Strain Energy Driven and Curvature Driven Grain Boundary Migration in 3D-IC Cu Vias

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Abstract

We use grain-focused models to study grain boundary (GB) migration (GBM) in polycrystalline Cu vias that interconnect MLM layers in 3D ICs. Curvature-driven GB velocities are calculated by PLENTE [1-3] using the local mean curvature of the GBs, as described in Ref. 2. We use Comsol Multiphysics [4] to calculate GB velocities due to thermally induced strain energy jumps across GBs [5]. The thermo-mechanical calculations needed for this are made using model structures that combine continuum models and grain-continuum (GC) models (see [1-3, 5]); we call these 'hybrid' grain-continuum (HGC) models. Curvature driven GB dominates in this work; however, there are uncertainties in the absolute stress values used and how the relative magnitudes of these phenomena will change as the structure evolves.

1 Introduction

We have used grain-focused simulations to study microstructure formation and evolution in Cu interconnects [1-3], because of their impacts on IC performance and reliability characteristics, including electromigration resistance [6,7], resistivity [8], and yield strength [9]. This paper reports on our on-going grain-focused modeling effort to understand microstructure evolution in polycrystalline Cu vias as they might be used in 3D-ICs [10]. In face-to-face bonded 3D-IC wafer stacks, as considered here [11], Cu vias can pass through several layers (see Fig. 1a); including, multi-level metallization (MLM), Si, SiO_2, and BCB. BCB is an organic polymer adhesive.

We focus on the relative roles of two driving forces for GBM: curvature driven GBM (CDGBM) and strain-energy driven GBM (SDGBM). CDGBM is traditionally cited as one major cause of post deposition self-annealing of ECD Cu [12], which is used to deposit Cu in our vias. The mechanism is based on the reduction of interface energy associated with GB area; *i.e.,* by reducing GB area. In contrast, SDGBM can become important when externally imposed loads or changes in temperature, combined with mismatches in coefficients of thermal expansion (CTE), cause non-uniform stress fields within a grain structure. Cu grains are mechanically anisotropic, allowing jumps in strain energy density, which act as driving pressures for GBM [13].

2 Methodology

In our grain continuum (GC) approach, we treat each grain as a continuum that interacts with other grains and the film boundaries [5,14,15]. For thermo-mechanical analyses of 3D-IC via structures, we use an extension of the GC approach that we call

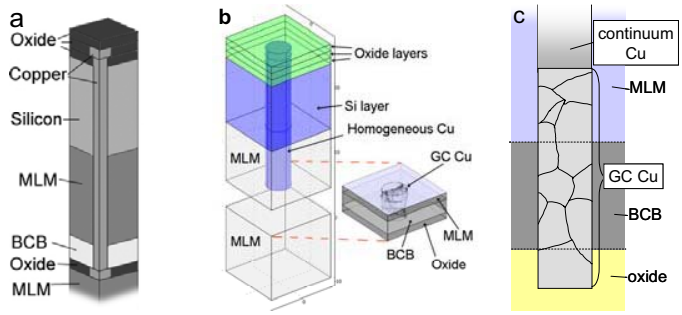

Figure 1: (a) Schematic of 3D-IC via passing through multilayer stack. (b) HGC representation containing both GC and continuum sections. (c) Cross section of HGC representation through center of Cu via showing grain structure.

'hybrid' grain-continuum (HGC) models [5]. In HGC models, parts of the Cu grain structure are replaced with continuum representations, while other parts retain GC representations (see Fig. 1b and 1c). HGC models reduce the computational burden while providing for detailed results in regions of particular interest.

To produce a starting grain structure, PLENTE [1-3] is used to model the deposition of Cu grains in a 1.5 μm diameter, 23.6 μm tall cylindrical via. With a nominal nucleation density of 0.7 μm^{-2} along the via sidewalls, Cu nuclei are allowed to grow as if they were produced by a kinetically limited electrochemical or electroless plating process [16] until the via is filled. This deposition model produces a reasonably realistic grain structure in the via, containing approximately 80 grains. The via is embedded in an oxide/BCB/oxide multilayer (as seen in Fig. 1a) with a BCB thickness of 3 μm and a via-to-via pitch of 15 μm. For the thermo-mechanical calculations, the explicit GC structure in the bottom 6 μm of the via is kept, and the upper section of the via is replaced with a continuum model. From previous modeling work [5], we know that the portion of the via that passes through the BCB has the highest stresses. The height of Cu to kept as GC above the BCB layer, determined as described in Ref. 5 is large enough that the answers in the BCB region do not change.

The structure is exported from PLENTE to Comsol Multiphysics [4] as an interface-fitted tetrahedral mesh. Thermo-mechanical calculations are made assuming a temperature drop of 100 K from an annealing temperature of 525 K. The structure is periodic by assumption and sits on a thick Si wafer, so displacement boundary conditions along the sides of the cell are imposed, mimicking the contraction of the underlying substrate. Strain energy density is computed throughout the via, and the set of all element faces that represent GBs are identified. The difference in strain energy density across each face is calculated. This difference in strain energy density is a driving pressure for SDGBM [14]. Multiplying this pressure by the mobility of Cu GBs, (1.3×10^{-16} m^4/J s at 425 K [13, 17]) we arrive at a normal speeds for each triangle on the Cu GBs, in the GC section of the structure.

