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Granularity Effects in Electromigration

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***Abstract*—The continued efforts to scale front-end-of-line transistors has resulted in simultaneous attempts to scale back-end-of-line coper metalization. However, just like is the case in scaled transistors, nanometer sized metal films behave quite differently to their thicker counterparts, primarily due to the increased influence that the microstructure and granularity plays on its conductive and reliability behavior. The grain boundaries and the roughness at the interface between a metal film and surrounding dielectric or isolation layers influence the movement of conducting electrons and diffusing atoms during electromigration. Therefore, fully understanding and thus modeling this phenomenon has become increasingly challenging, since the boundaries and interfaces must be treated independently from the grain bulk, for which continuum models are insufficient. In light of this, recent advances in modeling electromigration in copper nano-interconnects are described, which use spatial material parameters to identify the locations of the grain boundaries and material interfaces. This method allows to reproduce the vacancy concentration in thin copper interconnects properly.**

***Index Terms*—Materials reliability, Nano-interconnects, Electromigration, Modeling and simulation, Reliability TCAD, Back-end-of-line**

I. Introduction

CONTINUED transistor scaling along Moore's Law [1] has been accompanied by simultaneous miniaturization of the copper interconnect lines. The scaling of metal lines down to a few nanometers results in an increased impact of the material interfaces (MI) and grain boundaries (GB) on the conductivity and reliability of the thin film. Understanding and mitigating the impact of granularity in interconnects is essential for scaling to continue. This includes line and via sidewall roughness, the intersection of porous low-κ voids with the sidewall, copper (Cu) surface and copper/barrier interface roughness, and the presence of GBs [2]. Even though Cu is showing undesirable effects at the nanometer scale, including increased resistivity due to grain boundary and surface roughness scattering, and increased electromigration (EM) effects, it is expected to continue to be used for the next several technology nodes [2]. The critical layers are those closest to the front-end-of-line (FEOL) transistor, as they have the smallest cross sectional area and their size is determined only by the physical capabilities of the fabrication process, shown in Fig. 1.

It was found that, as the Cu thickness is reduced, the average crystal grain size decreases almost linearly for a wide range of processing conditions [4], [5]. The decreased grain size, combined with the overall reduction in metal thickness, means that GBs and MIs play an increasingly important role in determining the film behavior. The influence of these properties on electron scattering, and thus on conductivity, has been explored many decades ago by Fuchs [6] and Mayadas and Schatzkes [7]. In addition to the changes in its conductive behavior, the reliability of nanometer sized copper films is significantly influenced by their microstructure. EM degradation is the primary form of failure in metal films, which occurs due to the transport and accumulation of vacancies, which nucleate to form a void. Under a high current density, this void grows to increase the line resistance and ultimately to cause an open circuit failure [8].

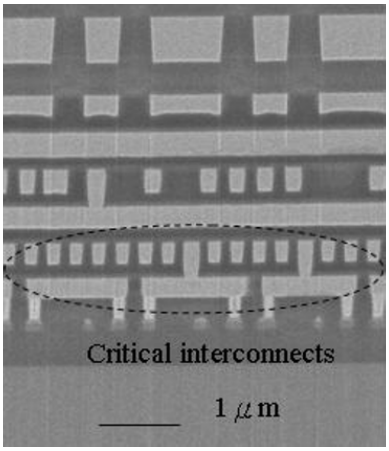

Fig. 1. TEM of multilayer copper interconnects, with the EM-critical layers circled. Reprinted by permission from Springer Nature: C.-J. Weng, 2011 [3].

While attempts are underway to replace the critical Cu interconnects (e.g., middle-of-line, M1 level, and tight-pitch level metalization) with EM-resistant alternatives, such as cobalt or carbon nanotubes [9], [10], the accepted reality is that we will have to live with copper for the forseeable future, at least down to the 5nm node [2]. Therefore, it must be ensured that EM is properly modeled in order to be able to appropriately estimate interconnect lifetimes. In this review a framework developed to accelerate EM simulations of grained copper interconnect lines is presented.

