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A finite-element analysis of in-grain microcracks caused by surface diffusion induced by electromigration

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ABSTRACT

Based on the classical theory of surface diffusion and evaporation–condensation, a finite-element method is developed for simulating the shape instability of in-grain microcracks in metallic materials caused by surface diffusion induced by electromigration. The validity of the method is confirmed by the agreement of the numerically simulated migration behavior, of a small, circular void with that predicted theoretically. The results indicate that the microcrack shape is governed by the electric field, χ, and the initial aspect ratio of the microcrack, β, and there exist critical values for these parameters. When $\chi < \chi_c$ or $\beta < \beta_c$, the microcrack will evolve into a stable shape as it migrates along the conductor, while when $\chi \geqslant \chi_c$ or $\beta \geqslant \beta_c$, the microcrack will split into two smaller microcracks. The splitting time of the microcrack decreases with an increase in the electric field or the aspect ratio, indicating that the increase of the electric field or the aspect ratio accelerates microcrack splitting. In addition, the critical electric field χ_c decreases as the aspect ratio increases, and the critical aspect ratio β_c decreases as the electric field increases. In other words, the increase of the electric field or the aspect ratio is beneficial to microcrack splitting.

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1. Introduction

With the development of miniaturization and integration of microelectronic systems, the feature size on the integrated circuit chip continues to decrease, following the sharp increase in current density. However, scattering by a high current density enhances atomic displacement in the direction of the electron flow. The enhanced atomic displacement and the accumulated effect of mass transport under the influence of an electric field (mainly, electric current) are called electromigration (Tu, 2003). The main causes of electromigration failures in metallic materials are the non-homogenous distribution of physical characteristics and some defects, such as voids and cracks (Zhang et al., 2006). It is therefore essential to understand microcrack evolution caused by the diffusion processes of electromigration so that the failure mechanism can be understood and controlled to achieve a desired engineering requirement.

The main research methods in microstructure evolution can be divided into experimental observation and numerical simulation. It has been observed experimentally that a high density of nanometer-sized bubbles exists in the aluminum and electromigration-induced voids form away from the interconnect sidewall (Lee et al., 2002). Failures often occur when a void changes its shape to form a crack-like slit oriented perpendicular to the line, which causes an open circuit (Arzt et al., 1994; Wang et al., 1996). In situ scanning electron microscope investigations suggested that the mass transport during electromigration mainly occurs along the material surface (Meyer et al., 2002; Huang et al., 2009). Extensive efforts have been made to simulate the evolution of microstructures. Many of them focus on modeling electromigration-induced diffusion via phase-field methods (Gugenberger et al., 2008; Kassner et al., 2010; Sadasiva et al., 2012; Meca et al., 2013) or finite difference with boundary element methods (Averbuch et al., 2003; Choy et al., 2004). Some progress has been made in developing finite-element methods to solve problems. Three-dimensional finite-element methods were developed to simulate the current density distribution in a flip-chip solder joint (Liang et al., 2007), obtain the electric fields with the migration failure (Liu et al., 2008) and predict the critical conditions necessary to nucleate electromigration-induced voids (Singh et al., 2010). However, two-dimensional finite-element methods are most prevalent. Electromigration-induced void nucleation, growth and evolution have been extensively studied by the finite-element method (Bower and Shankar, 2007; Wei et al., 2008; Yao et al., 2009; Dwyer, 2010; Maroudas, 2011). The results showed that increasing parameters such as the electric field strength or the void size may lead to morphological transitions from steady to

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time-periodic states, once certain critical values are exceeded (Maroudas, 2011).

Sun and Suo (1997) first built a weak formulation incorporating surface diffusion and evaporation–condensation, which formed the basis of the finite-element method for simulating large shape change due to surface diffusion. They used this idea to develop a general finite-element program for analyzing thermal grooving on a polycrystalline surface. Their approach has since been extended and applied to a range of problems. Huang et al. (2003a,b) and Huang and Sun (2004) simulated the morphological evolution of two-dimensional and three-dimensional microcracks, and the results showed that microcrack evolution was not only sensitive to its initial shape but also influenced by the environment. Yu and Suo (1999) and Liu and Yu (2006) found that the pore-grain boundary separation condition was insensitive to the dihedral angle and the influence of the mobility ratio of surface diffusion and evaporation–condensation on the surface grooves. He and Huang (2014) simulated the shape instability of in-grain microcracks caused by surface diffusion induced by stress migration, and found that the microcrack might split into three parts under certain conditions. Most works on the microstructure evolution induced by electromigration are on the basis of the weak formulation including electric field and curvature (Bower and Shankar, 2007; Xia et al., 1997; Fridline and Bower, 1999; Wang et al., 2006). However, the weak formulation including surface diffusion and evaporation–condensation induced by electromigration has not been reported in the literature up to now.

