Electromigration Modelling of Void Nucleation in Open Cu-TSVs

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Abstract

Recently, Through Silicon Vias (TSVs) have attracted much attention in three-dimensional (3D) integration technology due to their function as vertical connections of the different stacked semiconductor dies. Since electromigration (EM) will continue to be a key reliability issue in modern structures, 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 interconnect time to failure. In this work we investigate the applicability of Black's equation to open copper TSV structures using TCAD. TCAD can significantly contribute to the comprehension of EM failure mechanisms, in particular for the understanding of the early failure mode dominated by the void nucleation mechanism. The simulation procedure is applied to an open copper TSV technology in order to find the sites where void formation is most likely to occur. The time to failure is determined as the time needed to reach the stress threshold for void nucleation. Simulations are carried out for different current densities and successfully fitted to Black's equation. In this way, we have shown that failure development in studied TSV structures obeys Black's equation.

1. Introduction

Today, semiconductor device development has found one of the most advantageous avenues for achieving higher electronic device capabilities in 3D integration technology. The efficient use of the third dimension provides wider functionality, increased integration density, and higher performance per unit area in 3D interconnects as well as reduced interconnect length and power consumption. 3D integration can be carried out in different ways, and the most innovative way is based on direct TSV technology [1]. Due to the high mechanical stresses generated around the TSV as a result of the mismatched thermal expansion coefficients of the copper and the silicon substrate, a new TSV concept for wafer-to-wafer integration technology has been introduced. By approaching an unfilled copper TSV design, so called open copper TSV, the thermo-mechanical issues induced by the materials properties are minimized. 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, which is the process of mass transport due to current flow in a metal line and the most important metallization wear-out failure mechanism in interconnects. Fundamentally, EM is a quantum mechanical effect caused by the local electric field and the scattering of conducting electrons on lattice atoms. An EM wear-out mechanism is normally characterized by the formation of a void that eventually grows and triggers a chip failure [3]. In particular, the fabrication process induced imperfections and the geometric features of the metallic layers at the TSV bottom can lead to the nucleation of a small void under the TSV causing an additional 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. In turn, the late mode is governed by the void evolution mechanism [4]. Since interconnect EM reliability is primarily determined by the void nucleation mechanism [5], 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. EM time to failure, i.e., the time needed to reach the threshold stress for void formation in an interconnect, is typically based on a semi-empirical model, the well known Black's equation [6]. It has been shown that Black's equation well describes the time to failure for a wide spectrum of different interconnects from linear aluminum lines to copper-based dual damascene structures. The failure time depends on different factors, such as current density, stress gradient, and temperature [6], [7]. In this work, we describe a detailed EM analysis for 3D open Cu-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 Cu-TSV technology.

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2. Theoretical Background

EM early failure is caused by the formation of voids due to the migration of atoms in the metal interconnect. During this phase the lifetime of a line under EM is given by the time elapsed until void nucleation. Therefore, the understanding of this failure mode is required for modeling EM lifetimes. The material transport responsible for EM failure is induced by different driving forces and described by the vacancy flux $\vec{J}_{\mathrm{v}}$

$$\vec{J}_{\mathrm{v}} = -D_{\mathrm{v}}\nabla C_{\mathrm{v}} - \frac{D_{\mathrm{v}} e|Z^*|}{k_{\mathrm{B}}T} C_{\mathrm{v}}\nabla\phi + \frac{D_{\mathrm{v}}Q^*}{k_{\mathrm{B}}T^2} C_{\mathrm{v}}\nabla T - \frac{D_{\mathrm{v}} f\Omega}{k_{\mathrm{B}}T} C_{\mathrm{v}}\nabla\sigma, \tag{1}$$

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, Q^* the heat of transport, f the vacancy relaxation factor, Ω the atomic volume, and σ the hydrostatic stress. The first term in the vacancy flux equation represents the flux induced by the gradient of the vacancy concentration, the second represents the flux induced by EM, and the third and the fourth terms are related to the fluxes caused by the gradients of the temperature and the mechanical stress in the material, respectively. These driving forces cause a redistribution of the vacancies in the metal line. The vacancy concentration obeys the balance equation

$$\frac{\partial C_{\mathrm{v}}}{\partial t} = -\nabla\cdot\vec{J}_{\mathrm{v}} + G. \tag{2}$$

