Microstructure and Stress Aspects of Electromigration Modeling

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Abstract. The modifications and extensions of standard continuum models used for a description of material transport due to electromigration with models for the copper microstucture are studied. Copper grain boundaries and interfaces are modeled as a network of high diffusivity paths. Additionally, grain boundaries act as sites of vacancy recombination. The connection between mechanical stress and material transport is established for the case of strain build up induced by local vacancy dynamics and the anisotropy of the diffusivity tensor caused by these strains. High diffusivity paths are set on the surfaces of polyhedral domains representing distintcive grains. These polyhedral domains are connected by diffusive, electrical, and mechanical interface models. For a numerical solution a three-dimensional finite element method is used.

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INTRODUCTION

The electromigration behavior of copper interconnects realized in damascene architecture indicates macroscopic and microscopic electromigration divergence sites. Macroscopic divergence sites exist at the cathode end of via bottoms where the barrier layer can be a blocking boundary for the electromigration flux. The sites where two or more grain boundaries intersect can be considered as microscopic electromigration divergence sites. In the cases where failures are induced far away from a via, it has been shown that their activation energies are often below the expected value for the grain boundary diffusion [1]. This is a strong indication that copper interfaces to the barrier and/or capping layer are dominant diffusion paths [1]. Considering interfacial diffusion as main contribution to electromigration was a significant simplification for modeling and simulation of both void nucleation and void evolution [2, 3]. Surface treatment aiming at strengthening the copper/capping layer interface has been successfully applied to suppress interfacial diffusion [1, 4] and to increase electromigration life time. Reducing the diffusivity at the interfaces to the level of bulk and grain boundaries diffusivities necessities modeling of the grain boundary network and the crystal orientation in the grains. Moreover, intrinsic stress, introduced by the dual damascene process, has a strong impact on the bulk and grain boundary diffusion which has also to be considered [5].

The main challenge in electromigration modeling and simulation is the diversity of the relevant physical phenomena. Electromigration induced material transport is accompanied with the material transport driven by the gradients of material concentration, mechanical stress, and temperature distribution. A comprehensive, physically 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. In the present work we study a possible extensions of the vacancy transport model described in [2] in order to include effects of the copper microstructure and mechanical stress. characteristic features of an extended model are verified by a three-dimensional simulation example.

THEORETICAL BACKGROUND

The most comprehensive models of electromigration and accompanying phenomena are described by Mullins [6], Korhonen *et al.* [7], Sarychev *et al.*, and Kirchheim [8]. The major ideas and concepts of these models are set here into a general framework which enables their application to simulation of realistic three-dimensional interconnect layouts.

Vacancy Continuity

The bulk chemical potential of vacancies in a stressed solid can be expressed as [9, 10],

$$\mu(\sigma, C_v) = \mu_0 + \mu(0, C_v) + \frac{1}{3} f\,\Omega_a\,\mathrm{tr}(\sigma), \tag{1}$$

where, according to [9], the chemical potential in the absence of stress is:

$$\mu(0, C_v) = k_B T\,\ln\left(\frac{C_v}{C_v^0}\right). \tag{2}$$

C_v^0 is the equilibrium vacancy concentration in a stress free solid, μ_0 is the corresponding chemical potential, and σ is the tensor of the applied mechanical stress. A vacancy flux $\vec{J}_v$ driven by gradients of chemical potential and electromigration is given by,

$$\vec{J}_v = -\frac{C_v}{k_B T}\mathbf{D}(\mathrm{grad}\,\mu + |Z^*|e\,\mathrm{grad}\,\varphi). \tag{3}$$

φ is the electric potential which obeys Laplace's equation ($\Delta\varphi = 0$). Since a vacancy is a point defect with cubic symmetries and copper is an fcc crystal, the tensor of diffusivity $\mathbf{D}$ is diagonal ($\mathbf{D} = D_0\mathbf{I}$).

Vacancy transport fulfills the continuity equation,

$$\frac{\partial C_v}{\partial t} = -\,\mathrm{div}\,\vec{J}_v + G, \tag{4}$$

with G as a source function which describes the vacancy generation and annihilation process. The equations (1)-(4) model electromigration of vacancies in the perfect fcc monocrystal stressed by σ.