II. Physics of Electromigration

The physics of EM phenomena is described in great detail in, e.g., the work of Ceric and Selberherr [11]. There are two driving forces for EM, the *direct force* $\vec{F}_{direct}$, initiated by the direct action of the external field on the charge of the migrating ion, and the *wind force* $\vec{F}_{wind}$, arising due to the scattering of the conduction electrons by impurities or point defects. The total force $\vec{F}$ is given by the sum of the two forces

$$\vec{F} = \vec{F}_{direct} + \vec{F}_{wind} = (Z_{direct} + Z_{wind})\, e\, \vec{E} = Z^*\, e\, \vec{E}, \qquad (1)$$

where Z^* is the effective valence of the defect and is the sum of the direct (Z_{direct}) and wind (Z_{wind}) valences, e

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is the elementary charge, and $\vec{E}$ is the electric field. In free-electron-like metals (e.g., Cu) $\vec{F}_{wind}$ is dominant. To experimentally determine EM failure on a new technology, the failure behavior of all materials making up the interconnect must be characterized. This is commonly performed under accelerated conditions (i.e., high temperature and high current) to find the mean time to failure (MTTF) which is then extracted to operating conditions using a log-normal plot following Black's equation [12]. It should be noted that simulations, just like measurements, are carried out using the same accelerated conditions in order to as closely as possible match the experimental conditions.

A. Vacancy Dynamics

The main driver of EM is the accumulation of vacancies which then form a void. The diffusion of vacancies through a material D_v is determined by

$$D_v = D_{v0} \exp\left(\frac{\Omega\,\sigma - E_a}{k_B\,T}\right), \tag{2}$$

where D_{v0} is a pre-exponential constant, E_a is the activation energy, Ω is the atomic volume, T is temperature, k_B is Boltzmann's constant, and σ is the hydrostatic stress. The vacancy diffusion determines its flux $\vec{J}_v$ using

$$\vec{J}_v = -D_v\,(\sigma)\left[\nabla C_v + \frac{C_v}{k_B\,T}\left(e\,Z^*\,\rho\,\vec{j} - \frac{Q^*}{k_B\,T}\nabla T + f\,\Omega\,\nabla\sigma\right)\right], \tag{3}$$

where C_v is the vacancy concentration, ρ is the resistivity, $\vec{j}$ is the current density, Q^* is the heat of transport, and f is the vacancy relaxation ration. The subsequent accumulation and depletion of vacancies is found using the continuity equation

$$\frac{\partial C_v}{\partial t} = -\nabla\cdot\vec{J}_v + G, \tag{4}$$

where G is a surface function which models vacancy generation and annihilation. Furthermore, from Eq. (3) it is clear that the resistivity ρ plays a significant role in determining the vacancy flux and thereby in the overall EM behavior. The discussion thus far describes the EM process in a bulk material, which can be modeled assuming a continuum in the material properties. However, granularity can modify this view significantly, as discussed in the next section.

B. Effect of Granularity on Electromigration

1) Granularity and Resistivity: The resistivity (or conductivity) is one of the key material properties which influences the EM behavior of metal films. A high current density and a high electron wind frequently lead to diffusion of metal atoms in the direction of electron motion under $\vec{F}_{wind}$. To include granularity for modeling a film's resistivity, three main components must be included:

- The intrinsic resistivity of the bulk material, limited only by the electron mean free path (MFP);
- The increase in resistivity due to surface scattering off MIs;
- The increase in resistivity due to GB scattering.

With each new technology node, the resistivity of copper interconnects has steadily increased. This is expected to continue into future nodes, primarily due to the minimum half-pitch of the copper lines. TSMC and Intel are planning a minimum copper half-pitch of 20nm and 16nm, respectively at the 7nm node [5]. At these thicknesses, the expected copper resistivity is about $15\mu\Omega\,cm$, almost an order of magnitude more than the bulk value of $1.68\mu\Omega\,cm$. Therefore, to include the influence of granularity, a continuum equation was derived by Clarke et al. based on the works of Fuchs, Mayadas, and Schatzkes [13], namely

$$\frac{\rho_f}{\rho_i} = 1 + \frac{3\,\lambda}{4\,w}(1-p) + \frac{3\,\lambda}{2\,D}\left(\frac{R}{1-R}\right), \tag{5}$$

