Analysis of Electromigration Void Nucleation Failure Time in Open Copper TSVs

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***Abstract*—Through silicon vias (TSVs) are innovative interconnects which provide wider functionality and higher performance per unit area in three-dimensional (3D) integrated circuits. The reliability of TSVs in integrated circuits constitutes an important issue in microelectronics. One of the most relevant degradation mechanisms in interconnects is electromigration (EM). Therefore, the prediction of the EM failure behavior is a crucial necessity. Traditionally, Black's equation has been used from the early times of EM investigations for the estimation of the time to failure (TTF) for a wide spectrum of different interconnects. In this work we investigate the applicability of Black's equation for the estimation of the EM failure time in open copper TSV technologies. The EM void nucleation model has been solved by numerical calculations. Simulations have been carried out for different current densities. The results are in good agreement with Black's equation.**

I. Introduction

Today, semiconductor device development has found in 3D integration technology one of the most advantageous avenues for achieving higher electronic device capabilities. Innovative 3D interconnects provide increased integration density and reduced package total size thanks to their shorter lengths and power consumption [1]. Recently, TSVs have attracted much attention in 3D integration technology due to their function as vertical connections of the stacked semiconductor dies. Due to the high mechanical stresses generated around the TSV as a result of the mismatched thermal expansion coefficients of the metal core and the substrate, a new concept for wafer-to-wafer integration based on open TSV technology has been introduced [2]. By utilizing the unfilled copper TSV design (Fig. 1) the thermo-mechanical issues induced by the material properties are reduced. Furthermore, distinctive benefits of this specific TSV technology include a relatively large TSV sidewall surface area and thicker copper layer [2]. Since the TSV process has almost reached the status of being a full-grown progress, the understanding of the reliability issues that can occur in these interconnect structures is now a necessity.

A key aspect for reliability assessment of TSVs is EM. EM refers to the process of mass transport due to current flow in a metal line and is the most important metallization wear-out failure mechanism in interconnects. On the atomistic level EM is a quantum mechanical effect caused by the local electric field and the scattering of conducting electrons on the ionized lattice atoms. The EM wear-out mechanism is normally due to the formation of a void that eventually grows, causing a chip failure [3]. In 3D open TSV technology, the severe dimension mismatches between landing pads, TSV sidewall, and metal wires can lead to a nucleation of a small void triggering a failure mechanism. In general, EM modeling and simulation represent a multi-physics problem which can be divided into two parts, namely, the early mode of void nucleation and the late mode of void growth. During the first mode, voids can nucleate at some locations in the interconnect due to the stress, especially where the adhesion between the copper layer and the surrounding material is weak. The nucleation of a void is the beginning of the late mode. During this phase, the void evolution mechanism leads to a rapid increase of the interconnect resistance resulting in an open circuit failure. Since interconnect EM reliability is primarily determined by the void nucleation mechanism [4], the understanding of the early failure mode becomes decisive for a precise reliability assessment. Consequently, the prediction of the void nucleation time provides a realistic EM lifetime estimation of a given interconnect. Typically, EM TTF is based on a semi-empirical mathematical model known as Black's equation [5]. The EM TTF is defined as the time needed to reach the threshold stress at the sites of the void nucleation. In this work, we describe a detailed EM analysis for 3D open copper TSVs, considering the impact of the EM-induced stress on the failure time of the interconnect. The stress evolution which leads to the void nucleation in the TSV is simulated by using the finite element method (FEM). Finally, simulation results are used to show that Black's equation is applicable for the prediction of the lifetime of the open copper TSV technology.

