Advanced Modeling and Simulation of Cu Nano-Interconnects Reliability

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***Abstract*-The need to develop new interconnect technologies as devices scale below 10nm introduces new reliability challenges that need to be addressed by new models and modeling methods. In this work, we present a complete modeling framework that considers all relevant physical aspects of the reliability problem.**

***Keywords*-Cu nano-interconnects, simulation, electromigration, scaling effects.**

I. Introduction

The development of interconnect technology in recent years has brought to the fore two crucial questions regarding its future. The first question is how far we can go with Cu as an interconnect metal without reaching a point where the increase in interconnect resistivity and reduction in electromigration (EM) reliability become unacceptable, and the second, which metal can optimally replace Cu in the future. In the pioneering work by Sarychev, Zithnikov *et al.* [1], the general framework for EM degradation modeling of metallic interconnects in microscaled regions is provided. Since then, the original model has been extended and refined to include treatment of various microstructural properties of metal and interfaces, such as crystal anisotropy, stress-dependent diffusivities, etc. [2]. As interconnect technology moves to the nano-scale, changes in the basic technology produce a need for updated EM models. As the thickness of interconnects decreases, the importance of EM-induced material transport along grain boundaries (GBs) and interfaces increases. The lifetime of interconnects thus becomes more sensitive to the values of the parameters that determine this transport, such as effective valences and diffusivities. Interconnect thickness also has an impact on interconnect resistivity and the effective valence that needs to be considered. The material transport is additionally determined by GB density and the orientation of single grains. The goal of this work is to present and discuss a modeling concept that is not unnecessarily complex and that can be optimally combined with experimental data in order to assess the relative impact of different factors on interconnect reliability.

II. Models for the Prediction of Nano-Interconnect Lifetime

As the framework for the proposed modeling the work presented in [2] is used, which represents a further development from the original work of Sarychev, Zithnikov *et al.* [1]. There are three principal challenges in the modeling of nano-scaled interconnects. The first challenge involves the layout of the studied interconnect structure. In order to reproduce realistic mechanical conditions all materials in the layout and their corresponding properties need to be included in the overall modeling framework. The second challenge is the physics of GB and interfaces that can be modeled with different levels of complexity, either by applying dedicated local submodels or by using cumulative and average values. The third challenge is the modeling of void growth, which leads to an increase in interconnect resistance and to its final failure, at the necessary level of accuracy. According to the usual modeling approach, the lifetime of an interconnect structure, t_f, consists of a void nucleation, t_N, and void evolution time, t_E, corresponding to two failure development phases,

$$t_f = t_N + t_E. \tag{1}$$

Each of these two phases demands its own modeling approach.

Work undertaken by C. S. Smith [3] in 1952 on grain shape topology forms the basis of effective diffusivity formulas in many EM models. One of Smith's theorems states that the volume fraction, ϵ, of GBs in the metal body with an average grain size $\langle d \rangle$ is given by $\epsilon = 2\delta/\langle d \rangle$. This relationship enables an estimation of the effective values for diffusivities, effective valences, and recombination times for interconnect metal containing a network of GBs and embedded in different types of interface layers.

Effective values: The volume fraction dependent effective values of the Rosenberg-Ohring term, G_{eff}, the effective valence, Z^*_{eff}, and the effective diffusivity, D_{eff},

are given by the following terms, respectively:

$$G_{\text{eff}}(C_v) = -(C_{\text{eq}} - C_v)\Big(\frac{1-\epsilon}{\tau_{\text{bulk}}} + \frac{\epsilon}{\tau_{\text{gb}}}\Big), \tag{2}$$

$$Z^*_{\text{eff}} = Z^*_{\text{bulk}}(1-\epsilon) + Z^*_{\text{gb}}\epsilon, \tag{3}$$

$$D_{\text{eff}} = D_{\text{bulk}} + D_{\text{lin}}\Big(\frac{2}{w} + \frac{1}{h}\Big)\delta_{\text{I-lin}} + D_{\text{cap}}\frac{\delta_{\text{I-cap}}}{h} + \epsilon D_{\text{gb}}, \tag{4}$$

where h is the interconnect thickness and w is the interconnect width.

Effective valence and resistivity: The effective valence, Z^*, and resistivity, $\rho(T)$, are related on a fundamental level since both of these values characterize different aspects of electron scattering in a current carrying metal.

$$Z^*_{\text{bulk}}(T) = Z_d + Z_w(T) = Z_d + \frac{K(T)}{\rho(T)} \tag{5}$$

Different advanced models can be used in the modeling of interconnect resistivity, ρ. In regards to the effective valence in GBs, the work by Sorbello [4] in which the author makes an estimate $Z^*_{\text{gb}} \approx 0.8 Z^*_{\text{bulk}}$, is referenced.