where ρ_i is the bulk resistivity, λ is the electron MFP, w is the metal width, p is the probability of electron scattering from a material interface, D is the average grain diameter, and R is the probability of electron scattering from a GB. This equation provides a continuum model with adapted parameters based on granularity. However, in order to model the local effects of granularity (GBs and MIs) on copper's resistivity, a spatial representation is needed, where the resistivity is a function of the electron's distance from a potential scattering event (assuming only GB and MI scattering). This has recently been implemented by using the distance from a GB or MI d_b as a parameter for the local resistivity ρ_l with the equation

$$\rho_l = \rho\left(1 + \frac{3\,\lambda}{8\,d_b}\right). \tag{6}$$

2) Granularity and Electromigration: In addition to the resistivity, the diffusion of vacancies D_v is different between atoms located in the GB, MI, or in the grain bulk. From Eq. (2) both D_{v0} and E_a depend on the atom's location in the granular structure for copper according to Table I. Of note is that the atomic diffusivity in MIs is three orders of magnitude larger than the bulk value, which explains why MIs play such an increasing role in EM phenomena for nanometer sized interconnects. Therefore it is essential that these parameters are treated as spatial parameters in EM simulations.

TABLE I
GRANULARITY-DEPENDENT PARAMETERS FOR VACANCY DYNAMICS [8].

Vacancy diffusion parameter	Grain	GB	MI
Pre-exponential factor (D_{v0}) cm^2/s	0.52	52	520
Activation energy (E_a) eV	0.89	0.7	0.5

Another aspect of EM, which is ignored in continuum models, is that the generation and annihilation of vacancies G, according to Eq. (4) only takes place inside the GBs and MIs. The equation which governs this process is given by

$$G = \frac{\partial C_{v,T}}{\partial t} = \frac{\chi}{\tau}\left[C_{v,eq} - C_{v,T}\left(1 + \frac{\omega_R}{\omega_T\,C_v}\right)\right], \tag{7}$$

where $C_{v,T}$ and $C_{v,eq}$ are the trapped and equilibrium vacancy concentrations, respectively, τ is the relaxation time, and ω_R and ω_T are the vacancy release and trapping rates, respectively. In Eq. (7) χ is introduced, which is a spatial parameter assigned a value of 1 in the GB and MI, and 0 otherwise. Therefore, a total of four spatial parameters are used to

sufficiently include granularity in EM models, those being ρ_l, D_{v0}, E_a, and χ. A simulation framework designed to implement this model is described in the next section.

III. Electromigration Modeling Framework

Our framework relies on three components, namely Voronoi tessellation to generate the grained interconnect line, the assignment of the relevant granularity-dependent parameters discussed in the previous section, and the solution of the EM problem to find the vacancy accumulation and EM-induced stress, as visualized in Fig. 2.

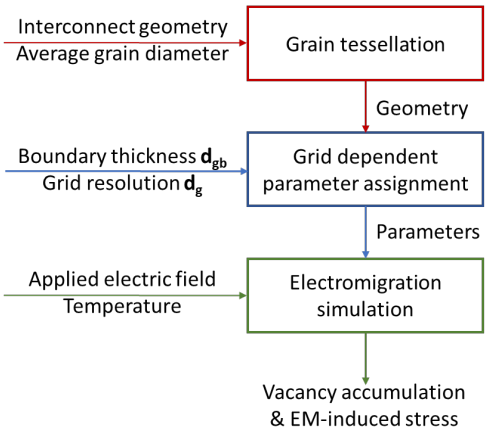

Fig. 2. Three phases of the modeling framework to properly simulate electromigration in copper nano-interconnects taking grain boundaries and material interfaces into consideration.

A. Tessellation

The stochastic polycrystalline copper line is generated using a Voronoi tessellation. Assuming spherical grains and knowing the average grain size, the total number of grains which fit into the volume is found. For each grain a seed point is placed at a random location inside the metal line, which then grows isotropically, until the entire volume is filled. When grains hit each other, they merge to form a GB. The Neper tessellation tool can be used to generate the required tesselated structures, which allows for the generation of a Vonoroi tessellation with ideal copper orientations of $(1\,1\,2)\,[1\,1\,\bar{1}]$ and $(\bar{1}\,1\,2)\,[1\,\bar{1}\,1]$ [14].

