EM-INDUCED DEGRADATIONS IN DUAL-INLAID COPPER INTERCONNECTS

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1. Introduction

Electromigration (EM), i.e., electric current-induced transport of atoms in metals, becomes the main cause violating reliability of integrated circuit interconnects as the sizes of features go below 65 nm. Transfer of metal atoms from the cathode to the anode of the interconnect line is accompanied by the stress evolution: a tensile hydrostatic stress originates in the cathode region, resulting in the void formation, while a compressive stress near the anode creates hillocks and extrusions. Detailed study of EM is required for elaboration of design rules which can provide long-term chip reliability.

An important problem for the dual-inlaid copper interconnects is the effect of the copper microstructure on EM resistance. The texture of the metal can affect this process through dependence of grain boundary (GB) diffusivity on misorientation angles. Besides, the orientation dependence of the elastic constants is also extremely important for stress evolution.

The aim of this paper is to present a novel physical model of EM-induced stress evolution that accounts for vacancy migration and atoms plating on interfaces and GBs, and to describe the consequent void formation and development. The effect of the copper microstructure is studied both in voidless and void migration regimes.

2. Theoretical model

Two-step modeling is used for the interconnect degradation simulations: the first step describes the stress evolution in the voidless regime and determines possible void nucleation sites, while in the second step the growth and motion of nucleated voids are simulated.

A vacancy mechanism for the mass transfer was assumed in the simulations. The redistribution of the vacancy concentration N under the action of electromigration forces is balanced by the backflow caused by the $\nabla\sigma_{Hyd}$ hydrostatic stress gradient evolution, as well as by the self-diffusion of vacancies. This process is described by the continuity equation that accounts for a possible generation-recombination of vacancies:

$$\frac{\partial N}{\partial t} + \vec{\nabla}\left(-D\vec{\nabla}N - \frac{DN}{kT}\left(\Omega\vec{\nabla}\sigma_{Hyd} + eZ\vec{\nabla}V\right)\right) + G = 0 . \qquad (1)$$

Here Ω is the atomic volume, e is the electron charge, *eZ* is the effective charge of the migrating atoms, *V* is the local electrical potential, *k* is Boltzmann's constant, and *T* is the absolute temperature. The deviation of the vacancy concentration from its equilibrium value $N_e = N_i \exp\left(\Omega\sigma_{Hyd}/kT\right)$ (here N_i is the concentration in the absence of stress) is accompanied by vacancies generation or annihilation at GBs or interfaces during a time τ : a process that is described by the term $G = \left(N - N_e\right)/\tau$.

The generation-annihilation of vacancies is accompanied by the variation of concentration M of atoms plated on interfaces and GBs:

$$\frac{\partial M}{\partial t} = G . \tag{2}$$

The difference in atom and vacancy volumes, characterized by the parameter $f = \Omega_v/\Omega$, results in the strain ε_{ij} which generates in encapsulated copper line both hydrostatic and shear stresses through interaction with the confinement. The strain tensor ε_{ij} includes the elastic component ε_{ij}^{el} and inelastic volume deformation due to change in the concentration of vacancies and plated atoms ε_{ij}^{inel} [1]:

$$\begin{aligned} \varepsilon_{ij} &= \varepsilon_{ij}^{el} + \varepsilon_{ij}^{inel} , \\ \varepsilon_{ij}^{inel} &= \frac{\Omega}{3}\left(-\left(1-f\right)\Delta N + \Delta M\right)\delta_{ij} . \end{aligned} \tag{3}$$

The generated stress is related to the elastic deformation by the stiffness matrix $\{C_{ij,kl}\}$:

$$\sigma_{kl} = C_{ij,kl}\varepsilon_{ij}^{el} , \tag{4}$$

and for the hydrostatic stress we have

$$\sigma_{Hyd} = C_{ij,kk}\left[\varepsilon_{ij} + \frac{\Omega}{3}\left(\left(1-f\right)\Delta N - \Delta M\right)\delta_{ij}\right]. \tag{5}$$

The copper is a well-studied fcc metal having the elastic constants $C_{11} = 168\times10^9$ Pa, $C_{12} = 121\times10^9$ Pa, $C_{44} = 75\times10^9$ Pa. We are especially interested in the elastic anisotropy of copper; the ratio of the shear modulus $\mu = C_{44}$ (for the (100) shear) and the shear modulus $\mu' = \left(C_{11} - C_{12}\right)/2$ (for the (110) shear) is $\mu/\mu' \approx 3$. Therefore, we have modeled a polycrystalline line with anisotropic elastic grains described by the stiffness matrix $\{C_{ij,kl}\}$.

