One approach to 3D-ICs:

- Bond processed wafers with BCB.
- "Damascene" processing to interconnect the MLM on the wafers.
- Differences in the coefficient of thermal expansion between materials is a concern.
- We have studied the stresses generated in 3D-IC via structures due to temperature changes.
- There is reason to be concerned.

Thermal Stresses in 3D ICs

- CTE mismatches is a reliability concern in 3D ICs.
- 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.

Continuum Calculations

- 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.

- 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

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

- \(<100> \ C_{11} = C_{22} = C_{33} = 168.4 \ GPa\)
- \(<110> \ C_{11} = C_{33} = 220.3 \ GPa: \ C_{22} = 168.4 \ GPa\)
- \(<111> \ C_{11} = C_{22} = 220.3 \ GPa: \ C_{33} = 237.6 \ GPa\)

\[
\sigma_i = C_{ij} \varepsilon_j
\]

Stress-Strain Relationship

Spherical Plot of the Directional Dependence of Young’s Modulus

Typically

Comsol

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.

Efficient HGC Splitting

Von Mises stresses for different division of structure into GC and continuum. Arrow indicates the position of boundary coupling between regions.
3D-IC via Result

- 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 structure
D) structure evolved for 25 hours at 425K, dark lines show initial positions of GBs at Cu interfaces with surrounding materials.
Continuum vs. HGC: DoE Results

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.
Summary

• Grain-focused models can give different results than simulations using continuum approximations.
  – It is important to capture the microstructural details.
• PLENTE provides a 3D, multiple material geometry tracking tool; e.g., for forming and evolving polycrystalline microstructures.
• PLENTE interfaces with other software (e.g., Comsol Multiphysics) that provide models of transport and reaction; i.e., process and microstructure models.