B. Spatial Parameter Assignment

The assignment of spatial parameters (ρ_l, D_{v0}, E_a, and χ) on a Cartesian grid with spacing d_g ensures that the GB and MI locations are explicitly defined and that the EM framework properly treats the granular nature of the interconnect line. Linear interpolation is used in the EM model in order to populate the entire material domain between the defined points. This proceeds according to the flow chart in Fig. 3. A boundary thickness of 1nm was assumed here as this was found to be appropriate from previous publications [15].

A test geometry with dimension 20nm×2000nm and a grain diameter of 25nm was used to test the given framework. The results of the spatial parameter assignment for the conductivity,

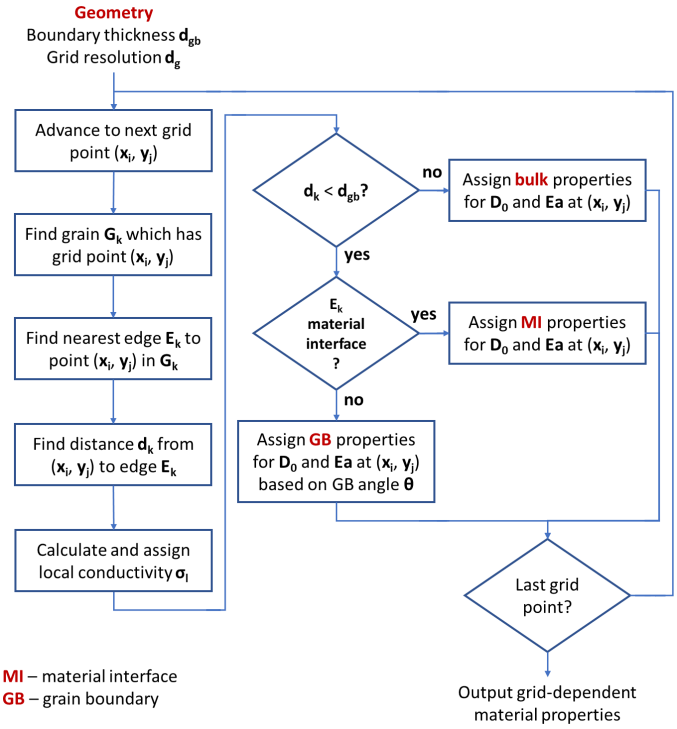

Fig. 3. Flow chart for the process of assigning the necessary material parameters to each grid point in the simulation space.

diffusivity, and step function χ on one section of the structure are shown in Fig. 4. The GBs' and MIs' impact is evident for all parameters which are subsequently passed to the EM simulation using the finite element method (FEM).

C. Electromigration Simulation

The simulation of EM physics is described in Section II. It requires the solution of three physical phenomena simultaneously, including the solution of the electro-thermal problem (current density, self-heating, and temperature), the vacancy dynamics problem, and the solid mechanics problem (EM-induced strain and stress). Ultimately, the EM-induced stress is desired, as shown in a sample in Fig. 5. Therein, the influence of the GBs and MIs on EM is evident. Notably, the framework is able to reproduce the stress generation at triple points σ_{TP} (where a GB intersects a MI), shown in the circled regions in Fig. 5. With the presented method, this stress can be accurately modeled, even with very coarse meshes. In fact, when the FEM mesh for EM simulations was varied from 0.4nm to 2nm (25x speedup in 2D), the variation was under 5% (the parameter grid d_g was set to 0.1nm).

The proposed framework allows for a very quick and efficient estimation of EM phenomena while taking the film's granularity into consideration. In Fig. 6 the simulation time is plotted against the chosen grid spacing, when the FEM grid is varied. The spatial parameter grid d_g is either set to 0.1nm (■) or is varied together with the FEM grid (●). A drastic reduction in the simulation time can be achieved by increasing the coarseness of the mesh with little loss of accuracy.

