Electromigration in Interconnect Structures of Microelectronics Circuits

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Abstract - We present a comprehensive physical model for the whole life cycles of electromigration induced voids. Special emphasis is put on explaining the void morphology and its impact on interconnect resistance. Investigations for common two- and three-dimensional interconnect structures are presented. Implications of the theoretical analysis and the simulation results for modern interconnect design are discussed.

I. INTRODUCTION

The downscaling of transistors in integrated circuits in order to achieve higher performance goes hand in hand with the reduction of the interconnect cross sections. At the same time the average interconnects' length is increased to accommodate larger chips with increasing functionality. These tendencies make interconnects more and more sensitive to electromigration and accompanying electro-thermal and thermo-mechanical effects which became one of the main reliability issues in modern integrated circuits.

Copper with its lower resistivity, higher melting point, good mechanical strength, and better electromigration performance [1] has replaced aluminum as advanced metalization solution. However copper based interconnects have introduced new problems, since copper electromigrates along fast diffusion paths at the interfaces to surrounding layers [2].

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 basis for deriving sophisticated design rules which will ensure higher steadfastness of interconnects against electromigration.

The material transport driven by electromigration is most commonly modeled by the dynamics of crystal vacancies.

A high concentration of vacancies indicates sites where the nucleation of intrinsic voids is very probable.

The evolution of voids inside the interconnect lines is the cause of the resistance change and failure of the line.

II. ELECTROMIGRATION FAILURE MECHANISM

The development of intrinsic voids, which leads to interconnect failure, goes through two distinctive phases. These phases exhibit the different influence on the operating abilities of interconnects and are based on different physical phenomena.

The first phase is the void nucleating phase in which electromigration-generated voids do not exist and a significant resistance change is not observable. The second phase starts when a void is nucleated and becomes visible in SEM pictures [3]. This is the so-called rapid phase

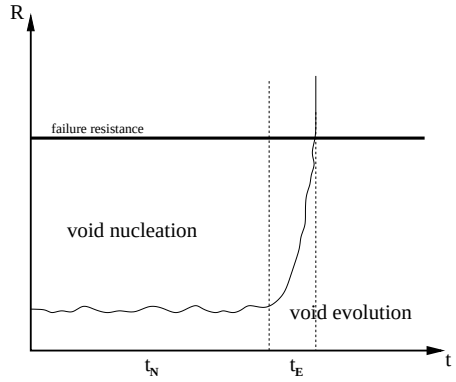

Figure 1: Resistance behavior and failure development phases.

of void development. The void expands from its initial position (nucleation site) to a size which can significantly change the resistance or completely sever the connection. If we denote the void nucleation time with t_N and the void evolution time with t_E, the time to failure t_F is,

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

The expected resistance development during these time periods is sketched in Fig. 1.

The development of a general electromigration model demands a careful analysis of physical phenomena in both phases of void development.

III. VOID NUCLEATION

The electromigration model applied in this work is based on propositions made in [4]. The model connects the evolution of the mechanical stress with the diffusion of vacancies under full account of the influence of the geometry of the metalization.

The dynamics of the vacancies is described by the following two equations [4]

$$\mathbf{J}_v = -D_v\Big(\nabla C_v + \frac{Z^*e}{k_B\,T}C_v\nabla\varphi + \frac{f\Omega}{3\,k_B\,T}C_v\nabla\,\mathrm{tr}(\sigma)\Big), \quad (2)$$

$$\frac{\partial C_v}{\partial t} = -\nabla\mathbf{J}_v + G(C_v), \quad (3)$$

where C_v is the vacancy concentration, f is the vacancy relaxation ratio, Ω is the atomic volume, D_v is the vacancy diffusivity, k_B is Boltzmann's constant, T is the local temperature, Z^*e is the effective valence, and $G(C_v)$ is the source function which models vacancy generation and annihilation processes. A closer look at equation (2) reveals that three major driving forces induce the dynamics of vacancies: the electromigration which is proportional to $\nabla\varphi$, the concentration gradient, and the mechanical stress gradient $\nabla\,\mathrm{tr}(\sigma)$.

If we have no residual mechanical stress from the technological process flow and an initially uniform distribution of vacancies (as is normally the case), it is obvious that the rise of mechanical stress and concentration gradients is a response to the electromigration stressing of the interconnect material. The overall behavior of temperature gradients depends on the material choice, the geometry of the interconnect layout, and the operating conditions. Both scenarios, in which temperature gradients enhance or retard vacancy transport induced by electromigration are possible.

