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 copper 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].

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 foreseeable 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 $\vec{F}_{\text{direct}}$, initiated by the direct action of the external field on the charge of the migrating ion, and the wind force $\vec{F}_{\text{wind}}$, 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

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

where $Z^*$ is the effective valence of the defect and is the sum of the direct ($Z_{\text{direct}}$) and wind ($Z_{\text{wind}}$) valences, $\epsilon$
The increase in resistivity due to surface scattering off MIs; 
• 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 15µΩ cm, almost an order of magnitude more than the bulk value of 1.68µΩ 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

\[
\rho_f = \frac{3\lambda}{4w(1-p)} + \frac{3\lambda}{2D} \frac{R}{(1-R)},
\]

where \(\rho_t\) is the bulk resistivity, \(\lambda\) 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 \(\rho_l\) with the equation

\[
\rho_l = \rho \left(1 + \frac{3\lambda}{8\mu_d} \right),
\]

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>
<thead>
<tr>
<th>TABLE I</th>
<th>GRANULARITY-DEPENDENT PARAMETERS FOR VACANCY DYNAMICS [8].</th>
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<tbody>
<tr>
<td>Vacancy diffusion parameter</td>
<td>Grain</td>
</tr>
<tr>
<td>Pre-exponential factor ((D_{v0})) cm(^2)/s</td>
<td>0.52</td>
</tr>
<tr>
<td>Activation energy ((E_a)) eV</td>
<td>0.89</td>
</tr>
</tbody>
</table>

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

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

where \(C_{v,T}\) and \(C_{v,eq}\) are the trapped and equilibrium vacancy concentrations, respectively, \(\tau\) is the relaxation time, and \(\omega_R\) and \(\omega_T\) are the vacancy release and trapping rates, respectively. In Eq. (7) \(\chi\) 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 \( \rho_l, D_{v0}, E_a, \) and \( \chi \). 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 granied 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.

- **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 tessellated structures, which allows for the generation of a Voronoi tessellation with ideal copper orientations of \((1\ 1\ 2)\ [1\ 1\ 1]\) and \((\bar{1}\ 1\ 2)\ [\bar{1}\ 1\ 1]\) [14].

- **B. Spatial Parameter Assignment**
  The assignment of spatial parameters \( \rho_l, D_{v0}, E_a, \) and \( \chi \) 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 \( 20\text{nm} \times 2000\text{nm} \) and a grain diameter of 25nm was used to test the given framework. The results of the spatial parameter assignment for the conductivity, diffusivity, and step function \( \chi \) 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 \( \sigma_{TP} \) (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 (\( \square \)) or is varied together with the FEM grid (\( \bullet \)). A drastic reduction in the simulation time can be achieved by increasing the coarseness of the mesh with little loss of accuracy.
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 ($\rho$, $D_v$, $E_a$, and $\chi$) 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.

REFERENCES