The Effect of Microstructure on Electromigration Induced Voids

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***Abstract*- We present the application of a state of the art electromigration model on a dual damascene interconnect with typical copper microstructure. The influence of the microstructure on the formation and development of an electromigration induced void is studied by simulation and the results are compared with experiments. A close investigation has shown that the network of grain boundaries has a decisive impact on the formation of void nucleation sites and void development.**

I. INTRODUCTION

Contemporary integrated circuits are often designed using simple and conservative design rules to ensure that the resulting circuits meet reliability goals. This precaution leads to reduced performance for a given circuit and metallization technology. An ultimative hope of integrated circuits designers today is to have a computer program at hand, which predicts the behavior of thin film metalizations under any imaginable condition. Due to intensive development in the last decade, physical models of electromigration have reached a level of maturity which enables predictions of failure behavior. The cause of failure is always an electromigration induced void in the interconnect structure. We present our recent development in modeling of void nucleation and void evolution.

A new model for grain boundary physics is applied as extension and refinement of the standard electromigration continuum model. The model differentiates between mobile and immobile vacancies. Immobile vacancies are captured at grain boundaries and triple points, causing a build-up of tensile stress.

High tensile stress leads to nucleation of intrinsic voids. These voids evolve through the interconnect causing a resistance change and, occasionally, a complete failure.

Different approaches have been applied to model evolving void surfaces in the last ten years. However, all of these models lack an appropriate description of the void development process, neglecting relevant physical phenomena that lead to interconnect failure. Moreover, these models are only suitable for simulations of simple two-dimensional interconnects and cannot realistically describe the void evolution mechanisms in modern complex interconnect structures.

In this paper a three-dimensional Level Set module is applied to simulate the evolving void surface. The site of void nucleation and the morphology of the evolving void accurately reproduce experimental observations.

II. MODELING OF GRAIN BOUNDARIES

The diffusion of point defects inside the grain boundary is faster compared to grain bulk diffusion due to the fact [1] that a grain boundary generally exhibits a larger diversity of point defect migration mechanisms.

Moreover, formation energies and migration barriers of point defects are in average lower than those for lattice.

In 1951, Fisher published his nowadays classic paper [2] presenting the first theoretical model of grain boundary diffusion. That pioneering paper, together with concurrent measurements by Turnbull and Hoffman [3], initiated quantitative studies of grain boundary diffusion in solids. The fact that grain boundaries in metals provide high-diffusivity paths was known already in the 1930s, mostly from indirect and qualitative experiments. For example, the enhanced rates of sintering, creep, discontinuous precipitation, and other processes and reactions in polycrystalline samples were attributed to an accelerated atomic transport along grain boundaries.

The grain boundary model used in this work is designed as an extension of continuum electromigration model [4,5]. The grain boundary is treated as a separate medium with the capability of absorbing and releasing vacancies (Fig.1). Vacancies are trapped from both neighboring grains with the trapping rate ω_T and released to these grains with a release rate ω_R.

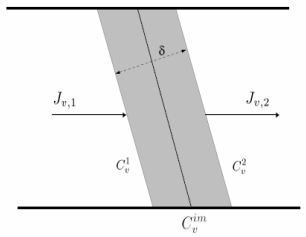

Fig. 1. The fluxes $J_{v,1}$ and $J_{v,2}$ change the concentration of mobile and immobile vacancies.

The vacancy concentration from both sides of the grain boundary is denoted as $C_{v,1}$ and $C_{v,2}$. Correspondingly, fluxes are calculated as

$$J_{v,1} = \omega_T (C_v^{eq} - C_v^{im}) C_{v,1} - \omega_R C_v^{im}, \quad (1)$$

$$-J_{v,2} = \omega_T (C_v^{eq} - C_v^{im}) C_{v,2} - \omega_R C_v^{im}. \quad (2)$$

The vacancies are captured at the grain boundary and converted into immobile vacancies (C_v^{im}). This is mathematically expressed as

$$\frac{\partial C_v^{im}}{\partial t} = \frac{J_{v,1} - J_{v,2}}{\delta} = -\left(\frac{\partial C_{v,1}}{\partial t} + \frac{\partial C_{v,2}}{\partial t}\right), \quad (3)$$

where δ is the grain boundary thickness. By combining equations (1),(2), and (3) with the vacancy balance equation, the following equation is obtained

$$\frac{\partial C_{v,\alpha}}{\partial t} = -\mathrm{div}\vec{J}_{v,\alpha} + \frac{1}{\tau}\left(C_v^{eq} - C_v^{im}\left(1 + \frac{2\,\omega_R}{\omega_T (C_{v,l} + C_{v,r})}\right)\right), \quad (4)$$

$\alpha = l$ and $\alpha = r$ indicate the left and the right side of the grain boundary, respectively. $\vec{J}_{v,\alpha}$ is the vacancy transport driven by electromigration and a stress gradient. τ is expressed by

$$\frac{1}{\tau} = \frac{\omega_T (C_{v,1} + C_{v,2})}{\delta}. \quad (5)$$

The capacity of the grain boundary to accept trapped vacancies is expressed by the stress-dependent equilibrium concentration [4]

$$C_v^{eq} = C_v^0 \exp\left(\frac{\sigma_m \Omega}{k_B T}\right), \quad \sigma_m = \vec{n}\cdot\sigma\cdot\vec{n}, \quad (6)$$

where we assume a unique equilibrium vacancy concentration C_v^0 in stress free copper, both, in grain bulks and boundaries. $\vec{n}$ is the normal to the grain surface.

