TCAD Solutions for Submicron Copper Interconnect

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Abstract- **The demanding task of assessing a long range interconnect reliability can only be achieved by combination of experimental and TCAD methods. A basis for TCAD tools is a sophisticated physical model which takes into account the microstructural characteristics of copper. In this work a general electromigration model is presented with a special focus on the influence of grain boundaries and mechanical stress. The possible calibration and usage scenarios of electromigration tools are discussed. The physical soundness of the model is proven by three-dimensional simulations of typical dual-damascene structures used in accelerated electromigration testing.**

I. INTRODUCTION

The main challenge in electromigration modeling and simulation is the diversity of the relevant physical phenomena.

Electromigration induced material transport is also accompanied by material transport driven by the gradients of material concentration, mechanical stress, and temperature distribution. A comprehensive, physics based analysis of electromigration for modern copper interconnect lines serves as the basis for deriving sophisticated design rules which will ensure higher steadfastness of interconnects against electromigration.

An ultimate hope of integrated circuit designers today is to have a computer program at hand which predicts the behavior of thin film metallization under any imaginable condition. 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.

Relaying of previous work we present our model which reveals an improvement in two mayor points. Firstly a complete integration of mechanical stress phenomena in the connection with microstructural aspects in the classical multi-driving force continuum model was performed, and, secondly, a new finite element based scheme enabling an efficient numerical solution of the three-dimensional formulation of the problem was developed. The satisfying assessment of electromigration reliability can only be achieved through combination of experimental methods and utilization of TCAD tools. Therefore, we also discuss a possible usage scenario of TCAD tools in connection with results of accelerated interconnect tests.

Competitive reliability targets of chip failure rates have been in the order of one per thousand throughout the anticipated life time in the field. The central problem of the interconnect design for reliability is the determination of the long term interconnect behavior.

The TCAD analysis of the electromigration reliability of interconnect structures has to be carried out on at least two levels. The first level is without any doubt a physical one, that means application of most complete and comprehensive models to interconnect portions of moderate size. The restriction in size and complexity arises from the capacity of computers (memory, computational time) but has also a cause in numerical issues.

The first level analysis is based on the simulation of the behavior of characteristic portions of the interconnect, which, known from experiments, represent a high electromigration risk. The goal of the analysis by simulation is to determine the time-to-failure distribution for this specific interconnect part. The second level analysis combines the results of the first level in order to assess electromigration reliability of an entire chip.

II. PHYSICALLY BASED MODELING

Preceding the consideration of the electromigration model equation an electro-thermal problem has to be solved with the goal to obtain an accurate temperature distribution.

All diffusivities in the electromigration model are thermally activated and even a small error in the temperature calculation can lead to a substantial error in the vacancy concentration and stress calculation.

The bulk vacancy transport is given by the following balance equation [1]:

$$\mathbf{J}_v = -\mathbf{D}\Big(\nabla C_v + \frac{Z^* e}{k_B T} C_v \nabla \varphi + \frac{f\Omega}{3 k_B T} C_v \nabla\, \mathrm{tr}(\bar{\bar{\sigma}})\Big), \quad \frac{\partial C_v}{\partial t} = -\mathrm{div}\mathbf{J}_v. \tag{1}$$

Here, $k_B T$ is the thermal energy, $Z^* e$ is the effective valence, Ω is the volume of atom, and f is the vacancy to atom volume ratio. **D** is the tensorial vacancy diffusivity which is in stress free state set as $D_{ij} = D_{bulk}\delta_{ij}$, where D_{bulk} is the isotropic bulk diffusivity.

Divergences of the vacancy flux produce local strain

$$\frac{\partial \varepsilon^v_{ij}}{\partial t} = \frac{1}{3}\Omega(1-f)\mathrm{div}\mathbf{J}_v \delta_{ij}, \tag{2}$$

which is equilibrated by induced displacements in the copper bulk $\vec{u} = (u_1, u_2, u_3)$ according to the Lamè-Navier equations,

$$\mu \Delta u_i + (\mu + \lambda)\frac{\partial}{\partial x_i}(\nabla \mathbf{u}) = B\frac{\partial \operatorname{tr}(\varepsilon^v)}{\partial x_i}, \quad i = 1,2,3 \tag{3}$$

Here λ and μ are the Lamè coefficients and $B = \lambda + 2\mu/3$. Generally, an elastic deformation of the metal is assumed:

$$\sigma_{ij} = \sum_{ijkl} \mathbf{C}_{kl}\varepsilon_{kl}, \tag{4}$$

with the small displacement approximation:

$$\varepsilon_{ij} = \frac{1}{2}\Big(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\Big), \quad i,j = 1,2,3. \tag{5}$$

Residual process stresses, thermo-mechanical stresses, and electromigration induced stresses cause anisotropy of material transport and therefore in (1) a tensorial diffusivity **D** must be taken into account.