The G term models creation and annihilation of vacancies at particular sites inside a metal [8]. These sites are grain boundaries, extended defects, and interfaces. The so called Rosenberg-Ohring term is given by

$$G = \frac{C_{\mathrm{v,eq}} - C_{\mathrm{v}}}{\tau_{\mathrm{v}}}, \tag{3}$$

where $C_{\mathrm{v,eq}}$ is the equilibrium vacancy concentration and τ_{v} the relaxation time. The flow as well as the creation and annihilation of vacancies 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. Dynamics of ε_{v} are described by the following equation:

$$\frac{\partial \varepsilon_{\mathrm{v}}}{\partial t} = \Omega[(1-f)\nabla\cdot\vec{J}_{\mathrm{v}} + fG]. \tag{4}$$

Inelastic strain rate equation has contributions from both the pile up and the generation/annihilation of vacancies. Distribution of mechanical stress in a 3D interconnect structure is calculated by solving (1)-(4) together with the mechanical equilibrium equation, and also by coupling the standard electro-thermal equations [9]. Korhonen *et al.* derived a simple solution for the stress evolution in time in which the stress has a square root time dependence [10]. As will be shown later, this model is implicitly valid for large size interconnects.

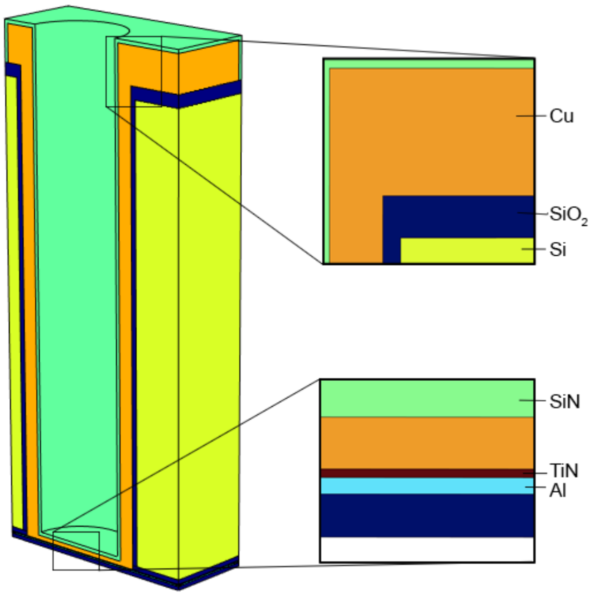

Figure 1. Profile view of the open copper TSV structure. TSV top: inset zoom-in of the backside thick copper RDL. TSV bottom: inset zoom-in of the front side layers stack.

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. The time period until the stress threshold is reached is called void nucleation time. After a void has nucleated, it grows and moves. During this period, called void evolution time, the resistance of the interconnect increases. Normally, after a resistance increase of 20% we consider the interconnect failed. The sum of void nucleation time and void evolution time is the interconnect failure time which is classically described by Black's equation. It has been shown by many experiments [6] that Black's equation well approximates the time to failure (TTF) of a metal interconnect subjected to EM:

$$TTF = \frac{A}{J^n}\exp\left(\frac{E_{\mathrm{a}}}{k_{\mathrm{B}}T}\right). \tag{5}$$

Here, A is a constant depending on the geometries and the material properties of the interconnect structure, J is the current density, n is the current density exponent, and E_{a} is the vacancy activation energy. In the following we will show that the application of Black's equation is a good tool for the understanding of EM in open Cu-TSV layouts and for the estimation of the time to failure of these structures.

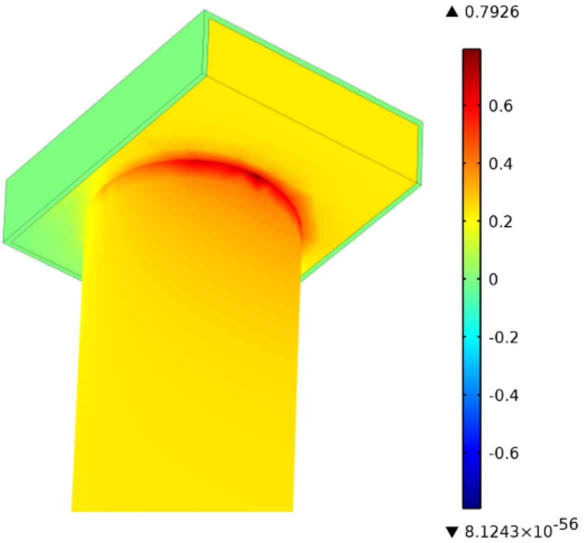

Figure 2. Current density in the TSV structure (MA/cm^2). Current crowding happens at the TSV top corner.