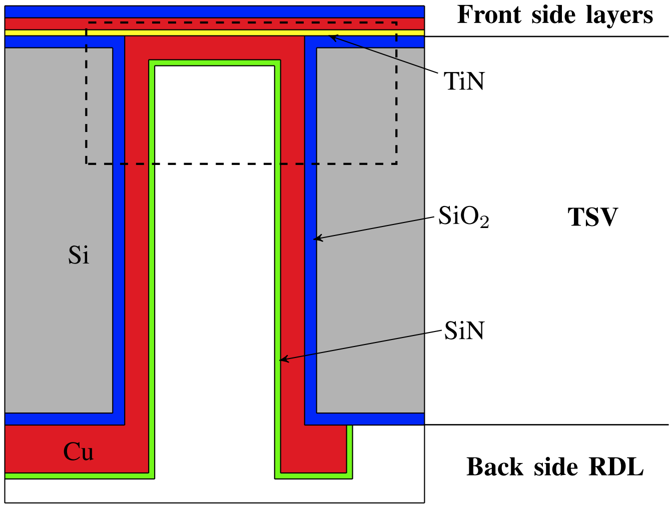


Fig. 1: General cross section view of the 3D integration technology using TSV, front side rerouting layer and back side RDL. The upper part of the interconnect layout is known as TSV bottom while the lower side is the TSV top. The TSV aspect ratio is 5:1 (TSV height / TSV width). The portion of the structure considered for simulations is highlighted (dashed rectangle).

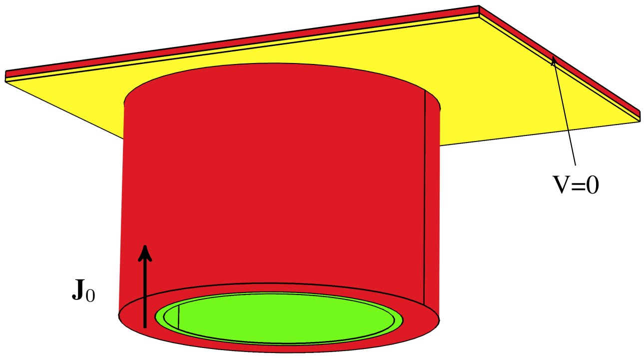


Fig. 2: Profile view of the analyzed TSV structure. The arrow shows the direction of the current flow.

II. Approach

A schematic overview of 3D integrated technology using TSV, front side rerouting layer and back side redistribution layer (RDL) is shown in Fig. 1. In general, the lower part of the structure is called TSV top while the upper part is the TSV bottom. It is normally considered that the TSV top is the part where the TSV comes out to the back side thick copper RDL, and the TSV bottom is the part of the TSV in contact with the front side rerouting layer. The TSV top is opened with a silicon etch process, and silicon dioxide insulation is deposited. Metallization (copper) and passivation (silicon nitride) are deposited on the TSV surfaces using electrodeposition and PECVD (plasma enhanced chemical vapor deposition), respectively. In the upper part of the structure (see Fig. 1) the front side layers stack (TiN/Cu/SiO_2) is formed. On the opposite side the thick copper back side RDL is placed and passivated. The back side RDL will always be by convention the side on which a solder bump is mounted to connect the other wafers. Since that only the TSV bottom is affected by EM, we investigate the EM reliability issues in this region as depicted in the highlighted area in Fig. 1. The geometry considered to the study of EM early failures is shown in detail in Fig. 2. Since that copper has high sensitivity to EM, the process of mass transport that leads to void nucleation is considered only in the copper parts of the structure.

In general, EM void nucleation failure is caused by the formation of voids due to the migration of atoms in the interconnect line. The material transport responsible for EM failure occurs due to a combination of different driving forces and can be described by the vacancy flux $\vec{J}_\text{v}$

$$\vec{J}_\text{v} = -D_\text{v}\left(\nabla C_\text{v} + \frac{e|Z^*|}{k_\text{B}T}C_\text{v}\nabla\phi + \frac{f\Omega}{k_\text{B}T}C_\text{v}\nabla\sigma\right), \quad (1)$$

where D_v is the vacancy diffusion coefficient, C_v the vacancy concentration, e the elementary charge, Z^* the effective valence, ϕ the electrical potential, k_B the Boltzmann constant, T the temperature, f the vacancy relaxation factor, Ω the atomic volume, and σ the hydrostatic stress. The first flux term in the brackets represents the flux induced by the gradient of the vacancy concentration, the second represents the flux induced by EM, and the third is related to the flux caused by the gradient of the mechanical stress in the material. Due to the homogenous temperature distribution in the copper and titanium nitride, the flux term due to the gradient of the temperature in the material is negligible in this analysis. These driving forces cause a redistribution of the vacancies in the metal line according to the continuity equation

$$\frac{\partial C_\text{v}}{\partial t} = -\nabla\cdot\vec{J}_\text{v} + \frac{C_\text{v,eq} - C_\text{v}}{\tau_\text{v}}, \quad (2)$$

where $C_\text{v,eq}$ is the equilibrium vacancy concentration and τ_v the relaxation time. The second term in the right side of the drift-diffusion equation is usually called Rosenberg-Ohring term [6]. It models creation and annihilation of vacancies at particular sites inside a metal. These sites are typically grain boundaries, interfaces, and extended defects.