Void nucleation (estimation of t_N): The central governing equations of EM models are the vacancy flux (6) and vacancy balance equation (7):

$$\vec{J}_v = D_{\text{eff}}\Big(\frac{C_v}{kT}|Z^*_{\text{eff}}e|\rho\vec{j} + \frac{C_v}{kT}f\Omega\nabla p - \nabla C_v\Big), \tag{6}$$

$$\frac{\partial C_v}{\partial t} = -\vec{J}_v + G_{\text{eff}}(C_v). \tag{7}$$

All symbols and notations used in (6) and (7), and in the following equations, are the same as in reference [2]. The dynamics of vacancy flux, $\vec{J}_v$, plays a crucial role in the development of EM failure. When $\vec{J}_v = 0$, the stress equilibrium state is achieved, the interconnect is virtually "immortal" (arbitrarily long-lived). This situation corresponds to Blech's effect in 1D and it is its actual generalization.

Conditions for void nucleation: The conditions for void nucleation are established as being due to either the geometrical or the microstructural features of the interconnect metal and layout. One particular geometrical feature can hinder vacancy flux and thus cause a local increase in the concentration of vacancies, which in turn leads to a local increase in tensile mechanical stress. After a certain stress-threshold is attained, an initial void is nucleated [5]. A microstructural feature, such as GB, can also lead to a local disturbance of material transport and subsequent rise in tensile stress at the so-called triple points (the intersection of the GB with the interface). In order to accurately capture the mechanism of void nucleation at the triple-point, more detailed modeling than that provided by expressions (2), (3), and (4) is necessary. The corresponding model is fully described in [2]:

$$J_{v,1} = \omega_T(C_v^{\text{eq}} - C_v^{\text{im}})C_{v,1} - \omega_R C_v^{\text{im}} \tag{8}$$

$$-J_{v,2} = \omega_T(C_v^{\text{eq}} - C_v^{\text{im}})C_{v,2} - \omega_R C_v^{\text{im}} \tag{9}$$

The model describes the trapping and release of vacancies inside a GB with the rates ω_T and ω_R, respectively. The trapped vacancies, from both sides of the GB become immobile vacancies with the corresponding concentration C_v^{im}. The parameters ω_T and ω_R can ultimately be determined only by means of molecular dynamics. For the purpose of this study, they are set in such a way that the condition for void nucleation at the triple point is fulfilled. The relationship between the GB model (defined by (8) and (9)) and the Rosenberg-Ohring term (2) is discussed in [2].

Estimation of initial void size: After an initial void is formed, the previously built stress relaxes. The volume of the initial void is determined as:

$$V_0 = -\frac{1}{B}\int_V p(x,y,z)\,dx\,dy\,dz \tag{10}$$

In order to simplify the model's implementation, it is assumed that a cylindrical void is formed around the triple point and spans the entire interconnect width, w. This assumption allows for the calculation of the initial void radius, r_0:

$$r_0 = \sqrt{\frac{2V_0}{\pi w}}. \tag{11}$$

Void evolution (estimation of t_E): The normal velocity, v_n, of the void surface is calculated according to

$$v_n = \Omega(\vec{J}_v \cdot \vec{n} - \nabla \cdot \vec{J}_s), \tag{12}$$

$$\mu = \mu_0 + \Omega(W_s - \gamma\kappa), \tag{13}$$

$$\vec{J}_s = -\frac{D_s\delta_s}{kT\Omega}(|Z^*_s e|\rho\vec{j}\cdot\vec{t} + \nabla_s\mu). \tag{14}$$

By further assuming that the void not only begins as a half-cylinder but that it also remains in this shape throughout its growth, the calculations (12), (13), and (14), can be significantly simplified and the relationship $v_n = v_n(r)$ established, with r being the actual void (cylinder) radius. Now the void evolution time, t_E, is obtained by integration:

$$t_E = \int_{r_0}^{r_c}\frac{dr}{v_n(r)}. \tag{15}$$

Here, the critical void radius, r_c, is the solution of the equation $R_{\text{failure}} = R(r_c)$.