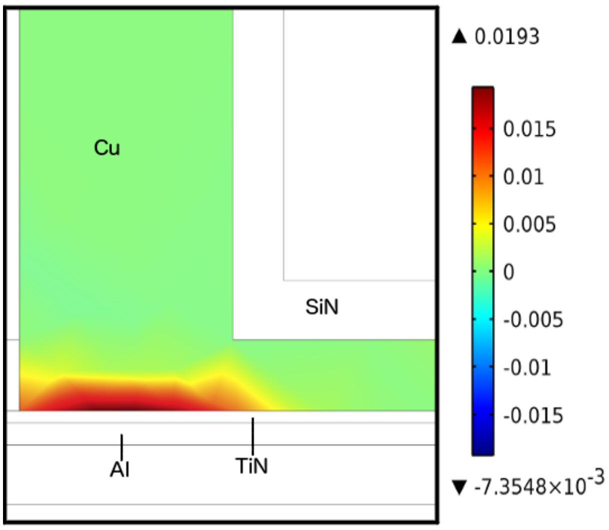

Figure 3. Relative vacancy concentration in the cross section view of the TSV bottom. The peak values are located at the interface region between copper and titanium nitride.

3. Results and Discussion

We have applied the above described physical model for analyzing EM in open copper TSVs. Figure 1 shows the geometry of an open Cu-TSV with a front side aluminum rerouting layer and a backside copper redistribution layer (RDL). The TSV bottom is the part of the TSV in contact with aluminum, and the TSV top is the part where the TSV comes out to the backside RDL. The TSV aspect ratio considered in our study is 5:1 (TSV height / TSV width). 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. Below the TSV bottom (see Figure 1) the front side layers stack (TiN/Al/SiO$_2$) is formed. In turn, on the top, the copper backside RDL is placed and passivated.

Due to the complexity of the mathematical model describing the physical phenomena presented in Section 2, application of numerical simulations is necessary. Model equations are solved by using the Finite Element Method (FEM). Simulation starts with solving the electro-thermal problem in order to obtain the electric potential and temperature distributions in the interconnect. 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 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.

The above simulation procedure is applied to the study of EM failures in the open copper TSV technology (Figure 1). 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 $I_0 = 1$ A is set at the left side of the copper RDL, and the zero electric potential condition is set at the copper/titanium nitride interface. For the mechanical problem, the following constraints as boundary conditions are imposed: the outer surfaces of the structure (see Figure 1) are fixed while the inner surface of the TSV (silicon nitride layer) is free to move.

The cross section view in Figure 2 shows the current density distribution in the open TSV geometry. Due to the different thicknesses of the copper lines, current crowding arises at the TSV top in the corner between the thick RDL line and the TSV sidewall. In the other regions of the TSV the current normally flows into the copper, reaching the minimum current density value at the Cu/TiN interface (zero electric potential boundary condition).

By monitoring the distributions of vacancy concentration and hydrostatic stress in the structure (see Figure 3 and 4), we identified the location with the highest probability of void formation. Tensile stress increases from the copper, which is closed to the interface, towards the interface regions of the copper and the titanium nitride, which leads us to the conclusion that void nucleation at these sites is very probable. As previously discussed, 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

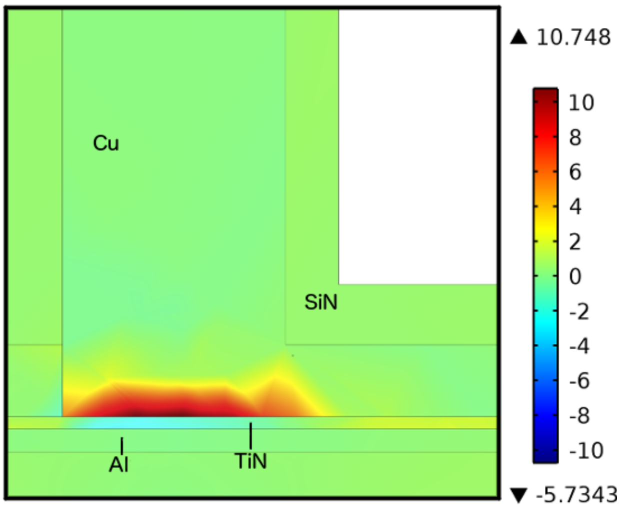

Figure 4. Stress in the cross section view of the TSV bottom (MPa). The maximum tensile stresses are located at the Cu/TiN interface.