The vacancy transport inside an interconnect leads to the development of an inelastic strain in the line. Metals respond to inelastic strain by deformation or the build-up of stress. Thus, the inelastic strain ϵ_v is the connection between material transport and mechanical stress in the interconnect. The dynamics of ϵ_v due to the pile up and the generation/annihilation of vacancies are described by the following equation:

$$\frac{\partial \epsilon_\text{v}}{\partial t} = \Omega\left[(1-f)\nabla\cdot\vec{J}_\text{v} + f\left(\frac{C_\text{v,eq} - C_\text{v}}{\tau_\text{v}}\right)\right]. \quad (3)$$

Distribution of mechanical stress in a 3D interconnect structure is calculated by solving (1) - (3) together with the mechanical equilibrium equation, and also by coupling the standard electro-thermal equations [7]. After a certain time the mechanical stress reaches a threshold value σ_t which is needed to nucleate a void at the sites of weakest adhesion. After a void has nucleated, it grows and moves. Typically, the void nucleation time is assumed much longer than void evolution time. Therefore, the void nucleation time well approximates the EM TTF of a metal interconnect which is classically described by Black's equation

$$TTF = \frac{A}{J^n}\exp\left(\frac{E_\text{a}}{k_\text{B}T}\right), \quad (4)$$

where A is a constant, J the electric current density, n the current density exponent, and E_a the vacancy activation energy. In the following we will show that the application of Black's equation is a good tool for the description of EM in open copper TSVs and for the estimation of the EM TTF of these structures.

III. Results

We have applied the above described physical model for analyzing EM in the portion of the open copper TSV technology shown in Fig. 2. Due to the complexity of the mathematical model describing the physical phenomena presented in Section II, the application of numerical simulations is necessary. Model equations are solved by using FEM. Simulation starts with solving the electro-thermal problem in order to obtain the electric potential and temperature distributions in the structure. Then the vacancy dynamics problem has to be solved followed by the mechanical stress problem in order to determine the distributions of vacancy concentration and stress. The simulation continues until the threshold stress for void nucleation is

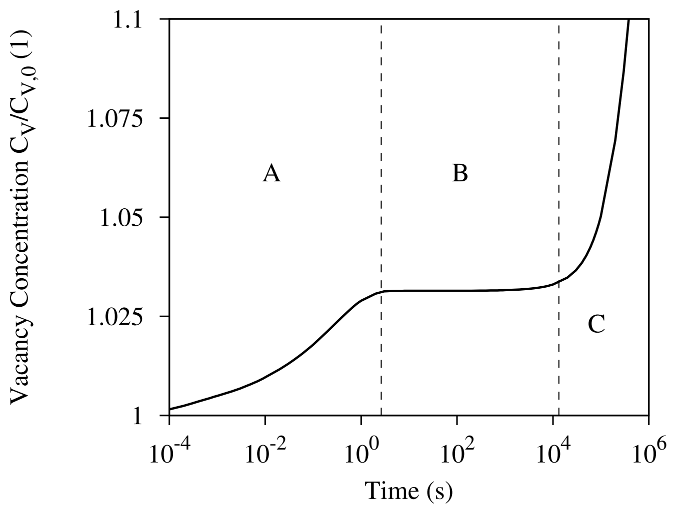
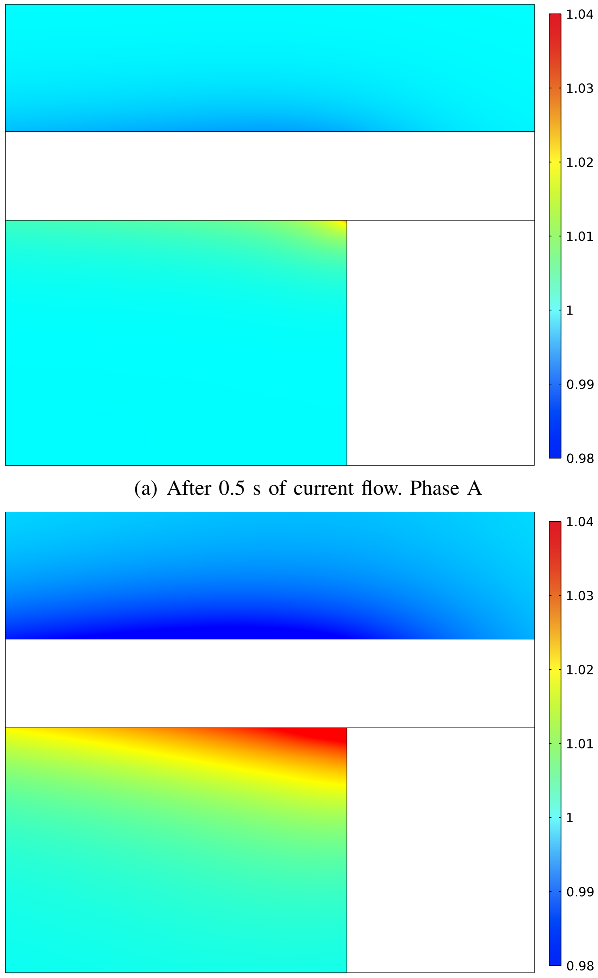