Considering the effective vacancy diffusivity we can distinguish between three basic diffusion paths and their diffusivities: bulk, grain boundaries, and copper interfaces to other layers. Interface self-diffusion is the dominant diffusion mechanism for the case of standard barrier layers such as TiN, as shown by many experimental observations [5].

The sites where the vacancies are generated or annihilated are grain boundaries or dislocations [6]. This effect is commonly modeled by a source function $G(C_v)$ [4, 7]. Following the work of Kirchheim [6] $G(C_v)$ is given by

$$G(C_v) = L_v kT \ln\frac{C_v}{C_v^{eq}}, \quad (4)$$

where L_v is a rate parameter and C_v^{eq} is the equilibrium vacancy concentration. Assuming only a small deviation of the vacancy concentration from its equilibrium value C_v^{eq}, (4) can be simplified to

$$G(C_v) = -\frac{C_v - C_v^{eq}}{\tau_s}, \quad (5)$$

with $\tau_s = -C_v^{eq}/(kTL_v)$. Rosenberg and Ohring [8] use (5) without any previous considerations and introduce τ_s as "*life time of a vacancy in the presence of sinks*". A more physical interpretation of τ_s declares it as a characteristic relaxation time needed for the vacancy concentration to reach the level which is in local equilibrium with stress [9].

(5) plausibly models production of vacancies, if their concentration is lower than the equilibrium value C_v^{eq} ($G(C_v) > 0$) and their annihilation ($G(C_v) < 0$) in the opposite case.

Relation (5) is frequently used to include the effect of vacancy recombination in electromigration models, however, one should consider that it is only a rough approximation of the real physical phenomena. A theoretical refinement of the source function concept was introduced and discussed by Clement [10].

In his pioneering work on electromigration Korhonen *et al.* [11] use a direct relationship between lattice density and hydrostatic stress. This approach is based on simplifications which are justifiable only for a straight aluminum line. Other researchers, such as Povirk [12] and Rzepka *et al.* [13], searched for a more general description and employed the idea that diffusion fluxes give rise to volumetric strain which serves to establish stress fields, thereby driving stress-migration fluxes.

Using a similar concept, Sarychev and Zhitnikov [4] introduced a contribution of local vacancy dynamics to stress build-up in a three-dimensional model of stress evolution during electromigration. The standard elastic model was extended by introducing inelastic loads due to vacancy migration and recombination. The total strain tensor is given by

$$\varepsilon_{ik} = \varepsilon_{ik}^{v} + \varepsilon_{ik}^{\sigma}, \quad (6)$$

where ε_{ik}^{v} and $\varepsilon_{ik}^{\sigma}$ denote the inelastic and elastic strain component, respectively. The kinetic relation for inelastic strain component is given by [14],

$$\frac{\partial\varepsilon_{ij}^{v}}{\partial t} = \Omega\Big[(1-f)\nabla\mathbf{J}_v + f\frac{C_v - C_v^{eq}}{\tau}\Big]\delta_{ij}. \quad (7)$$

During the material redistribution induced by any driving force, the lattice actually tries to keep the vacancy concentration at its equilibrium value.

An even more complete model than this presented above also includes diffusion in the grain boundaries together with an interaction model which describes the vacancy exchange between the grain boundaries and the bulk. A model of this type was first studied by Fisher [15] which represents a promising improvement for electromigration modeling.

The lack of well-established models for nucleation of initial voids remains a limitation in modeling the failure of interconnect lines. Typically used nucleation conditions are critical stress or/and critical vacancy concentration [9], but in both cases it is actually very difficult to motivate values of these thresholds.

Consideration based on classical thermodynamics and kinetics [16] have shown that for aluminum, the nucleation rates for bulk, grain boundary, and sidewalls are

very low. Such an analysis has, to the authors knowledge, not been carried out for copper technology.

III. VOID EVOLUTION

Modeling the micromechanics of void evolution is a long-standing scientific problem. It began with sharp interface models requiring an explicit finite element tracking of void surfaces during the course of evolution [17]. Later, prompted by the complexity of void surfaces, diffuse interface (DI) models were introduced [18].

Diffuse interface models circumvent computationally costly explicit surface tracking by application of a smooth order parameter field for the representation of void structures. An alternative diffuse interface model based on the double obstacle potential was proposed in [19], where the computation is simplified by reduction of order parameter profile evaluation to only the void-metal interfacial area.

The main disadvantages of these diffuse interface models are their requirement of underlying structured meshes for the order parameter evaluation and their restricted capability to reach higher resolution of an order parameter profile in the void-metal interfacial area.