We prescribed the above values of elastic constants to a grain oriented along the line (i.e., the crystallographic planes are parallel to the line facets). The transformation of the elasticity matrix due to the rotation of the grain is given by the expression $C'_{ij,kl} = T_{ig}T_{jh}C_{gh,mn}T_{km}T_{nl}$. Describing the disorientations of the grains relative to the line by Euler's angles (ϕ,θ,κ), we present the matrix T as the product of three matrices: $T = A_z(\phi)A_x(\theta)A_z(\kappa)$, where $A_i(x)$ are the rotation matrices.

Combining Eqs. (3) and (4) with the equilibrium condition

$$\frac{\partial \sigma_{kl}}{\partial x_k} = 0, \tag{6}$$

one can obtain the distribution of the stresses, using the finite-element method (FEM) modeling.

The incoming flux of vacancies, which is proportional to the positive hydrostatic stress outward the void: $J_{incom} = -M_s \nabla \sigma_{Hyd}$ (the parameter Ms describes the overcoming probability of the void surface by a vacancy), results in the void growth. On the other hand, the atomic flux along the void surface leads to the void migration in the direction opposite to the electric current. The resulting normal velocity of the void surface is expressed in the form [2]

$$v_n = \Omega \left(J_{incom} + \frac{\partial J_{surf}}{\partial s} \right). \tag{7}$$

Here the surface flux is driven by the EM and capillary forces

$$J_{surf} = \frac{D_s}{kT} \frac{\partial}{\partial s} \left(\Omega g K + eZV \right), \tag{8}$$

where K is the void surface curvature, g is the surface energy, D_s is the diffusivity of atoms on surface, and s is the curvilinear coordinate along the surface.

3. Simulation results

The Comsol Multiphysics FEM code was used for simulations of stress evolution and voiding dynamics. Considered system represents a dual-damascene M1-M2-M1 copper structure encapsulated by the tantalum liner from the bottom and both sides and by the silicon carbide from the top (Fig. 1). The bamboo-like microstructure is assumed for the copper line, with the crystallographic orientations (111), (110), and (100). The interfaces and GBs are characterized by fast diffusivities of the vacancies: $D_{Cu\text{-}SiC}=10^4 D_{Cu}$, $D_{Cu\text{-}Ta}=10^2 D_{Cu}$, $DGB=10^3 D_{Cu}$, where D_{Cu} is the vacancy diffusivity in the bulk.

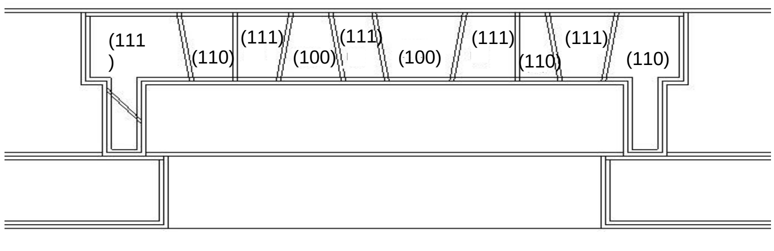
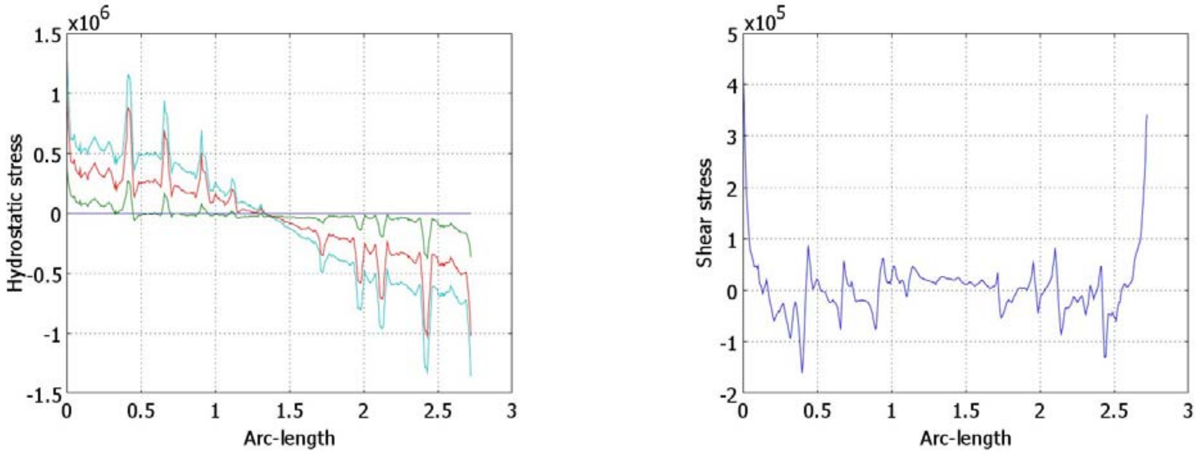