III. VOID EVOLUTION

When a sufficiently high stress level is reached at some interfacial spot, where a flaw can be assumed, the failure development enters the next phase and a different modeling method must be applied. Here, we have an evolving void surface shaped by two dynamic forces: the chemical potential gradient and the electron wind.

The development of fatal voids, i.e. voids which lead to a significant resistance increase, or even completely sever the line, which is the ultimate cause for the electromigration induced interconnect failure [6]. Therefore, the understanding and prediction of electromigration failure behaviour can only be achieved through a detailed study of the void evolution mechanisms.

Including both contributions, electromigration and chemical potential-driven surface diffusion, gives the total surface vacancy flux $\vec{J}_s = J_s \vec{t}$, where $\vec{t}$ is the unit vector tangential to the void surface [7]

$$\vec{J}_s = -D_s\left(eZ^* E_s + \Omega \nabla_s\left(\frac{\sigma:\varepsilon}{2} - \gamma_s \kappa\right)\right). \quad (7)$$

$\vec{E}_s = E_s \cdot \vec{t}$ is the local component of the electric field tangential to the void surface, ∇_s is the surface gradient operator, $1/2(\sigma:\varepsilon)$ is the strain energy density of the material adjacent to the void surface, and κ is the curvature of the void surface. D_s is given by an Arrhenius law:

$$D_s = \frac{D_0\,\delta_s}{k_B T}\exp\left(-\frac{Q_s}{k_B T}\right). \quad (8)$$

δ_s is the thickness of the diffusion layer, Q_s is the activation energy for the surface diffusion, and D_0 is the pre-exponential coefficient for mass diffusion.

Numerical tracking of the surface is necessary, since it fully determines the failure dynamics. The shape of the void together with local geometry conditions cause changes in the interconnect resistance and the speed of the void growth. Thus, the migration direction is strongly influenced by the shape of a void. The three-dimensional algorithms for simulation of the void surface evolution are computationally very demanding, and currently no satisfactory solution exists.

Level Set is a powerful method for simulating moving boundary problems, where the moving boundary is implicitly represented by the level set of a given function. The time evolution of the level set is governed by a Hamilton-Jacobi equation. A velocity field, which accounts for the physical effects acting on the moving boundary, dictates the evolution of the level set. Several algorithms and strategies to implement the level set method have been proposed [8].

For the case of the void surface evolving under the influence of electromigration and the gradient of the surface energy the Hamilton-Jacobi equation for a level set function ϕ is

$$\frac{\partial \phi}{\partial t} - \alpha \nabla_s \cdot \left(eZ^* \vec{E}_s - \gamma \Omega \nabla \cdot \left(\frac{\nabla \phi}{|\nabla \phi|}\right)\right) = 0, \quad \alpha = \frac{D_v \delta}{k_B T}. \quad (8)$$

$\vec{E}_s$ is the component of the electric field tangential to the void surface and γ is the surface energy. The value of the surface diffusivity D_s is set according to the region, where the void surface lays.

This region can be bulk, grain boundary, or the interface to capping or barrier layers. The role of the surface diffusivity variation is a potential cause for a huge diversity of void shapes, which have been observed in experiments.

IV. SIMULATION RESULTS

The site of void nucleation and the morphology of the evolving void accurately reproduce experimental observations.

The simulation is started by assuming a grain boundary network (c.f. Fig..2) in the studied dual-damascene interconnect.

The vacancy release rate and vacancy trapping rate are chosen in such a way that during simulation the following conditions are fulfilled:

$$\frac{2\omega_R}{\omega_T(C_{v,1}+C_{v,2})} \ll 1, \tag{9}$$

and

$$1\text{s} < \tau = \frac{\delta}{\omega_T(C_{v,1}+C_{v,2})} < 2\text{s}. \tag{10}$$

With these conditions the model for immobile vacancies behaves analogously to a classical Rosenberg-Ohring term, which was already successfully applied in [9], where τ=1 s and τ=2 s was used.

All parameters for simulation are set according to experiments published in [9]. The line width is $0.18\ \mu m$, the applied current density is $1.5\ \text{MA/cm}^2$, and the temperature is $300\ ^\circ C$. Barrier and capping layer are Ta/TaN and SiCN, respectively. SiOC is used as interlayer dielectric. The continuum equations (4) are solved, until a stress threshold (σ_{th}) for void nucleation is reached at some triple point (c.f. Fig. 3).

At this triple point an initial, small spherical void is set and the Hamilton-Jacobi equation (8) is solved.

For stresses $\sigma < \sigma_{th}$ an energy barrier exists between the void embryo and a stable-growing void. If the stress is above the threshold value ($\sigma > \sigma_{th}$), the free energy monotonically decreases with void volume and the energy barrier vanishes.