Fig. 3: Maximum relative vacancy concentration change over time in the simulated structure.



(a) After 0.5 s of current flow. Phase A

(b) After 10 ks of current flow. Phase C

Fig. 4: Relative vacancy concentration in the cross section views of the TSV bottom during the phase A and C of the vacancy dynamics in Fig. 3. The peak values are located close to the copper/titanium nitride interface.

reached at some location in the interconnect. Reaching of the threshold stress implies void nucleation and the beginning of the rapid failure development at this location.

Operating conditions for EM simulations are set by the following boundary conditions: the temperature is kept constant at $T_0 = 473$ K for all external surfaces of the structure; the electric current density $J_0 = 1$ MA/cm^2 is set at the bottom side of the copper TSV cylinder (arrow in Fig. 2), and the zero electric potential condition is set at the right side of the copper rerouting layer (V=0). For the mechanical problem, the following constraints as boundary conditions are imposed: the outer surfaces of the structure are fixed while the inner surface of the TSV (silicon nitride layer) is free to move.

As discussed before, our model describes the change of vacancies in time. In Fig. 3, three distinctive phases of the time evolution of the maximum relative vacancy concentration can be recognized. These phases are explained according to [8]. In the first phase (A), the transport of vacancies is dominated by the EM term. The reaction of the material in this phase due to the gradients of the stress and the vacancy concentration is considerably smaller than the EM itself. As a result vacancies tend to accumulate close to the interface region between copper and titanium nitride (Fig. 4a). After $t \sim 1$s the vacancy concentration reaches a quasi-steady state (phase B). In this phase the response of the material tends to balance EM perfectly. The quasi-steady state is followed by a rapid growth of the vacancy concentration (phase C) caused by stress activated vacancy sources (Fig. 4b).

By monitoring the distributions of the hydrostatic stress in the structure (Fig. 5), we identify the locations with the highest probability of void formation. Void nucleation mainly occurs in those locations where vacancies accumulate. Due to the small relaxation of the lattice surrounding a vacancy, vacancy accumulation produces volume contraction, causing tensile stress development at these areas. Therefore, the copper/titanium interface is recognized to be the site of void nucleation. Here, the tensile stress increases from the copper, which is closed to the interface, towards the interface regions of the copper and titanium nitride. In turn, in the opposite side, compressive stress arises due to the volume expansion caused by vacancy depletion.

The sites of void nucleation turn out to be the locations of current crowding as well. This outcome can be verified by analyzing the current density distribution in the open TSV geometry (Fig. 6). Due to the different electrical conductivities of the copper lines and the titanium nitride layer, current crowding arises at the TSV bottom close to the interface regions of void nucleation. In fact, in the areas where the titanium nitride is mechanically fixed to the copper the current is mainly flowing in the copper lines due to their lower electrical resistance. In this way, the current flow tends to accumulate vacancies at these locations leading to a development of tensile stresses and accordingly void nucleation. Furthermore, the impact of the different thicknesses of copper and titanium nitride layers can significantly contribute to the current crowding increase in these regions.