Fig. 1. Simulated structure and grain orientations in the studied M2 line.

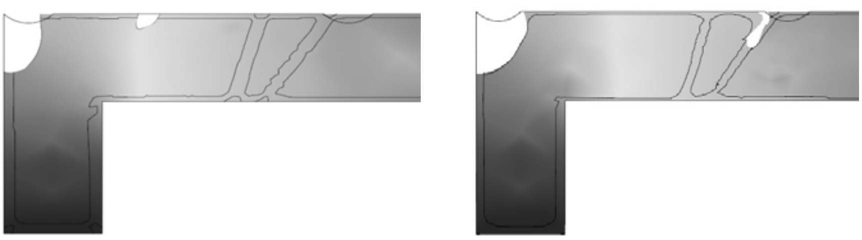
The hydrostatic stress evolution is shown in Fig. 2a. Since the electrical current-induced mass flow is tried to be balanced by the atoms backflow due to hydrostatic stress gradient, the linear stress distribution is established ultimately in the line. This is the prediction of the classic EM theory; it should be noted, however, that our model describes the transition from initial exponential stress distribution to linear distribution at arbitrary geometry of the test structure due to proper account of atoms plating effect. There are also some stress differences in the grains due to their crystallographic orientation. Sharp peaks in the hydrostatic stress are observed at intersections of grain boundaries with the interface.

If the generated stresses cause the copper delamination or cracking of the inter-level dielectric in any site, a flaw originates that will serve as a sink for vacancies. These fracture processes require a significant component of the shear stress. Fig. 3b demonstrates the shear stress distribution under the top interface, which is usually subjected to voiding. This stress has high values near edges; besides, peaks appear at GBs due to large differences in the elastic constants of neighboring anisotropic grains. It can be assumed that nucleation of a void can take place if the shear stress (in the tensile hydrostatic stress region) exceeds some critical value. This model of void nucleation has been validated by simulating the copper lines with real grain structure and comparison with the experiment.



a) b)

Fig. 2. Distributions of a) hydrostatic stress and b) shear stress under the top interface.



a) b)

Fig. 3. Migration and growth of voids in the case when the dominating mechanism of atomic transport is the diffusion a) along the top interface, and b) along grain boundaries. Only the near-cathode region of the structure is presented.

Having determined the void nucleation sites, we can proceed by describing the voiding dynamics, using relations (7) and (8). The results of voiding dynamics FEM simulations, performed using the arbitrary

Lagrange-Euler (i.e., mesh deformation) technique, are presented in Fig. 3. If the diffusion along the top interface prevails ($D_{int} >> D_{GB}$), the voids nucleated at delamination sites (depicted on the figures by the semispherical cutouts in the copper line) and moving toward the cathode are not affected by the grain boundaries (Fig. 3a). In the opposite limit $D_{int} << D_{GB}$ the grain boundaries provide an outflow for the void surface fluxes, so that the void propagates preferentially along the grain boundary and can be transformed into a slit (Fig. 3b). In the intermediate case $D_{int} \geq D_{GB}$ the grain boundary can pin the moving void. In all the cases the void nucleated at the line edge grows preferentially toward the bottom of the via. These results coincide well with the experimental data obtained by SEM study of the similar structures [3].

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