In the case of void evolution there are two main forces which influence the shape of the evolving void interface: the chemical potential gradient and the electron wind. The first force causes self-diffusion of metal atoms on the void interface and tends to minimize energy, which results in circular void shapes. The electron wind force produces asymmetry in the void shape depending on the electrical field gradients.

Including both contributions, electromigration and chemical potential-driven surface diffusion, gives the total surface vacancy flux, $\mathbf{J_s} = J_s\mathbf{t}$, where $\mathbf{t}$ is the unit vector tangent to the void surface [17, 20]

$$J_s = -D_s\Big(eZ^*E_s + \Omega\nabla_s\Big(\frac{\sigma:\varepsilon}{2} - \gamma_s\kappa\Big)\Big). \qquad (8)$$

$E_s \equiv \mathbf{E_s}\cdot\mathbf{t}$ is the local component of the electric field tangential to the void surface, ∇_s is the surface gradient operator, $0.5\,(\sigma:\varepsilon)$ 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:

$$D_s = \frac{D_0\,\delta_s}{k_B\,T}\exp\Big(-\frac{Q_s}{k_B\,T}\Big). \qquad (9)$$

Here, 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. Equation (8) is the Nernst-Einstein equation, where the sum in the parentheses on the right side expresses the driving force. Mass conservation gives the void propagation velocity normal to the void surface, v_n, through the continuity equation,

$$v_n = -\nabla_s\mathbf{J_s}. \qquad (10)$$

The full simulation scheme including void nucleation and void evolution is presented in Fig. 2.

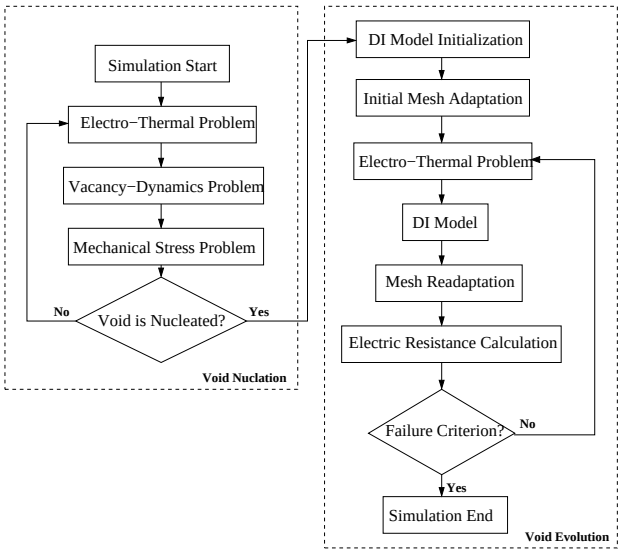

Figure 2: Two-phase electromigration simulation scheme.

V. THE EFFECT OF MICROSTRUCTURE

The network of grain boundaries influences vacancy transport during electromigration in several different ways. The diffusion of point defects in the grain boundary is faster compared to grain bulk diffusion due to the fact [21] 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

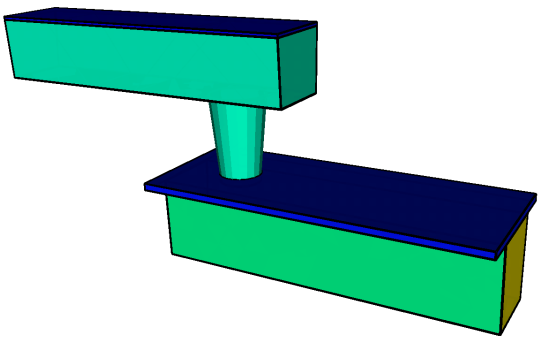

Figure 3: Typical dual-damascene layout used for simulation.

polycrystalline metals, grain boundaries are also recognized (together with dislocations loops) as sites of vacancy generation and annihilation [6, 10]. During the diffusion process vacancies generally seek to reach a concentration C_v^{eq} which is in equilibrium with the local stress distribution,

$$C_v^{eq} = C_v^0\exp\Big(-\frac{f\,\Omega\ \mathrm{tr}(\sigma)}{3\,k_B\,T}\Big). \qquad (11)$$

This tendency is supported by recombination mechanisms which are commonly modeled by a source function G (5).

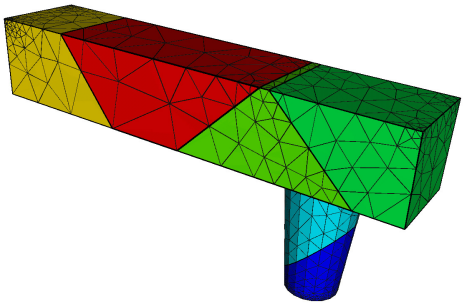

Figure 4: The copper segment is split into polyhedral grains and each polyhedron is separately meshed with initial mesh.

