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MORPHOLOGICAL STABILITY ANALYSIS OF POLYCRYSTALLINE INTERCONNECTS UNDER THE INFLUENCE OF ELECTROMIGRATION

K. E. Aifantis[1,2] and S. A. Hackney[2,3]

[1]Lab of Mechanics and Materials, Aristotle University of Thessaloniki, Thessaloniki, Greece
[2]School of Engineering and Applied Sciences, Harvard, Cambridge, MA, USA
[3]Materials Science and Engineering, Michigan Technological University, Houghton, MI, USA

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Abstract. Failure due to electromigration is one of the limiting factors encountered in reliability of integrated circuits. The key to fully understanding the morphological changes in metal interconnect lines in the presence of an electric field is to account for the variations of the electromigration flux as a function of the underlying factors, such as the microstructure. Although there is significant experimental and numerical simulation evidence documenting that grain structure is related to electromigration damage, a general analytical treatment that can explicitly account for such microstructure is lacking. In the present study the perturbation method is employed for the first time to the electromigration process in order to develop a general analysis of how morphological stability is correlated to microstructure induced spatial variations in the effective diffusivity.

1. INTRODUCTION

The lifetime of integrated circuits is dictated by the mass transport which occurs in metal lines upon application of an electric field (electromigration). As the electrons flow in the material, the atoms drift along the electron wind direction and depending upon the microstructure of the line, void (accumulation of vacancies due to atom movement) and hillock (accumulated mass extruding from the surface) formation takes place. This defect formation, which is accompanied by mechanical damage, leads to failure of such systems.

The investigation of the relationship between stress and electromigration has been investigated for at least 35 years. Studies concerned with electromigration can be classified into two main categories: 1) the first category investigates how the microstructure of the metal affects electromigration; these studies have shown that void and hillock formation takes place at areas in which the diffusion coefficient changes from the bulk value, such as at grain boundaries, surfaces, and interconnects [1-4]; 2) the second category is concerned with the stress evolution and distribution that is associated with void growth [5-7].

The present study combines both of the above approaches so as to try and relate the microstructure of metal lines with the stress associated with void growth. Of particular interest to this paper is the causative relationship established between flux divergence, microstructure and void/hillock pair electromigration damage. Many investigators have proposed that an electromigration flux divergence

Corresponding author: K. E. Aifantis, e-mail: kaifanti@seas.harvard.edu

resulting in electromigration damage may be correlated to grain structure within the conducting line (e.g. [1-4]). However, this tendency for flux divergence to create electromigration damage is balanced by the development of flux divergence induced stress gradients which oppose electromigration hillock/void damage [8-10]. Blech [8-10] was perhaps the first to quantify the balance between electromigration induced hillock/void formation and the stabilizing electromigration induced stress. The Blech stability condition is based on the examination of lines that were so short that the hillock formed at the cathode end of the wire and the void formed at the anode end of the wire. Blech *et al.* proposed the stability condition that the threshold for electromigration damage occurs when

$$j \cdot \lambda = \frac{\Omega \cdot \Delta\sigma}{eZ^{*}\rho}, \tag{2}$$

where j is the current density, λ the length of the conducting line, eZ^{*} the effective charge, ρ the resistivity, Ω the atomic volume and $\Delta\sigma$ is the stress differential caused by electromigration (or imposed artificially).

For very thin lines with high values of j, it is observed that line damage associated with hillock/void growth occurs along the length of the lines and is often correlated with grain boundary geometry and other interfaces [11]. The occurrence of hillock/void electromigration damage along the length of polycrystalline lines, and not just at the ends of the lines, has lead to investigations of correlations with microstructure, particularly grain structure. The correlation of grain boundary triple point geometry with electromigration flux divergence and resulting stress development has been explicitly analyzed theoretically in [12] and experimentally in [13]. In [12] it is pointed out that "geometrical divergences occur at grain boundary triple points, where the number of flux carrying paths in the region differs…and would be expected to give rise to damage". According to [13], "The electromigration flux, at low temperatures concentrated in the grain boundaries, is disturbed where a continuous path of grain boundaries is interrupted. This situation is schematically depicted in Fig. 1a. At the cathode end of the grain boundary path voids form, while at the anode end hillocks may form, as illustrated in the scanning electron microscopy (SEM) micrograph in Fig. 1b". Fig. 1 is adapted from [13] to qualitatively illustrate how an area averaged (with effective diffusivity, D_{eff}) would vary with position relative to the grain structure. Note that in Fig. 1a (according to [13]) the tensile stress that