Mechanical Stress

Since atoms and vacancies have a different volume of about 20-40% [8], the migration and recombination of vacancies induce local stress build up.

Vacancy Migration

We consider a small test volume V inside the interconnect metal. If n atoms leave this volume and n vacancies enter it, due to the different volume of the single vacancy and atom ($\Omega_v/\Omega_a = f < 1$) the new volume will be,

$$V_{new} = V - n\Omega_a + nf\Omega_a. \tag{5}$$

The relative volume change in this case is

$$\frac{\delta V}{V} = \frac{V_{new} - V}{V} = -(1-f)\Omega_a \frac{n}{V} = -(1-f)\Omega_a \delta C_v, \tag{6}$$

where δC_v is the increment of the vacancy concentration. With a time derivative of (6) and the well known mechanical relationship between volume increase and strain [11]

$$\frac{\delta V}{V} = \varepsilon^m_{xx} + \varepsilon^m_{yy} + \varepsilon^m_{zz} = 3\varepsilon^m, \tag{7}$$

we obtain

$$3\frac{\partial \varepsilon^m}{\partial t} = -(1-f)\Omega_a \frac{\partial C_v}{\partial t}. \tag{8}$$

For the test volume V the vacancy continuity holds

$$-\operatorname{div}\vec{J}_v = \frac{\partial C_v}{\partial t}. \tag{9}$$

From (8) and (9) we obtain for the components of the migration strain tensor

$$\frac{\partial \varepsilon^m_{ij}}{\partial t} = \frac{1}{3}(1-f)\,\Omega_a \operatorname{div}\vec{J}_v \delta_{ij}. \tag{10}$$

Vacancy Recombination

Using the same concept as given above we calculate the new volume V_{new} as a result of production (annihilation) of n vacancies inside the initial volume,

$$V_{new} = V \pm nf\Omega_a. \tag{11}$$

Now we can express a relative volume change as,

$$\frac{\delta V}{V} = \frac{V_{new} - V}{V} = \pm f\Omega_a \delta C_v. \tag{12}$$

Using relation (7) and the time derivative we obtain

$$3\frac{\partial \varepsilon^g}{\partial t} = \pm f \Omega_a \frac{\partial C_v}{\partial t}. \tag{13}$$

The time derivative $\partial C_v/\partial t$ in this case is equal to the vacancy production/annihilation source function G. Thus the time change of the strain caused by vacancy recombination is given by,

$$\frac{\partial \varepsilon^g_{ij}}{\partial t} = \frac{1}{3} f\, \Omega_a\, G\, \delta_{ij}. \tag{14}$$

From (10) and (14), we obtain a kinetic relation for the strain caused by vacancy migration and recombination,

$$\frac{\partial \varepsilon^v_{ij}}{\partial t} = \frac{\Omega_a}{3}\Big[(1-f)\,\mathrm{div}\vec{J}_v + f\,G\Big]\delta_{ij}. \tag{15}$$

Stress Equilibrium

According to [9] the general form of the mechanical equilibrium equation is

$$\sum_{j=1}^{3} \frac{\partial \sigma_{ij}}{\partial x_j} = 0, \quad \text{for} \quad i = 1,2,3. \tag{16}$$

Taking into account the strain induced by vacancy migration and recombination we obtain [12]

$$\sigma_{ij} = (\lambda\, \mathrm{tr}(\varepsilon) - B\, \mathrm{tr}(\varepsilon^v))\delta_{ij} + 2G\varepsilon_{ij}, \tag{17}$$

where λ and G are Lame's constants and $B = (3\lambda + 2G)/3$ is the bulk modulus. The strain tensor ε^v is defined by relation (15).

Anisotropic Diffusivity

In the case of a homogeneously deformed cubic crystal with strain field ε the vacancy diffusivity tensor obtains additional contributions [13]

$$D_{ij} = D_0\, \delta_{ij} + \sum_{k,l=1}^{3} d_{ijlk}\, \varepsilon_{kl}, \tag{18}$$

where d_{ijlk} is the elastodiffusion tensor. Equation (18) shows that strain causes an anisotropy of the diffusivity tensor. A comprehensive analysis of the point defect jump frequencies in a strained solid and calculation of the elastodiffusion tensor components is provided in [5].

