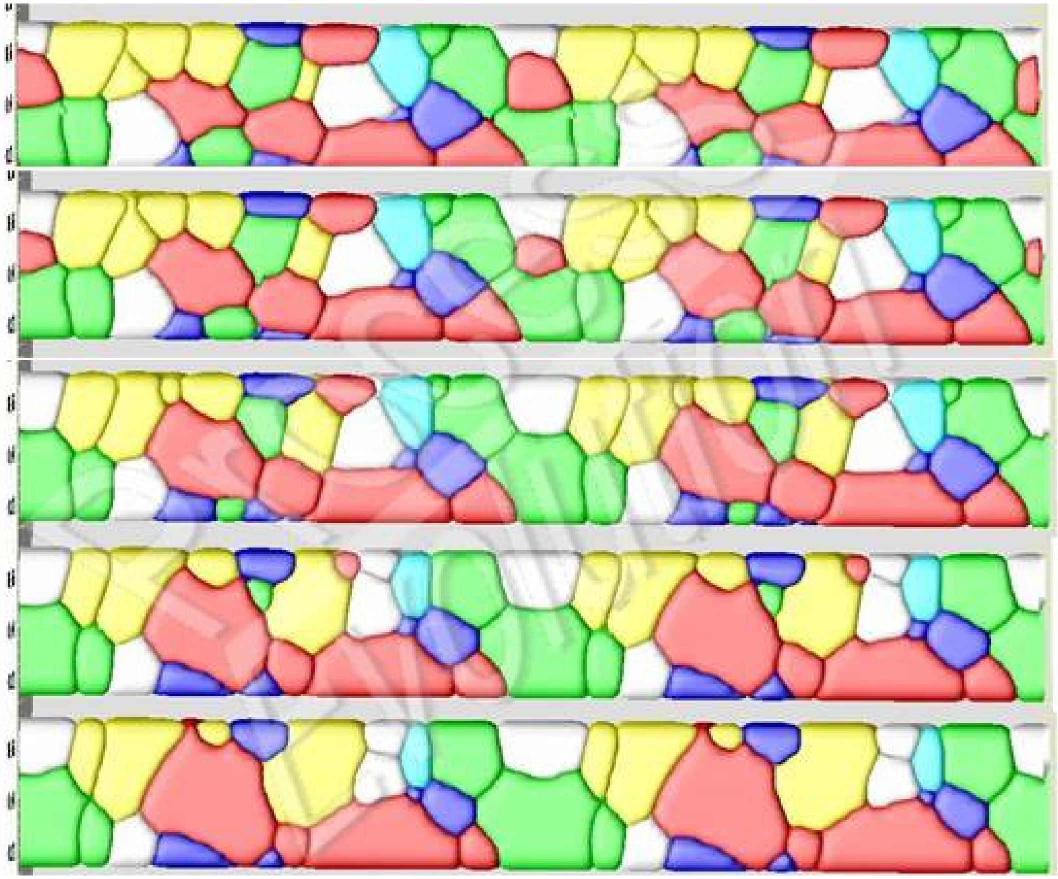
Example starting line, with Cu ‘grown’ by electroless plating model.



Grain size distributions at selected times during an annealing simulation

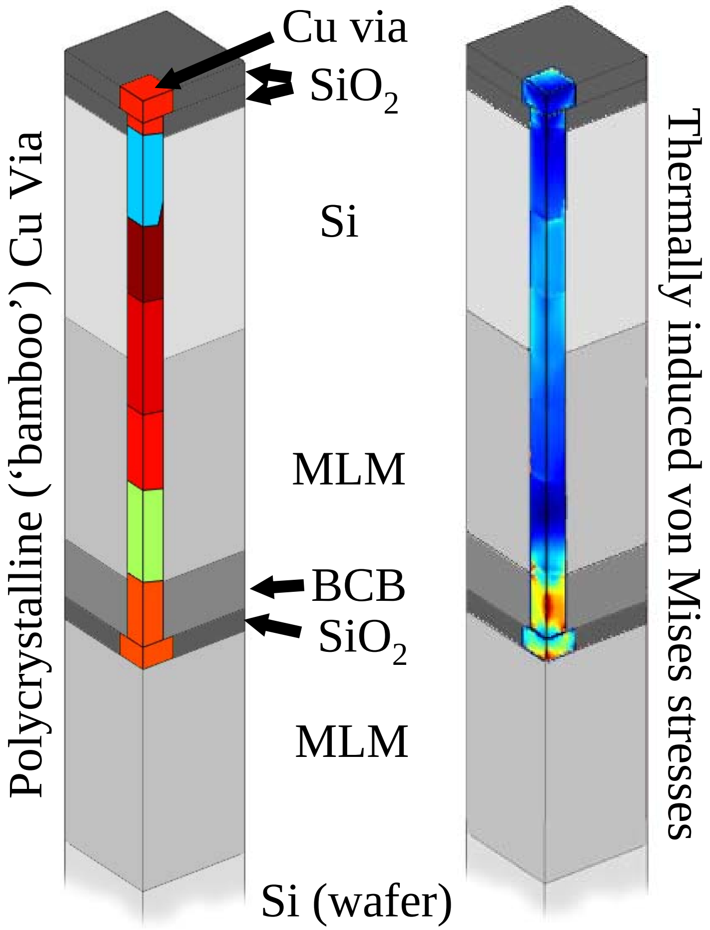


Still shots during the simulated evolution of grains due to curvature driven ripening (annealing)