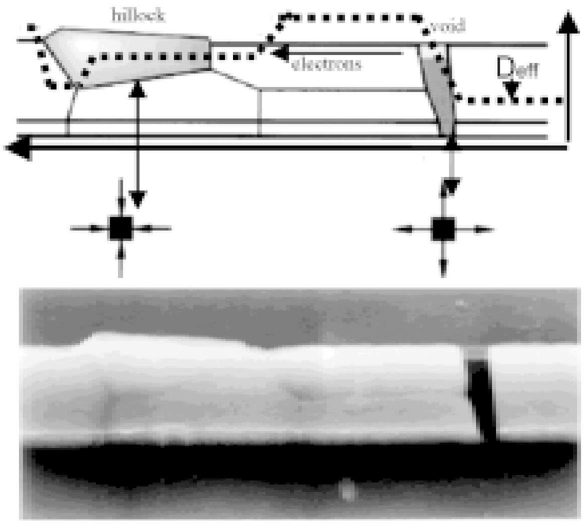

Fig. 1. Adapted from Kraft [13]. (a) Schematic, showing qualitatively how the diffusion coefficient varies along the electron wind flow direction as the microstructure changes. (b) SEM micrograph depicting the effects of electromigration in a 1.8μm wide Al wire (j=1.4M/cm^2, T=227 °C); it can be seen that the hillock and void formed at triple junctions.

supposedly develops at the triple junction (where the void forms) is due to a positive flux divergence while the compressive stress that develops at the hillock triple junction is due to a negative flux divergence (flux in the positive direction).

There is a broad agreement among the experimental and numerical simulation works that grain microstructure induced flux divergences are important to electromigration damage and production of mitigating stress gradients. However, there is no general treatment of electromigration that describes the influence of grain microstructure in an expression analogous to Eq. (1). This paper will employ the method of small perturbation to develop an expression analogous to Eq. (1) which incorporates the influence of microstructure through a smoothly varying 'effective' diffusivity that is a weighted average of the volume and boundary diffusivities. The use of the perturbation method in the analysis of interface and surface instability is well established in the materials science literature [14-21]. However, it does not appear that such an analysis has been undertaken in the examination of electromigration void/hillock formation coupled to spatial variations in the diffusion coefficient.

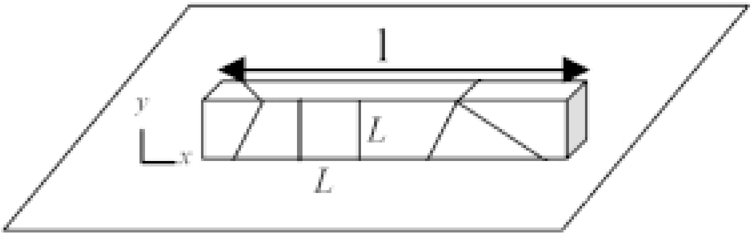

Fig. 2. Configuration of geometry considered.

2. THEORETICAL FORMULATION

The geometry to be considered in the sequel is a thin metal line (height=width=L) deposited on a planar substrate (Fig. 2) such that unconstrained expansion/contraction may occur normal to the substrate, while material in the line is constrained in the plane of the substrate. Following [2] the stress (σ) rate for this geometry (Fig. 2) is postulated to be given by

$$\frac{\partial \sigma}{\partial t} = \frac{E}{(1-\nu)kT}\left[\frac{\partial}{\partial x} D_{eff}(x)\left(\Omega \frac{d\sigma}{dx} + eZ^{*}\rho j\right)\right], \quad (2)$$

where: t is time, E the elastic modulus, ν is Poisson's ratio, k is Boltzmann's constant, T the temperature, Ω the atomic volume, eZ^{*} the effective charge, j the current density and $D_{eff}(x)$ the effective diffusivity as a function of position. The diffusion coefficient is allowed to be a function of position so as the local microstructure (triple junctions, grain boundaries) may be accounted for. As in [2] surface energy terms are neglected.

In order to examine the morphological stability of the conducting line, it is necessary to relate the state of stress to the change in the height of the unconstrained surface. We will follow Yost *et al*. [22] in relating flux divergence to atomic displacement, where a flux divergence results in a net deposition or removal of mass, and the resulting stress free displacement for a film of thickness L is considered to have magnitude τ, giving a stress free strain of τ/L. For plane stress, the stress for the two principle directions in the plane of the substrate is then

$$\sigma(x,t) = -\frac{\tau(x,t)}{(1-\nu)L}E, \quad (3)$$

while the displacement in the free surface of the film, $y(x,t)$, is

$$y(x,t) = \tau(x,t)\left[\frac{1+\nu}{1-\nu}\right]. \quad (4)$$

Eliminating τ from Eqs. (3) and (4) gives the required relationship between the stress and the free surface morphology, and thus allows Eq. (2) to be rewritten as

$$\frac{\partial y}{\partial t} = \frac{(1+\nu)L}{kT(1-\nu)}\frac{\partial}{\partial x}\left[D_{eff}(x)\left(\frac{\Omega E}{(1+\nu)L}\frac{dy}{dx} - eZ^{*}\rho j\right)\right]. \quad (5)$$