If we now assume the adhesion free patch with a radius of 10 nm (about 20 atoms), we obtain $\sigma_{th} \approx 344$ MPa [4].

After the void is nucleated at the triple point (c.f. Fig.4), which is a natural free adhesion patch, it moves in electric current direction. The void encounters the second grain boundary and transforms its shape (c.f. Fig.5). During evolution the void remains attached to the copper/capping layer interface which is also a fast diffusivity path. The strength of adhesion between copper and SiCN determines the speed of the void evolution. By choosing other capping materials and corresponding technology processes which increase adhesion the speed of the void is reduced and the interconnect life time is increased.

In Fig. 5 it can be clearly seen that the presence of a grain boundary induces a void surface movement toward the inner part of interconnects. Here grain boundary acts as fast diffusivity path. This result is consistent with numerous experimental observations and explains the fact that bamboo microstructures are prone to failures caused by slit-like voids [9].

In the further development this shape change is increased leading to a high increase in interconnect resistance (c.f. Fig. 6). The results of simulation and experiments demonstrate a decisive impact of the microstructure on the failure development [9].

The experimental result presented in Fig. 7 clearly shows that the applied models together with the assumed microstructure reproduce the experimentally observed void dynamics.

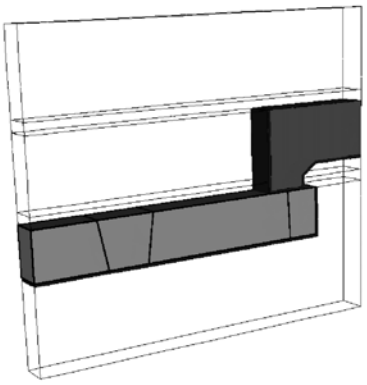

Fig. 2. Dual-damascene structure used for simulation.

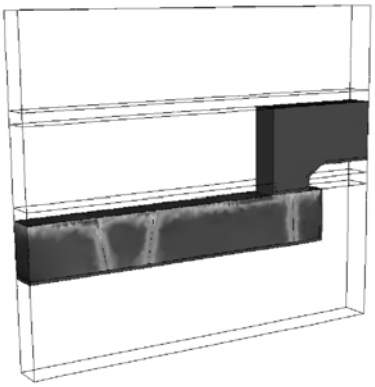

Fig. 3. Peak hydrostatic tensile stress distribution (light areas) caused by electromigration.

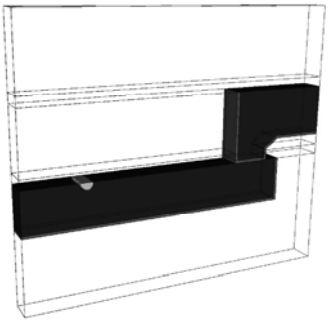

Fig. 4. Initial void placed at the nucleation site.

The distance between the grain boundaries and the angle between the grain boundaries and the copper/capping layer interfaces are crucial for void evolution. Triple points determine the void nucleation site and during the evolution the void is shaped by the grain boundaries it encounters.

In order to investigate the exact correlation between the microstructural properties and the void dynamics the statistical simulation using a large number of automatically generated microstructures is necessary.

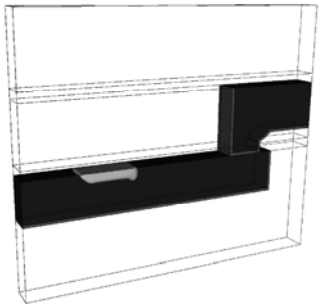

Fig. 5. The void moves and encounters the second grain boundary.

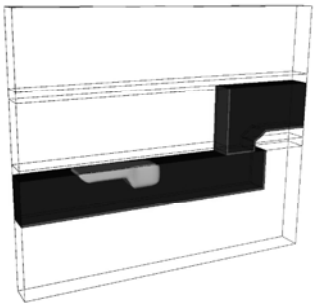

Fig. 6. The shape change is enhanced as the void drifts toward the via.

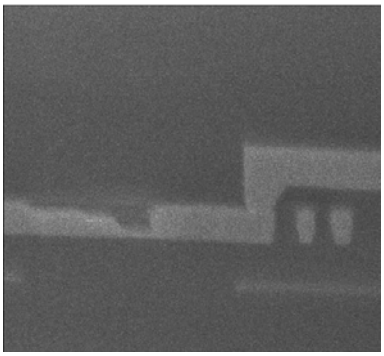

Fig. 7. FIB cross-section of an interconnect after an electromigration test [10] (courtesy of Dr. Lucile Arnaud).

IV. CONCLUSION

The ultimate cause of electromigration failure is an intrinsic void. In this work we study void nucleation and evolution for the case when the interconnect interface to the capping layer is the dominant material transport path and the void nucleation site is at the intersection of copper grain boundary and capping layer. A detailed, physically based grain boundary model is applied to model the void nucleation process. Void evolution is simulated using a three-dimensional level-set algorithm. The simulation results are successfully verified through comparison with experimental observations.

ACKNOWLEDGMENT

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