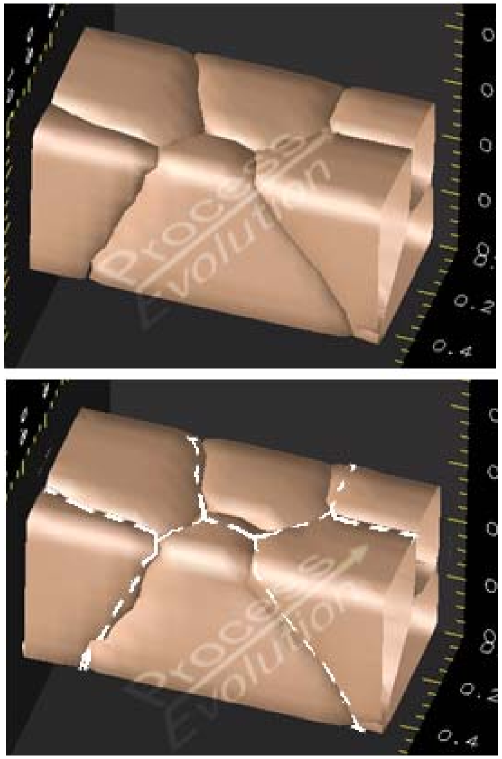
Stress Driven Grain Evolution [4,5]

We are studying stresses in 3D ICs, to help set design parameters for stable structures.



(L) Simulation domain for a Cu via through the multiple material stack seen for BCB-bonded wafer level 3D-ICs. (R) Von Mises stresses (red high, blue low) in the Cu via, due to CTE mismatches of material in the structure.

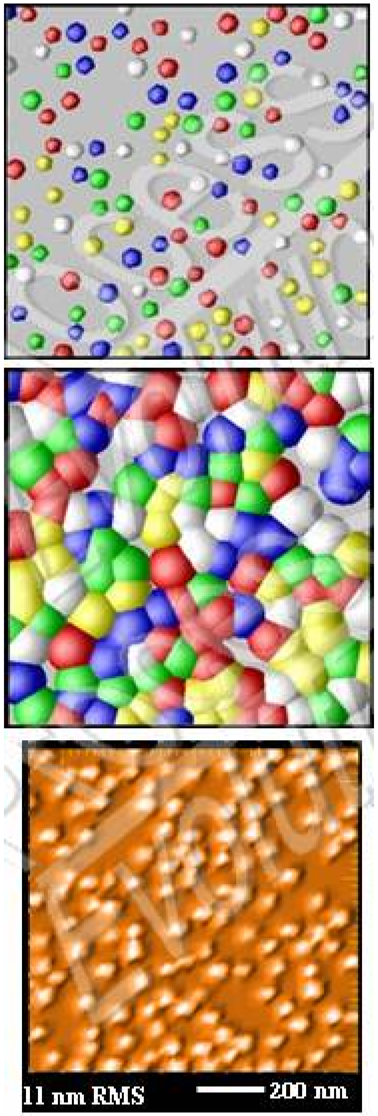
A starting point for grain evolution – focus on simpler structures.



Example of strain energy induced grain boundary motion in a polycrystalline Cu line surrounded by oxide (oxide is not shown). Stresses are induced by lowering the temperature from a stress-free state at 525 K to 425 K. The top image is the initial structure and the bottom is after motion. The white lines in the bottom image delineate the grain boundaries in the original structure (top). Anisotropic elasticity plays a large role.