It is necessary now to account for the presence of grain boundaries in the wire through the term D_{eff} following the work of Baker *et al.* [1]. In [1] it was suggested that a linear combination of the volume diffusivity and the grain boundary diffusivity, each term weighted by their respective area fraction, can produce an effective diffusivity controlling the total mass transport during electromigration. We modify the Baker approach [1] slightly to incorporate the dot product of the current direction unit vector (***q***) and the unit vector direction of diffusion in the plane of the grain boundary (***r***), and to also allow for the possibility that more than one grain boundary exists in any given line cross section

$$D_{eff}(x) = D_{volume} + \sum_{s=1}^{N}\frac{Area_{gb}(s)(q\cdot r(s))}{Area_{line}}D_{gb}, \quad (6)$$

where the $Area_{gb}$ and $Area_{line}$ refer to cross sectional areas of the grain boundary and conducting line in sections perpendicular to the line direction, respectively. For bamboo type grain structures, the effective diffusivity is expected to have spatial variations relative to the average diffusivity D correlated with the "geometrical divergences" [12] caused by the grain structure. That is, the presence of the grain boundaries provides a perturbation on the average diffusivity. For this case, a truncated Fourier cosine series is used to approximate $D_{eff}(x)$ as

$$D_{eff}(x) = \bar{D} + \sum_{n=1}^{N} A_n \cos\left(\frac{2\pi nx}{\lambda}\right), \tag{7}$$

where λ is the line length. In keeping with the perturbation method, the sum over the Fourier coefficients for all x is assumed to be small relative to the average diffusivity, $\sum_{n=1}^{N} A_n << \bar{D}$. Note that this makes no statements concerning the magnitude of individual Fourier coefficients as A_n may be positive or negative. Inspection of Eq. (5) in the context of the linear perturbation theory and orthogonality of sine and cosine functions suggests that $y(x)$ be written as a truncated Fourier sine series about the average $y(t)$=0 using a time dependent Fourier coefficient.

$$y\left(x,t\right) = \sum_{n=1}^{N} B(t)_n \sin\left(\frac{2\pi nx}{\lambda}\right). \tag{8}$$

A linear analysis of Eq. (5) is possible when $[\sum_{n=1}^{N} B(t)_n] \times [\sum_{n=1}^{N} A_n] \approx 0$, and then substitution of Eqs. (7) and (8) into Eq. (5), followed by application of the orthogonality of sine functions leads to

$$\frac{dB(t)_n}{dt} = \frac{\Omega E}{kT(1-\nu)} \bar{D} B(t)_n \left(\frac{2\pi n}{\lambda}\right)^2 - \frac{(1+\nu)}{kT(1-\nu)^3} eZ^* \rho j A_n \left(\frac{2\pi n}{\lambda}\right). \tag{9}$$

The simplest stability analysis that can be made based on the above formulation is to consider the case where growth of amplitudes of specific surface morphology frequencies does not take place, i.e. $dB(t)_n / dt = 0$.

$$\left(E\frac{(1-\nu)}{(1+\nu)L} B(t)_n\right)\left(\frac{2\pi n}{\lambda}\right) = \frac{eZ^* \rho j}{(1-\nu)\bar{D}\Omega} A_n . \tag{10}$$

Of course, if there is one dominant frequency, then the peak of the periodic surface undulation will correspond to a hillock and the valley to a void. We note that

$$2E\frac{(1-\nu)}{(1+\nu)L} B(t)_n = \Delta\sigma(t)_n$$

leading to a form of Eq. (10) suitable for direct comparison with Eq. (1)

$$j \times \frac{\lambda}{n} = \left(\frac{1}{2}\right) \frac{\Omega \pi \bar{D}(1-\nu)}{eZ^* \rho} \frac{\Delta\sigma(t)_n}{A_n}. \tag{11}$$

Thus, for a dominant surface morphology frequency, the distance between a void and a hillock is λ/(2n), where n is the index of the Fourier coefficient associated with the stress differential and the spatial variation in the effective diffusion coefficient. Eq. (11) then predicts how magnitude of the "geometrical divergences" [12] of the grain structure, represented by the magnitude of the Fourier coefficient, A_n, can influence the morphological stability at specific spatial frequencies. For the case where Eq. (11) is satisfied for a specific spatial frequency, (2πn)/l, and this frequency is correlated to a possible void/hillock pair, the distance between a hillock and a void below which the hillock/void pair will not grow is predicted to be l/(2n).

3. CONCLUSIONS

The new result embodied by Eq. (11) offers the first general analytical treatment incorporating grain structure into the Blech stability equation. If we divide Eq. (11) by Eq. (1), we obtain a stability criterion which includes a descriptor of the microstructure influence

$$n = \frac{A_n}{\pi \bar{D}(1-\nu)}. \tag{12}$$

Eq. (12) sets stability criteria by defining the relationship between the spatial frequency and amplitude for zero growth rate of surface perturbations. The value of n corresponding to the zero growth condition depends on the ratio of the local perturbation of the effective diffusivity (A_n) and the averaged effective diffusivity ($\bar{D}$). Thus, Eq. (12) reflects the qualitative statements of [12,13] in a general, quantitative result. The precision of the predictive power may be somewhat limited because of the smoothing action of Eq. (7) and the reliance on linearization. However, the result does reveal the physics behind experimental observations and will assist in the interpretation and configuration of numerical and *ab initio* simulations.

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