In order to consider the microstructure of copper, the bulk model (1) is extended by fast diffusivity paths models, the most significant of which is the grain boundary model, since it describes also vacancy recombination.

Our modeling approach is based on models of Herring [2] and Fisher [3], which deal with grain boundary mechanics and grain bulk/boundary material exchange, respectively. To connect these models a careful analysis of the chemical potential in the vicinity of a grain boundary and in a grain boundary is necessary.

For the chemical potential in the grain boundary we use Herring's expression [2]:

$$\mu_v^{gb} = \mu_0 + \Omega\sigma_{nn} + k_B T \ln\Big(\frac{C_v^{gb}}{C_v^0}\Big), \tag{6}$$

where we assume a unique equilibrium vacancy concentration C_v^0 in stress free copper, both, in grain bulks and boundaries. μ_0 is some chemical reference potential, $\sigma_{nn} = \vec{n}\cdot\bar{\bar{\sigma}}\cdot\vec{n}$ and $\vec{n}$ is the normal to the grain surface.

The chemical potential of the vacancies in the bulk is given by [4]:

$$\mu_v = \mu_0 + k_B T \ln\Big(\frac{C_v}{C_v^0}\Big) + \frac{1}{3} f\Omega \operatorname{tr}(\bar{\bar{\sigma}}). \tag{7}$$

In the continuum modeling approach the grain boundary as a vacancy transport medium is defined by the chemical potential. This chemical potential is constant through the grain boundary thickness and equal to the bulk chemical potential on the interfaces to the bulk regions, eg. $\mu^1{}_v(-\delta/2) = \mu^1{}_v(+\delta/2) = \mu_{gb}$, Fig. 1. The vacancy fluxes on both sides of the grain boundary given by:

$$J_v^1 = \frac{D_v\, C_v}{k_B\, T}\nabla\mu_v^1,$$
$$J_v^2 = \frac{D_v\, C_v}{k_B\, T}\nabla\mu_v^2. \tag{8}$$

The difference $J_v^2 - J_v^2$ is an actual loss (gain) of vacancies which is localized at the thin slice which represents the grain boundary (in continuum modeling).

The recombination rate can now be approximated as:

$$G = \frac{\partial C_v}{\partial t} = -\operatorname{div} J_v \approx -\frac{J_v^2 - J_v^1}{\delta}. \tag{9}$$

In order to include the effect of the grain boundary as a vacancy sink (source) into the bulk vacancy transport model the recombination term G has to be included in equations (1) and (2):

$$\frac{\partial C_v}{\partial t} = -\operatorname{div}\mathbf{J}_v + G,$$
$$\frac{\partial \varepsilon_{ij}^v}{\partial t} = \frac{1}{3}\Omega((1-f)\operatorname{div}\mathbf{J}_v + fG)\delta_{ij}. \tag{10}$$

The full description of the atomic mechanisms of vacancy generation and annihilation in grain boundaries goes beyond the capability of continuum modeling and can only be obtained by molecular dynamics methods.

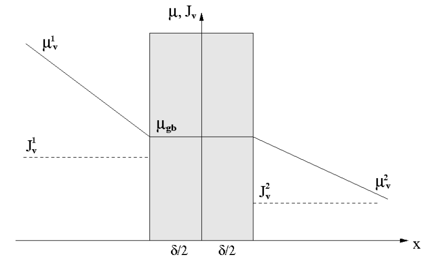

Fig. 1. The grain boundary according to Fisher's model and Herring's relationship.