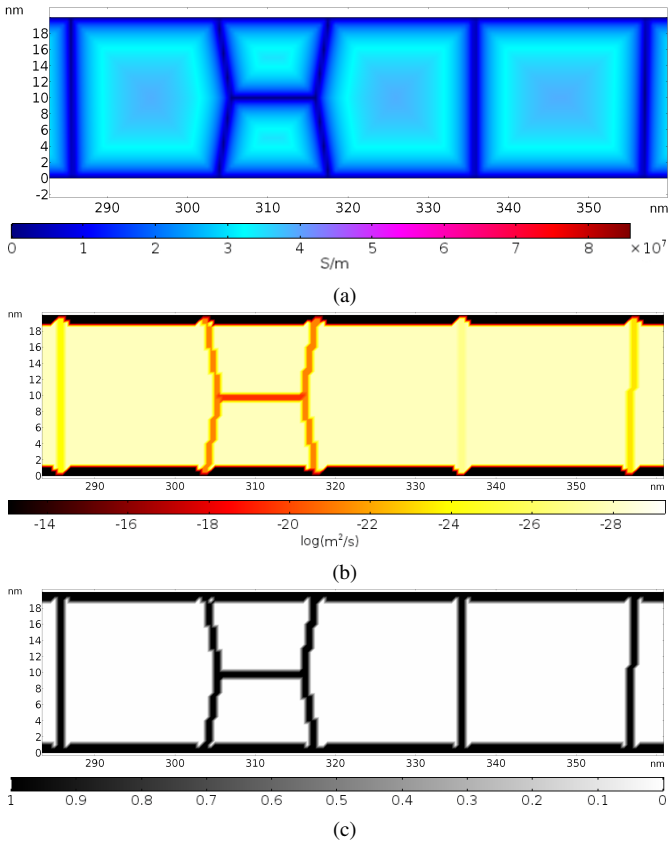

Fig. 4. Spatial parameters assigned to a section of the test structure, (a) the local conductivity under accelerated conditions (T=300°C) from Eq. (3), (b) logarithm of the vacancy diffusivity D_v from Eq. (3), and (c) the step function χ used for vacancy generation and annihilation from Eq. (7).

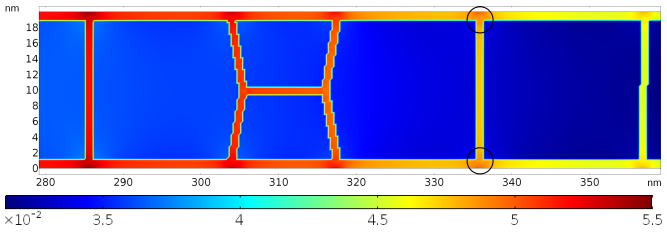

Fig. 5. EM-induced hydrostatic stress (MN/m^2) at t=200s. The average grain diameter is 25nm, the applied current density is 1MA/cm^2, and the applied temperature is 300°C. Circled regions show the stress at triple points $\sigma_{\mathbf{TP}}$.

IV. Conclusion

Continuum EM models frequently underestimate the time at which EM effects initiate, due to their inability to properly take into account the granularity of nanometer sized interconnects. The effects of granularity (GBs and MIs) have been known to exacerbate the EM phenomena, which is why therefore, it is essential that they are properly treated. Here, a sophisticated modeling framework is described, which considers granularity by applying spatial material parameters (ρ_l, D_{v0}, E_a, and χ) in EM simulation to identify the locations of the GBs and MIs. The framework allows to model EM-induced stress at triple points even when a very coarse mesh is used to accelerate the simulation time.

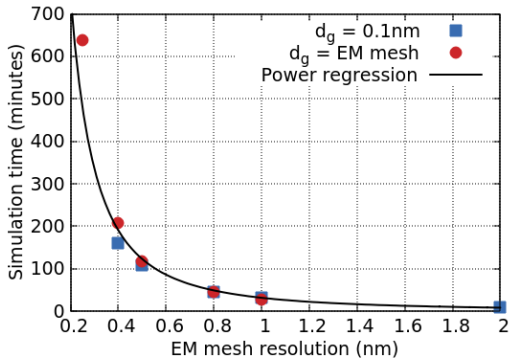

Fig. 6. The dependence of the mesh resolution on the simulation time for the EM simulations, when the FEM grid is varied, while the spatial parameter grid d_g is either set to 0.1nm (■) or is varied together with the FEM grid (●).

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