In the present paper, based on the work of Sun and Suo (1997), a finite-element formulation is developed to model the morphological evolution of an intragranular microcrack controlled by surface diffusion induced by electromigration. The problem to be solved is illustrated in Fig. 1. The conductor is idealized as a two-dimensional single crystal with a microcrack forming symmetrically along the axis of the conductor, which conducts electric current according to Ohm's law. The conductor is subjected to voltage V_0, and the distribution of voltage in the boundary is uniform. We assume that the conductor deforms in a state of plane strain and that the electric field in the conductor has no component normal to the plane of the figure. Diffusion through the bulk is assumed to be negligible. Therefore, in the absence of grain boundaries, the only mode of mass transport is diffusion along the microcrack surface. We have assumed that the surface energy of the solid is isotropic, in which case the energy-minimizing shape is a cylinder, and the surface energy does not interfere with the electric field energy.

For simplicity, the microcrack is characterized by the aspect ratio $\beta = a/h_0$, where a is the initial semi-major axis of the microcrack, h_0 is the initial semi-minor axis (taken as 0.1 in all calculations if not specifically indicated), L is the length of the conductor, and H is the width.

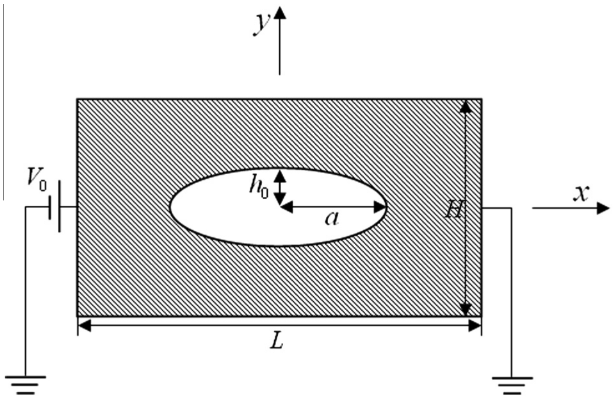

Fig. 1. A simplified model of an in-grain microcrack in a conductor under an electric field.

The remainder of this paper is organized as follows: in the next section we first briefly describe the weak formulation used in the model, that governs the coupled processes of surface diffusion and evaporation–condensation induced by electromigration and a brief description of the algorithm is provided. Section 3 proves the accuracy of the algorithm. Section 4 shows the surface morphology evolution of the microcracks under different electric fields and aspect ratios, and discusses the corresponding effects. The major conclusion will be presented in Section 5.

2. Basic theory

2.1. Weak formulation for combined surface diffusion and evaporation–condensation

Imagine two concurrent processes on a solid surface: the solid matter can relocate on the surface by diffusion and exchange with the surrounding vapor by evaporation–condensation. The general weak formulation for two-dimensional case was listed in Sun and Suo (1997). It is listed for self-containment of this paper.

Define the driving force for surface diffusion, F, as the free energy decrease associated with the amount of matter per unit volume moving per unit distance on the surface and the driving force for evaporation–condensation, p, by the free energy reduction associated with the amount of matter per unit volume added to per unit surface area of the solid. Following the principle of virtual work (Yang and Suo, 1996), we have:

$$\int_{\text{surface}} F \cdot \delta I ds + \int_{\text{surface}} p \cdot \delta i ds = -\delta G \tag{1}$$

where δI is the virtual mass displacement associated with surface diffusion, δi is the virtual volume of mass deposited from the environment on a unit area of the solid surface and δG is the free energy increment associated with the above virtual motion of the surface.

Based on Herring's classical theory (Herring, 1951), the kinetic law at every point on the grain surface can be described as that the flux of surface diffusion J is proportional to the driving force F:

$$J = MF \tag{2}$$

where M is the mobility of atoms on the surface. In this paper, the mobility is assumed to be isotropic and represented by a number

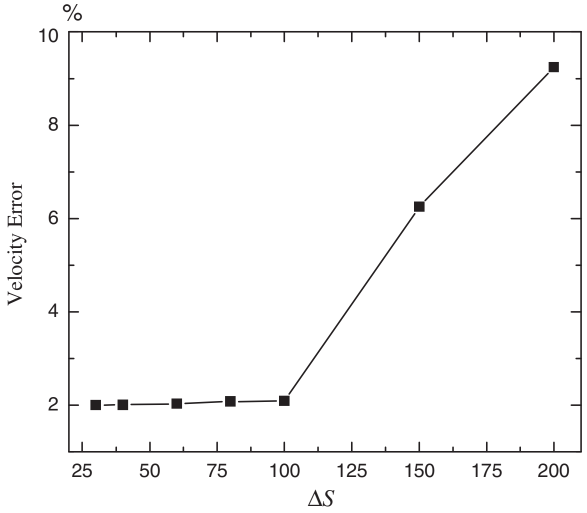

Fig. 2. The error of the void migration velocity as a function of ΔS for $\chi = 0.14$.

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