III. USAGE SCENARIO FOR TCAD TOOLS

Simulation can be used for extrapolation of long time interconnect behavior on the basis of results of accelerated electromigration tests. This capability is clearly superior to an extrapolation by standard statistical methods which rely on Black's equation and extrapolate a time-to-failure (TTF) for a single interconnect structure. The usage of TCAD tools enables a prediction of the behavior for structures which are obtained by variation of geometrical properties and operating conditions of a previously used initial test structure.

The assumed scenario for application of an electromigration reliability TCAD tool is:

1. *Model Calibration:*
For this purpose we use one layout and many test units. At the end of calibration all parameters of the model are fixed.

During this process, different microstructures are considered and simulation parameters are varied with the goal to reproduce experimental failure time statistics, cf. Fig. 2.

2. *Model Application:*.
The calibrated model is used for simulation. The simulation extrapolates the behavior of the interconnect under real life conditions.

For a given interconnect layout and monocrystalline material, simulation will provide a unique time-to-failure. All impact factors, e.g. geometry of the layout, bulk diffusivity, interface diffusivity, and mechanical properties are deterministic and so TTF is deterministic. However, the situation changes when the interconnect possesses a microstructure. The microstructure has a significant impact on electromigration, since it introduces a diversity of possible electromigration paths and local mechanical properties (the Young modulus and Poisson factor depend on the crystal orientation in each grain). However, the microstructure itself cannot be completely controlled by a process technology. In other words, the position of grain boundaries, angles in which they meet the interfaces, etc. cannot be designed, the process itself determines only statistics of grain sizes and textures.

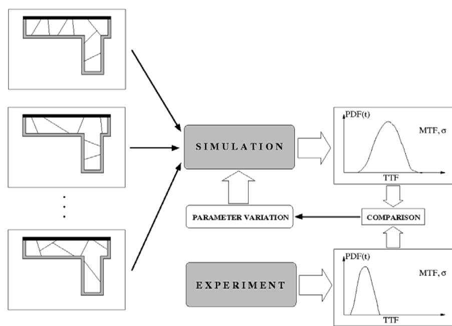

Fig. 2. Electromigration model calibration using a multitude of microstructural inputs.

IV. SIMULATION RESULTS

We have applied our model to the interconnect layout which has been extensively used for accelerated electromigration tests [6]. This layout is typical for dual-damascene 0.18 µm technologies. The Copper microstructure (Fig. 3) is set according to results of EBSD (Electron Backscatter Diffraction) measurements [5]. The peak values of stress and the vacancy concentration values are extracted from three extraction cylinders (C1, C2, and C3), which are presented in Fig. 4a).
The solution of the electro-thermal problem sets the operating conditions for electromigration simulation. The applied mechanical, thermal, and electrical boundary conditions are presented in Fig. 4b). The temperature T is set on constant 673 K which is the temperature level used in accelerated tests [6] and the voltage is V=10 mV. The obtained average current density is 10 MA/cm². Due to the geometry of the problem and the applied boundary conditions the temperature is only slightly changed by Joule heating.

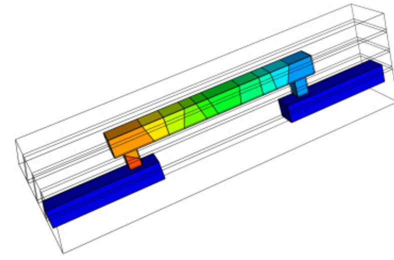

Fig. 3. Three-dimensional dual-damascene structure with polycrystalline copper metallization.

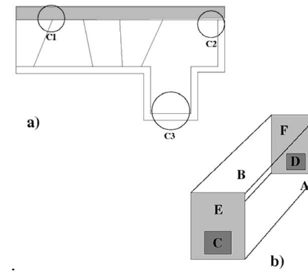

Fig. 4. a) Peak values for hydrostatic stress and vacancy concentration values are extracted from cylinders C1, C2, and C3. b) Applied boundary conditions: A, B: fixed temperature T=673K; C, D: voltage V=10 mV, upstream electromigration from C3 to C1; E, F: mechanically fixed.