VI. SIMULATION RESULTS

In order to illustrate capabilities and consequences of the introduced models we consider two examples. The vacancy dynamics leading to void nucleation is studied for the case of a dual damascene architecture consisting of copper, capping, and diffusion barrier layers (Fig. 3), and void evolution for the case of a void nucleated in the bulk of the interconnect (Fig. 6). The copper segment is split into polyhedral grains (Fig. 4). For the solution of the governing equations (2)-(7) an in-house finite element code is used. The diffusion coefficient along the grain boundaries and the copper interfaces to the capping and barrier layers is assumed to be 5000 times larger than that in the bulk regions. The Rosenberg and Ohring recombination term G is assumed to be active only in the close vicinity of the grain boundaries. The vacancy concentration on both ends of the via is kept at the equilibrium level during simulation and all materials are assumed to be relaxed. The obtained vacancy distribution is presented in Fig. 5. Consistent with experimental results [22] the peak values of the vacancy concentration develop at the intersection lines of the grain boundaries and the capping layer. As a setting for a void evolution example we consider a two-dimensional, stress free, electrically conducting interconnect via. A constant voltage is applied between points A and B (Fig. 6). At B a refractory layer is assumed.

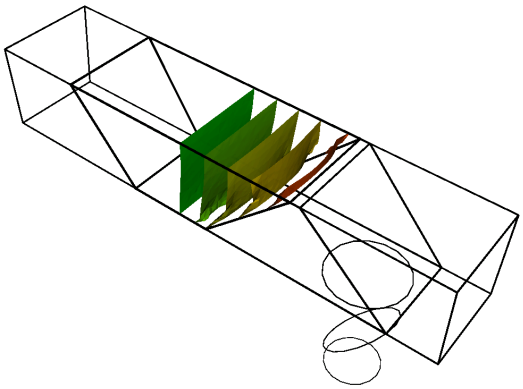

Figure 5: The peak value of vacancy concentration (displayed iso surfaces) is accumulated at the grain boundary/capping layer crossing line.

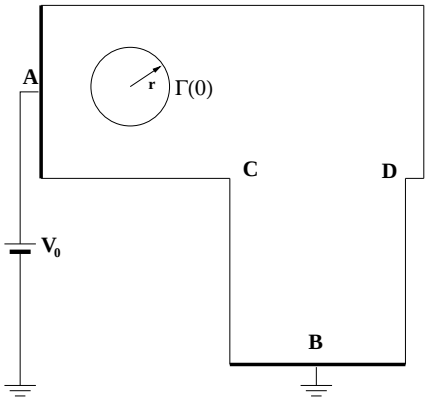

Figure 6: Interconnect via with initial void.

Because of geometrical reasons there is current crowding in the adjacencies of the corners C and D. High electrical field gradients in the area around the corner points increase the overall error of the finite element scheme, which is overcome by applying an additional refinement of the finite element mesh according to the local value of the electric field. A fine triangulated belt area which is attached to the void-metal interface [20] at the initial simulations step follows the interfacial area throughout the simulations whereby the interconnect area outside the interface is coarsened to the level of the inital mesh (Fig. 8).

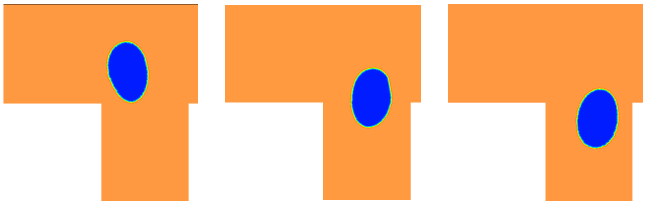

Figure 7: Void evolving through interconnect in the electric current direction

In our simulations a void evolving through the straight part of the interconnect geometry exhibits similar shape changes as observed in earlier models [17]. There is also no significant fluctuation of the resistance during this period of void evolution (Fig. 9). The situation changes, when the void evolves in the proximity of the interconnect corner. Due to current crowding in this area the influence of the electromigration force on the material transport on the void surface is more pronounced than the chemical potential gradient. This unbalance leads