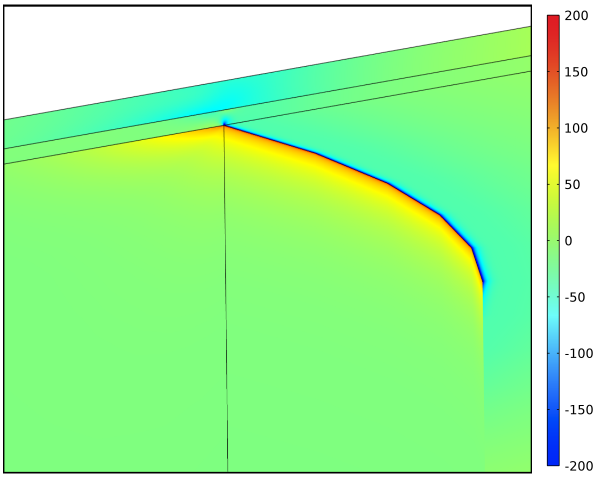


Fig. 5: Stress (MPa) in the profile view of the TSV bottom after 1Ms of current flow. The maximum tensile stresses are located at the copper/titanium nitride interface.

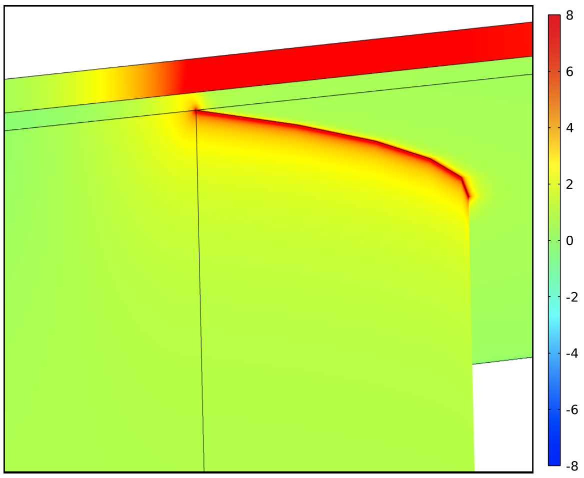


Fig. 6: Profile view of the current density distribution (MA/cm^2) in the open copper TSV structure. Current crowding happens at the sites of void nucleation at the TSV bottom.

Fig. 7 shows the time evolution of the stress built-up during the three phases of the vacancy dynamics in Fig. 3. During the first two phases we have observed that the maximum stress exhibits linear growth with time. After a certain time the stress increases with the square root of time, until it reaches the threshold value for void nucleation. This stress dependence has been derived by Korhonen *et al.* and it is implicitly valid for large size interconnects [9]. Therefore, reaching of certain threshold stress is a usual condition for EM void nucleation.

In order to estimate the void nucleation time, we have carried out simulations for several different current densities. From the simulation results we have obtained the time evolution of the stress due to EM for six current densities (Fig. 8). As expected, for higher current densities a shorter time is needed to reach the threshold stress for void nucleation than for lower current densities. The void nucleation time is related to the time elapsed until the achievement of the stress threshold at the sites of void nucleation. The value of the stress threshold is obtained by following [10, 11].

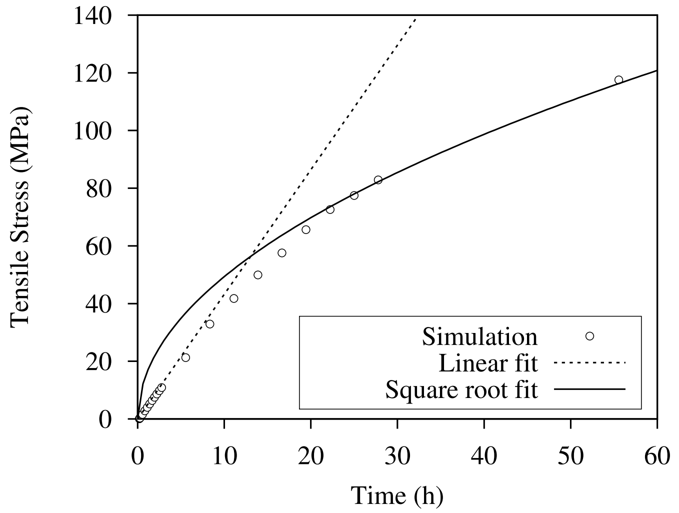


Fig. 7: Fitting of the time evolution of the maximum tensile stress in the open copper TSV using a linear and a square root model.