The mechanical problem: Both the void nucleation, as well as the void evolution model, are solved simultaneously with the equations of mechanical model [2]:

$$\frac{\partial\varepsilon^v_{ij}}{\partial t} = \frac{1}{3}\Omega\big[((1-f)\nabla\cdot\vec{J}_v + fG_{\text{eff}}(C_v)\big]\delta_{ij}. \tag{16}$$

$$\nabla\cdot\sigma = \mathbf{0}, \quad \sigma = \mathbf{E}(\varepsilon - \varepsilon^v) + \sigma_0. \tag{17}$$

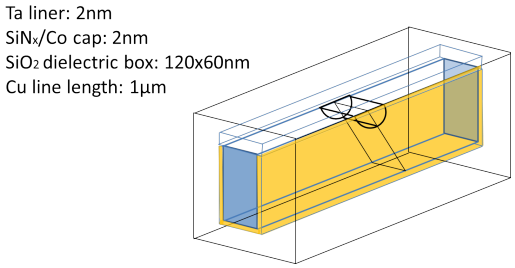

Fig. 1: Structure used for simulations. Cylindrical void nucleation is assumed at the triple point.

Overall schema: In order to estimate interconnect lifetime (t_F), both void nucleation (t_N), as well as the void evolution time (t_E), need to be estimated as accurately as possible. In its simplest form, an estimation of t_N demands that equations (6), (7), (16), and (17) be solved simultaneously. The same group of equations needs to be solved for the interconnect containing a void in order to determine the function $v_n(t)$ and subsequently to estimate t_E by the integral (15).

III. Simulation Results and Discussion

The modeling framework described above is used to study t_F dependence on: a) interconnect thickness, and b) the mechanical and material transport properties of SiN_x and Co caps. COMSOL Multiphysics [6] was used for the simulations. The 1μm long Cu interconnect is placed between two contacts and encapsulated in a Ta barrier layer on all sides except the top, which is covered with the cap layer. The Cu interconnect along with all interface layers is fully embedded in SiO_2 (cf. Fig.1). Realistic material properties for all involved materials and interfaces are assumed, including a 20MPa stress threshold for void nucleation at the SiN_x cap and a 30MPa at the Co cap. Interface diffusivity at the SiN_x/Cu interface is assumed to be 100 times higher than in the case of the Co/Cu interface. The temperature for both simulations is set at 300°C. A detailed modeling approach allows for the observation of different physical characteristics as failure develops. As we can see from (15), an estimation of the void evolution time (t_E) demands the extraction of the function $v_n = v_n(r)$, which can be studied in detail by the simulation results presented in Fig. 2. Interconnect lifetimes for both types of capping layers are significantly reduced for a thinner interconnect (cf. Table 1), but the benefits of replacing SiN_x with Co is clearly recognizable. Such behavior is confirmed by numerous experimental results (e.g [7]), as it is to be expected, since for thinner interconnect a larger portion of atoms is transported along the interfaces and a smaller void volume is needed to produce the fatal failure.

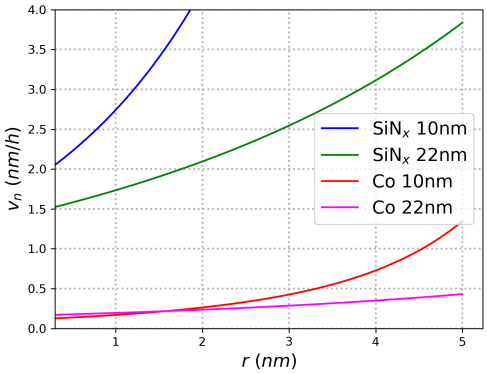

Fig. 2: Normal velocity (v_n) of the void surface in dependence on void radius thickness (h) for SiN_x and Co cap.

Table 1: Lifetime dependence on interconnect thickness.

Capping	thickness [nm]	t_N/t_F	t_E/t_F	t_f/t_F
SiN_x	10	0.200	0.099	0.299
SiN_x	22	0.395	0.605	**1.000**
Co	10	0.304	1.598	1.902
Co	22	0.608	5.379	5.987

IV. Conclusions and Outlook

An EM reliability model, which takes into account different effects related to the narrowness of the interconnect, as well as the particular material choice needed for a layout realization, is presented. Among the particular effects included are the effective valence's dependence on microstructure and interconnect thickness, the effects of interfacial EM paths and void growth under the assumption of a narrow interconnect. The dependence of interconnect lifetimes on length, thickness, and the diffusivities of the cap layers obtained through the simulation fully match known and published results. The presented modeling concepts will be further optimized and applied for reliability studies of nano-interconnects.

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