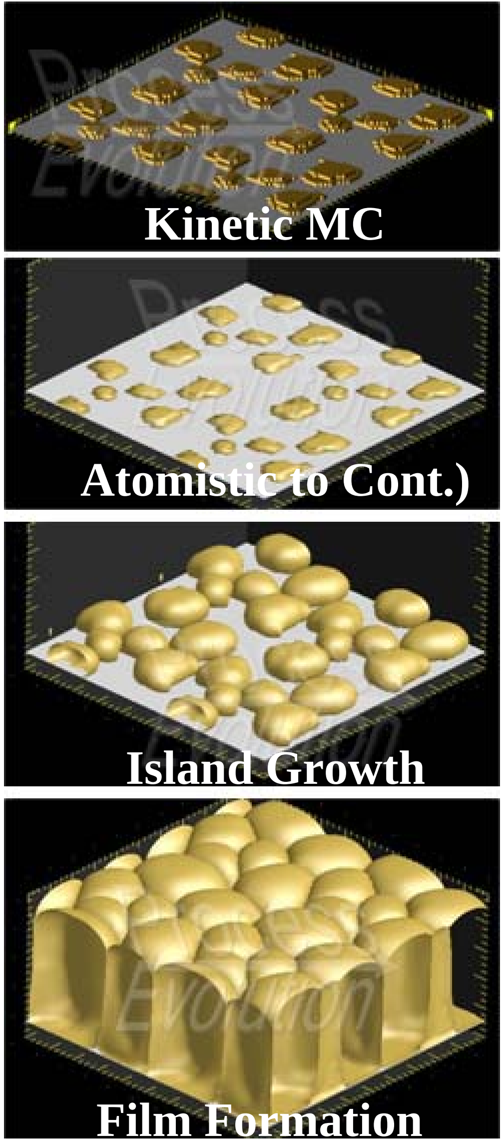
PLENTE for Process Simulations [6,7]

Atomic Layer Deposition

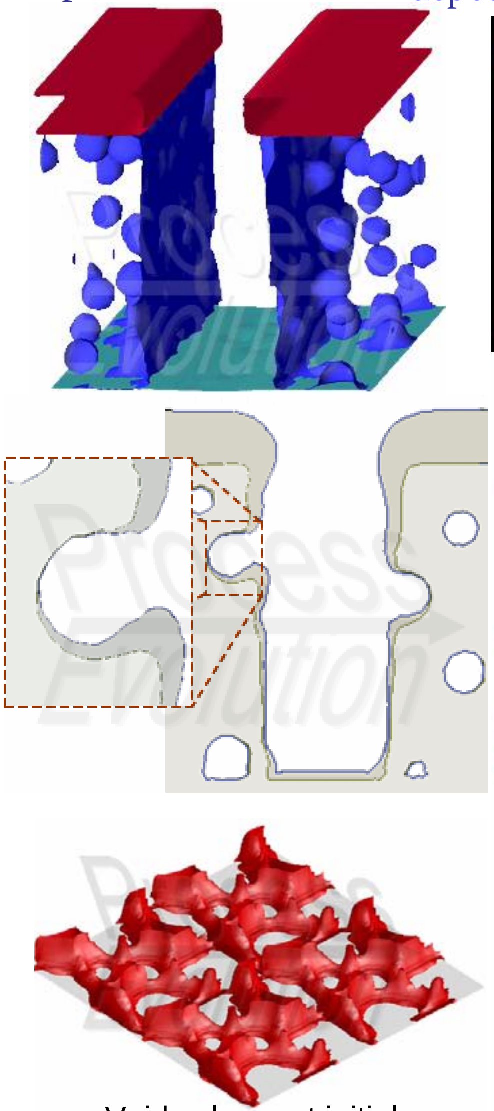


Simulated AFM during early ALD.

Physical Vapor Deposition



Deposition into Pores



Void volume at initial substrate surface

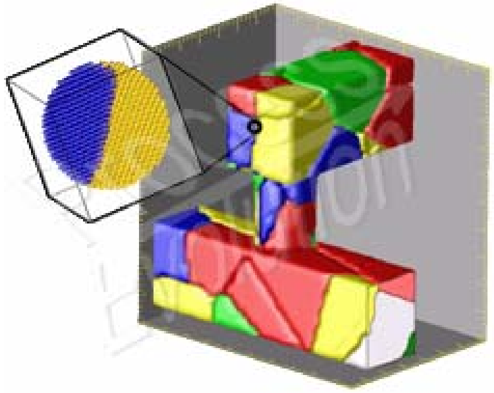
Kinetically controlled electroless deposition onto a rough substrate

PLENTE

For more information about PLENTE, please visit www.process-evolution.com. To discuss modeling and simulation projects, please e-mail Timothy Cale (cale@process-evolution.com). The papers below provide some details, as well as additional references to the software and applications to date.

A next Step:

Add atomistic information



Grain-continuous representation of a section of copper metalization, with an 'atomated' representation of a small section of an inter-granular region.

References

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2. "A computational framework for modeling grain structure evolution in three-dimensions", M.O. Bloomfield, D.F. Richards, and T.S. Cale, ***Phil. Mag. 83(31-34)***, 3549 (2003).
3. "Formation and Evolution of Grain Structure in Thin Films", M.O. Bloomfield and T.S. Cale, ***Microelectr. Eng. 76(1-4)***, 195 (2004).
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6. "Modeling Thermal Stresses in 3D IC Inter-Wafer Interconnects", Jing Zhang, Max O. Bloomfield, Jian-Qiang Lu, Ronald Gutmann, and Timothy S. Cale, ***IEEE Trans. Semi. Manuf.***, in press.
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