In dual-damascene copper technologies interfaces to capping (etch-stop) layers are recognized as the fastest material transport paths for standard capping dielectrics SiN_x [6]. Experimental investigations have shown that for such cappings critical voids are formed at the top corner of the cathode edge of the metal line [7].
In order to properly include the effect of fast diffusivity paths, grain boundary, barrier, and capping layer diffusivities are set as 10^2 D_{bulk}, 10^2 D_{bulk}, and 10^5 D_{bulk}, respectively.
For a possible void nucleation high tensile stress and a local interface defect are necessary. Therefore, the primary goal of our investigation is to determine the sites, where high stresses arise.

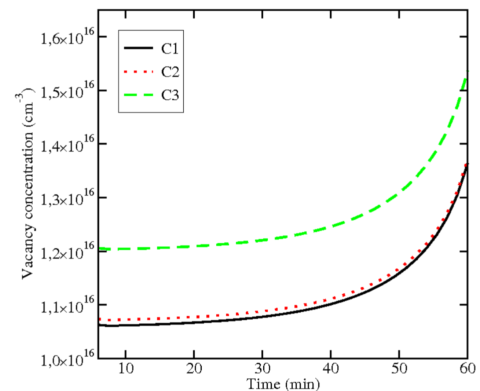

Fig. 5. Time evolution of vacancy concentration at three characteristic spots of the via.

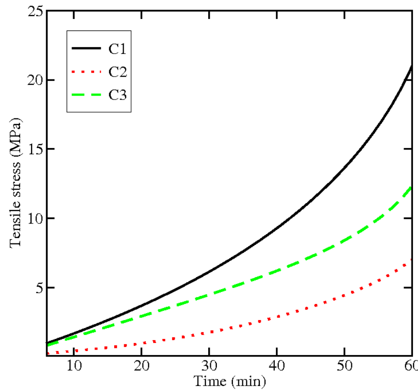

Fig. 6. Time evolution of tensile hydrostatic stress at three characteristic spots of the via.

For this purpose we monitor the hydrostatic stress development in three cylinders placed at the triple point next to cathode end of the via (C1), at the portion of the capping layer which lays directly above the via bottom (C2), and at the via bottom itself (C3), cf. Fig. 4a).

Due to the geometry layout, the highest vacancy concentration always develops at the bottom of the cathode end of the via (C3), cf. Fig. 5.

The peak vacancy concentration on the sites C1 and C2 develops approximately in the same way, but the site of highest stress (C1) does not coincide with the site of highest vacancy concentration (C3) (Fig. 6).

The connection between tensile stress and local vacancy concentration is defined through the relationships (10) and overall mechanical equilibrium (3).

The local stress behavior does not depend only on the local vacancy concentration, but also on mechanical conditions in the neighboring areas. It is obvious that a defect site is necessary for void nucleation and the coincidence of high vacancy concentration and high tensile stress regions with triple points (Fig. 7) indicates that triple points are natural locations of weak adhesion. This assumption was also expressed in the discussion of results of accelerated tests published in [5, 6].

The scenario of weak triple points in combination with a stress threshold would allow multiple void nucleations in the short time interval as it has actually already been observed [6].

These voids can migrate along the copper/capping layer interface, from one triple point to another, and stop at the corners above the via. Here, further void growth takes place eventually resulting in a critical decrease in the effective interconnect cross section leading to failure.

V. CONCLUSION

A comprehensive electromigration model is used as a basis for development of a three-dimensional simulation tool. An influence of residual and electromigration induced strains on material transport is discussed and an earlier electromigration model is extended by introduction of tensorial self-diffusivity. A discussion of grain boundary physics is provided, whereas a special focus was put on the enlightenment of the stress influence on the grain boundary dynamics.

The physical soundness of the extended electromigration model is verified with several simulation examples. The simulated dynamics of early failure development is in good agreement with experimental observations. The role of triple points regarding void nucleation is discussed on the basis of simulation and corresponding experimental results. A concept for usage of TCAD tools in combination with experimental tests is presented.

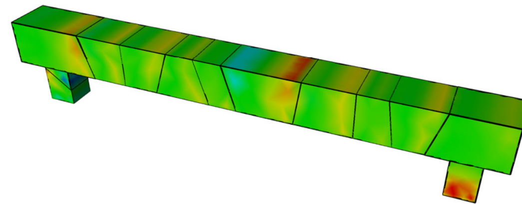

Fig. 7. Peak tensile stress tensor component distribution. Red (dark) color areas marks peak tensile stress.

ACKNOWLEDGMENT

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