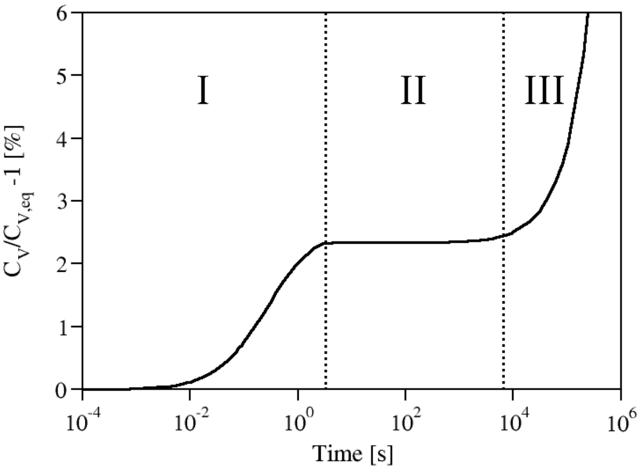

Figure 5. Maximum relative vacancy concentration change in time in the open copper TSV.

these areas. Therefore, the Cu/TiN interface is recognized to be the site of void nucleation.

As discussed before, our model describes the change of vacancies in time. In Figure 5, three distinctive phases of the time evolution of the maximum vacancy concentration can be recognized. These phases are explained according to [7]. In the first phase (I), 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 Cu/TiN interface. After $t = 1$s the vacancy concentration reaches a quasi-steady state. In this phase (II) the response of the material tends to balance EM perfectly. The quasi-steady state is followed by a rapid growth of the vacancy concentration (III).

The time evolution of the stress built-up during the three phases of the vacancy dynamics is shown in Figure 6. During the first two phases we have observed that the maximum stress exhibits linear growth with time. After a certain time ($> 10^4$ s) the stress increases with the square root of time, until it reaches the threshold value for 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 a total of five current densities (Figure 6). 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 time to failure is determined as the time needed to reach the stress threshold. The value of the stress threshold is obtained from [11]. Time to failure/current density curves are subsequently fitted to Black's equation (5). The estimation of the fitting parameters A and n are obtained. Once A is known, we have been able to demonstrate that the void formation times in open Cu-TSV structures follow Black's behavior, as shown in Figure 8. Furthermore, the result yields a current density exponent n of 1.65 which indicates that the void nucleation is the dominant mechanism of EM failure. This is in good agreement with experimental values obtained for a filled copper TSV [12].

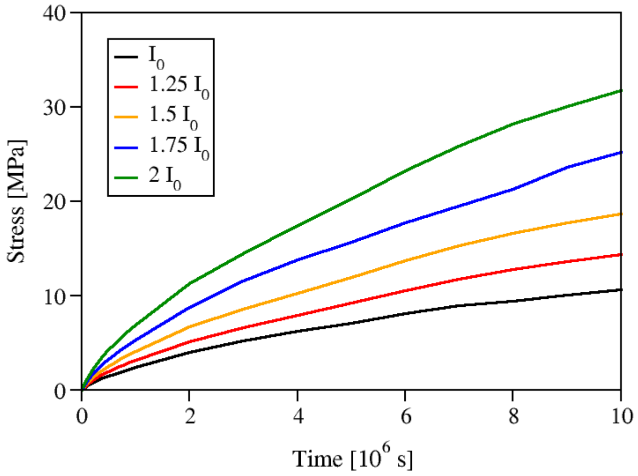

Figure 6. Time evolution of the maximum tensile stress in the open copper TSV for five different current densities.

4. Conclusions

In this work we have investigated the applicability of Black's equation for the assessment of the early EM failure times of open Cu-TSV structures. For this purpose

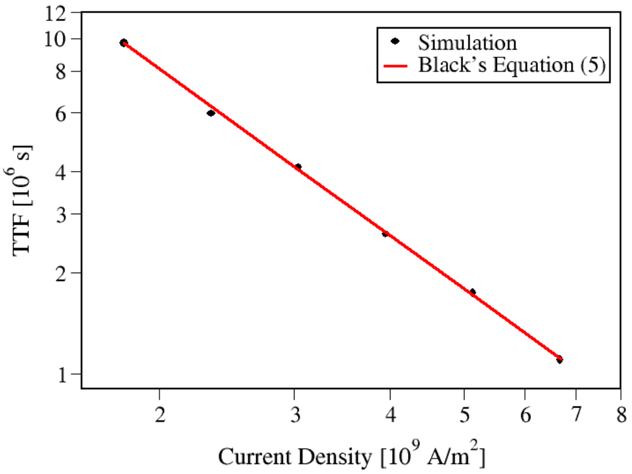

Figure 7. Time to failure dependence on current density (in log-log plot). The red line indicates the fitting according to Black's equation.

a 3D simulation based on a multiphysics EM model has been utilized. Model equations have been solved by means of FEM. The locations with the highest tensile stress in the TSV structure identify the sites with the highest probability of void nucleation. Time to failure 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 time to failure/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 time to failure for open Cu-TSV structures.

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