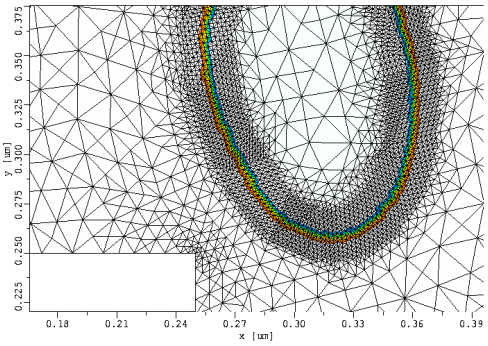

Figure 8: Refined mesh around the void in the proximity of the interconnect corner.

to higher asymmetry in the void shape then observed in the straight part of the interconnect. A void evolving in the proximity of the interconnect corner causes significant fluctuations in the interconnect resistance due to void asymmetry and position. The resistance change shows a charasteristical profile with the two peaks and a valley (Fig. 9). The extremes are more pronounced for

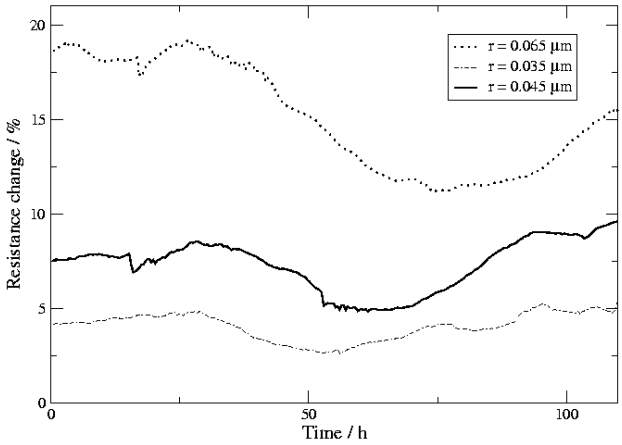

Figure 9: Time dependent resistance change during void evolution for the different initial void radius r.

larger initial voids. The capability of the applied adaptation scheme is also presented in the simulation of void collision with the interconnect refractory layer (Fig. 10).

Our simulations have shown that for all considered initial void radii, voids follow the electric current direction (Fig. 9) and do not transform in slit or wedge like formations which have been found to be a main cause for complete interconnect failure [23].

The applied diffuse interface model extends readily to incorporate additional physical phenomena such as anisotropy, temperature variations, and bulk and grain boundary diffusion.

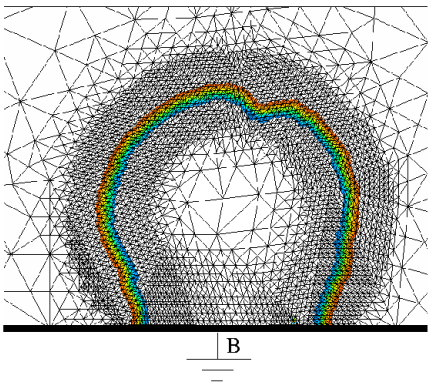

Figure 10: Mesh adaptation in the case of void collision with the refractory layer.

V. CONCLUSION AND OUTLOOK

The electromigration reliability analysis of modern inteconnects demands simulation tools which are based on comprehensive physical models. In order to predict an interconnect failure, modeling and analysis of complete life cycles of electromigration induced intrinsic voids are needed.

A careful analysis of the connection between the local vacancy dynamics and strain build-up must be carried out. The obtained relations have been coupled to an electromigration model using the concepts of stress driven diffusion and anisotropy of the diffusivity tensor. For correct physical handling of the grain boundary network as the network of high diffusivity paths and at the same time as sites of vacany recombination, a method of splitting a copper segment into grain segments is introduced. The grain boundary segments are treated as simulation sub-domains connected to each other by diffusive, mechanical, and electrical interface conditions. A dual-damascene architecture example layout is used to illustrate and verify the introduced modeling approach. The obtained simulation results qualitatively resemble the behavior observed in experimental investigations.

A governing equation for the void evolution is solved using the finite element scheme. A dynamically adapted mesh is maintained by a refinement-coarsening algorithm controlled by position, curvature, and width of the simulated void-metal interface, which distributes the mesh density in such a way that it allows efficient simulation of evolving voids through large portions of a complex interconnect geometry. Due to high electrical current gradients in the proximity of the interconnect corners and overall asymmetry of the electrical field, voids exhibit specific faceting which was not observed in the case of straight interconnect geometries.

The presented method is well suited for long time prediction of resistance change due to electromigration during the interconnect life time. The applied diffuse interface model can be extended readily to incorporate addi-

tional physical phenomena such as anisotropy, temperature variations, and bulk and grain boundary diffusion.

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