TTF/current density curves are subsequently fitted to Black's equation (4). The estimation of the fitting parameters A and n is obtained. In particular, the result yields a current density exponent n of 1.9. It has been shown that a value close to 2 indicates that the void nucleation is the dominant mechanism of EM failure [12]. Furthermore, this is in good agreement with experimental values obtained for a filled copper TSV [13]. Once the parameters are known, we are able to demonstrate that the void formation times in open copper TSV structures follow Black's behavior, as shown in Fig. 9.

IV. Conclusions

In this work we have investigated the applicability of Black's equation for the assessment of the EM void nucleation failure times in open copper TSV structures. Since that EM has a localized behavior, the analysis of EM has been restricted to a critical area of the geometry rather than the entire TSV. For this purpose 3D simulations based on a multiphysics EM model have been performed. Model equations have been solved by means of FEM.

The locations with the maximum tensile stress in the TSV structure identify the sites with the highest probability of void nucleation. The peak values are observed close to the copper/titanium nitride interface regions. The largest current crowding in the via is observed near the regions of void nucleation as well. TTF is determined as the time needed to reach the stress threshold at the sites of the void nucleation. Simulations are carried out for different current densities and TTF/current density curves are fitted to Black's equation. In this way, we have shown that Black's equation provides a convenient compact model for the prediction of the void nucleation time and for an estimation of the TTF for open copper TSV technologies.

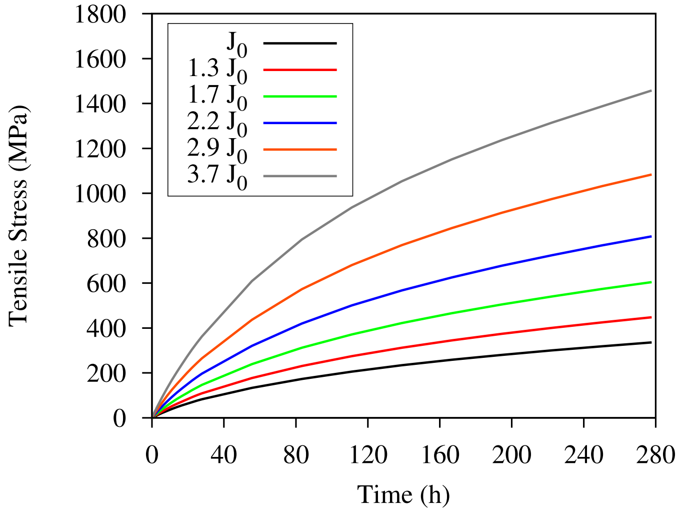


Fig. 8: Time evolution of the maximum tensile stress in the open copper TSV for six different current densities.

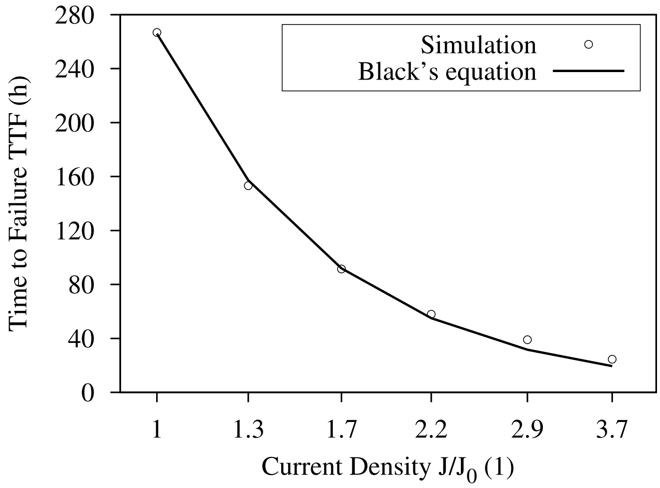


Fig. 9: Time to failure dependence on current density. The line indicates the fitting according to Black's equation.

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