Microstructure

The network of grain boundaries influences vacancy transport during electromigration in several different ways. The diffusion of point defects inside the grain boundary is faster compared to grain bulk diffusion due to the fact [14] that a grain boundary generally exibits 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 polycrystalline metals, grain boundaries are also recognized (together with dislocations loops) as sites of vacancy generation and annihilation [8, 15]. During the diffusion process vacancies generally seek to reach a concentration C_v^{eq} which is in equilibrium with the local stress distribution,

$$C_v^{eq} = C_v^0 \exp\left(-f \frac{\mathrm{tr}(\sigma)\Omega}{3 k_B T}\right). \tag{19}$$

This tendency is supported by recombination mechanisms which are commonly modeled by a source function G in the form introduced by Rosenberg and Ohring [16],

$$G = -\frac{C_v - C_v^{eq}}{\tau}, \tag{20}$$

which means production of vacancies, if their concentration is lower than the equilibrium value C_v^{eq} and their annihilation in the opposite case. τ is the characteristic relaxation time [17]. The full understanding of the source function G is still missing but it surely has to comprise three processes: exchange of point defects between adjacent grains, exchange of point defect between grains and grain boundaries, and point defect formation/annihilation inside the grain boundaries.

SIMULATION EXAMPLE

We consider an interconnect via realized in dual damascene architecture consisting of copper, capping, and diffusion barrier layers (Figure 1). The copper segment is split into polyhedral grains (Figure 2). For the solution of the governing equations (1)-(4) an in-house finite element method 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 Figure 3. Consistent with experimantal results [18] the peak values of the vacancy concentration develop at the intersection lines of the grain boundaries and the capping layer.

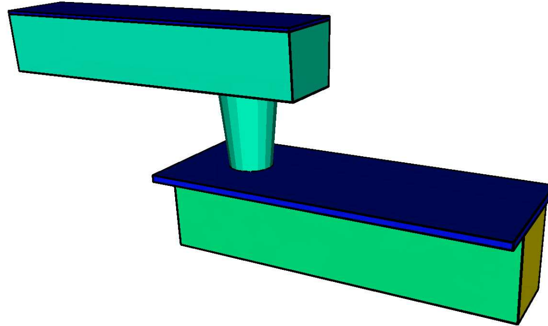

FIGURE 1. Typical dual-damascene layout used for simulation.

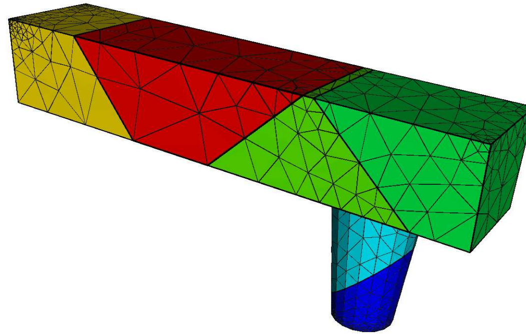

FIGURE 2. The copper segment is split into polyhedral grains and each polyhedron is separately meshed with initial mesh.

CONCLUSION

A careful analysis of the connection between the local vacancy dynamics and strain build-up has been 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 a 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, the method of splitting of 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.

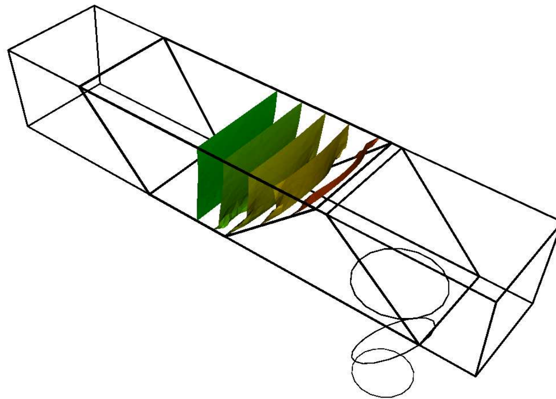

FIGURE 3. The peak value of vacancy concentration (displayed iso surfaces) is accumulated at the grain boundary/capping layer crossing line.

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.

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