

Microstructure and Stress Aspects of Electromigration Modeling

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The electromigration behaviour of copper interconnects realized in damascene architecture indicates macroscopic and microscopic electromigration divergence sites. Macroscopic divergence sites exist at the cathode end of via bottoms where the barrier layer can be a blocking boundary for the electromigration flux. As microscopic divergence can be considered triple point sites of the grain boundary network. In the cases where failures are induced far away from a via, it has been shown that their activation energies are often below the expected value for the grain boundary diffusion [2]. This is a strong implication that copper interfaces to the barrier and/or capping layer are dominant diffusion paths [2]. Considering interfacial diffusion as main contribution to electromigration was a significant simplification for modeling and simulation of both void nucleation and void evolution [3,4].

Surface treatment aiming at strengthening the copper/capping layer interface has been successfully applied to suppress interfacial diffusion [1,2] and to increase electromigration life time. Reducing the diffusivity at the interfaces to the level of bulk and grain boundaries diffusivities necessities modeling of the grain boundary network and the crystal orientation in the grains. Moreover, intrinsic stress, introduced by the dual damascene process, has a strong impact on the bulk and grain boundary diffusion which has also to be considered [5].

We adjusted previously studied models [3,4] by including effects of grain boundaries and grain crystal orientation. The impact of grain boundaries is twofold. First they act as fast diffusivity paths and second they serve as sites of intensive vacancy generation/annihilation. Therefore, the scalar and cumulative value (for all possible paths) of vacancy diffusivity is replaced by a diffusivity tensor for fcc crystal lattices [5],

$$D_{ij} = D_0 \delta_{ij} + \sum_{kl} d_{ijkl} \epsilon_{kl} ,$$

deformed by the strain field ϵ_{kl} . d_{ijkl} is the elastodiffusion tensor [5]. The expression above is applied inside the grains. The grain boundaries are modeled as planes crosssectioning interconnect lines and vias. In these grain planes constant diffusivity values are assumed. In addition we have developed a simulation scheme which enables to study intrinsic stress build-up as consequence of the transition from initial nanostructure to polycrystalline structure. The model can predict shrinkage of the deposited copper lines after deposition and tensile stress build up which is subsequently applied to electromigration simulation.

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