Curvature driven speeds are determined entirely within PLENTE, as discussed in Ref. 2. In brief, the level set method PLENTE uses to represent grain structures is used to find a value for the mean curvature of all of the triangles representing. Using a

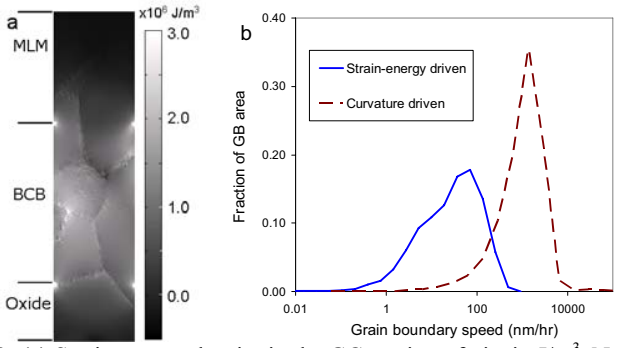

Figure 2: (a) Strain energy density in the GC section of via, in J/m^3. Note that the scale does not include the entire range of energies, to better highlight the details of the grain structure. (b) Speed probability distribution of the Cu grain boundaries velocities for SDGBM (solid line) and CDGBM (dashed line) cases.

Gibb-Thompson-like relation [2], the product of the mean curvature and the surface energy density is identified as a driving pressure, and normal speeds are determined using the same mobility as for SDGBM.

3 Results and Discussion

Computed strain energy densities resulting from a temperature drop of 100 K are shown in Fig. 2a for a cross section through the via. The materials surrounding the Cu grains are indicated by the solid lines. The mechanical effects of the grain structure in this system are significant enough that the grains can be roughly seen in this field. However, it is difficult to see the magnitude of the discontinuities in energy density across the GBs. It is revealing to look at the distribution of normal speeds over the GBs as speed probability distributions. SDGBM and CDGBM speed distributions are plotted in Fig. 2b for comparison. These curves show the fraction of the Cu-Cu GB area moving at a given differential speed interval. The SDGBM distribution exhibits a broad peak around 70 nm/hr. In contrast the CDGBM curve peaks sharply at 1400 nm/hr. Note that neither distribution gives information about where particular speeds occur. To answer such questions, additional visualization is required. However, it can be said that because CDGBM rates are only a function of the local shape of grains, they are, on average, uniform throughout the via. Thus the entire via is used (not just the bottom 6 μm) to determine the CDGBM speed distribution.

The speeds associated with CDGBM are 1-2 order of magnitude higher than those for SDGBM. It is tempting to say that CDGBM is the dominant of the two mechanisms, but that statement may be limited to short times after deposition. CDGBM is highly dependent on the local shape of the GBs. As grains relax under CDGBM, high curvature areas from the as-deposited structure will tend to smooth out and the peak in the distribution will shift to the left [2]. Further, although the driving energy for CDGBM is stored in the structure, the driving energy for SDGBM is induced in the structure by the work done upon changing its temperature, or in other cases, by work

done by an imposed load. Therefore, the CDGBM rates may drop off much faster than the SDGBM rates as the system relaxes.

5 Conclusions

Thermomechanical and geometric calculations on a realistic grain structure show that, at least for short times after deposition, CDGBM is larger than SDGBM, having a most probable interface speed about an order of magnitude higher. A more complete exploration of the relative role of these two mechanisms should involve the evolution of the grain structure, in order to reveal how the behavior changes with time. Additionally, more advanced models may be appropriate for some systems [18]. It should be noted that von Mises stresses exceeded some estimates of the yield strength of Cu in some locations in the results summarized here. The elastic model used cannot account for plastic deformation that would dissipate strain energy.

The extra work required to account for grain structure in the thermomechanical calculation is justified, as evidenced by visualizing the strain energy density field. The visiblity of the underlying grain structure in the computed result (Fig. 2a) underscores the presence of a grain-based effect on the mechanical response.

Acknowledgments

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References

[1] M.O. Bloomfield, D. F. Richards, and T. S. Cale, *Phil. Mag.*, **83,** 3549 (2003).
[2] M.O. Bloomfield *et al.*, *Microelectron. Eng.*, **76,** 195 (2004).
[3] M.O. Bloomfield *et al.*, *JEM*, accepted April 2007.
[4] Comsol Multiphysics 3.3, http://www.comsol.com, May 2007.
[5] M.O. Bloomfield, *et al.*, in *2007 IEEE International Reliability Physics Symposium Proceedings*, IEEE, pp. 644 (2007).
[6] L. Vanasupa, *et al.*, *J. Appl. Phys.*, **85,** 2583 (1999).
[7] C. Ryu*, et al.*, *IEEE Trans. on Elect. Dev.*, **46,** 1113 (1999).
[8] K. Yamaguchi, *J. of Appl. Phys.*, **89,** 590 (2001).
[9] E.O. Hall, *Proc. of the Phys. Soc. Section B*, **64,** 742 (1951).
[10] J.-Q. Lu*, et al.*, in *Proc. of 2002 IITC*, IEEE, p. 78 (2002).
[11] R.J. Gutmann, *et al.*, in *2003 Advanced Metallization Conference,* Mater. Res. Soc., p. 19 (2004).
[12] S. Lagrange*, et al.*, *Microelectron. Eng.*, **50,** 449 (2000).
[13] G. Gottstein, L. S. Shvindlerman, *Grain Boundary Migration in Metals: Thermodynamics, Kinetics, Applications*, CRC Press,1999.
[14] M. O. Bloomfield*, et al.*, in *Proc. of the 2006 VLSI Multilevel Interconnect Conference*, IMIC, p. 234, (2006).
[15] M.D. Thouless, J. Gupta, and J. M. E. Harper, *J. Mat. Res.*, **8,** 1845 (1993).
[16] M.O. Bloomfield, Y. H. Im, and T. S. Cale, in *2003 IEEE Intl. Conf. on Sim. of Semicon. Processes and Dev.*, IEEE, p. 19 (2003).
[17] M.O. Bloomfield, *et al., Microelectron.Eng.*, accepted May 2007.
[18] *International Journal of Non-linear Mechanics*, Elsevier Ltd., 1966-present.