Journal of the Korean Crystal Growth and Crystal Technology
Vol. 14, No. 2 (2004) 58-62

Effect of anisotropic diffusion coefficient on the evolution of the interface void in copper metallization for integrated circuits

J.H. Choy†

Department of Physics, Simon Fraser University, Canada

(Received March 16, 2004)
(Accepted March 24, 2004)

Abstract The shape evolution of the interface void of copper metallization for intergrated circuits under electromigration stress is modeled. A 2-dimensional finite-difference numerical method is employed for computing time evolution of the void shape driven by surface diffusion, and the electrostatic problem is solved by boundary element method. When the diffusion coefficient is isotropic, the numerical results agree well with the known case of wedge-shape void evolution. The numerical results for the anisotropic diffusion coefficient show that the initially circular void evolves to become a fatal slit-like shape when the electron wind force is large, while the shape becomes non-fatal and circular as the electron wind force decreases. The results indicate that the open circuit failure caused by slit-like void shape is far less probable to be observed for copper metallization under a normal electromigration stress condition.

Key words Electromigration, Void, Copper metallization, Surface diffusion

1. Introduction

Modern integrated circuit (IC) technology scales the minimum feature size down to 0.13 μm for the commercial chips. In accordance with the aggressive scaling, there has been high demand for electrically lower resistive interconnecting material, and for the insulator with lower dielectric constant (low-k), in order to reduce resistance-capacitance (RC) time delay of the circuit. Copper (Cu) has already been adopted as the interconnecting material due to its lower electrical resistivity compared to aluminum (Al) metallization (by 40%). In addition, Cu is known to have higher activation energy for atomic diffusion through grain boundaries and lattice, and offers the improved resistance against electromigration compared to that of Al metallization [1]. Being one of the major reliability issues of the IC metallization, electromigration is the atomic transport induced by the momentum transfer from electron "wind" to atoms when a relatively large current density flows along the interconnects [1, 2]. Table 1 lists the activation energies for atomic diffusion of Cu and Al-base metallization along major paths [1, 3-5]. As shown in Table 1, grain boundary diffusion offers the fast diffusion path for Al metallization. As the line width shrinks, the number of such fast diffusion paths decreases since the microstructure becomes near-bamboo, in which the grain boundaries align perpendicular to the length direction in order to reduce the energy associated with them. Even in this case, however, experimental studies report short lifetime against electromigration stress by the development of a transgrannular void [6-9]. It is now well known that a void may develop its shape into a slit-like shape across the metal cross section, and cause open circuit failure within a short time since it does not require a large volume. Modeling studies were performed to simulate the failure mechanism in bamboo Al metallization, and concluded that a relatively large size void may change its shape into a slit-like void by surface diffusion when the diffusion coefficient is anisotropic [10-14].

Table 1
Activation energies (eV) for diffusion along the major pathways

Material	Grain boundary	Interface	Lattice	Surface
Al/Cu	0.7	0.9~1.0	1.2	-
Cu	1.2	0.7~1.0	2.3	0.7

For Cu metallization system, however, the failure caused by slit-like void has not been observed even though the line width and thickness becomes smaller than those of Al metallization. Instead, voids forming and growing along the Cu/Si_3N_4 interface and grain boundaries are frequently observed [15, 16]. The problem with the less adherent Cu/Si_3N_4 interface is well known as the interface offers the major void nucleation site as well as fast diffusion path [1, 17-19]. As the interconnecting tech-

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†Corresponding author
Tel: +604-291-4082
Fax: +604-291-3592
E-mail: junhoc@sfu.ca

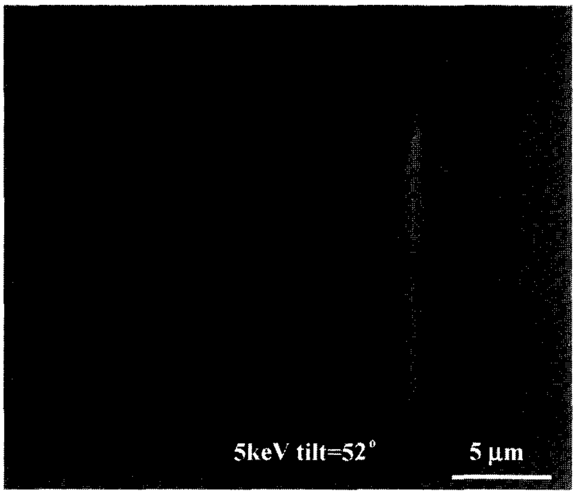

Fig. 1. SEM observation of the IMD (inter-metal dielectric) delamination at Cu/low-k dielectric interface. The sample image is tilted 52°. Focused ion beam is used to make the cross section.

nology moves on to adopt low-k dielectric, the problem is likely to persist. Figure 1 shows, as an example, the sample failed by delamination after cyclic thermal stress of 100°C. The sample employs the dual damascene Cu metallization with low-k inter-metal dielectric. The cross section image of the failed site was prepared by focused ion beam and scanning electron microscope. The arrow in the photo indicates the delamination occurred at Cu/low-k dielectric interface. There are, however, the experiments reporting the improvements on the interface adherence, where the Cu/barrier metal interface becomes the dominant diffusion path for electromigration voiding [20, 21]. Therefore, it is also instructive to predict whether the fatal slit-like void will be formed for Cu metallization or not. In the present study, we will employ the 2 dimensional finite difference numerical method for void shape evolution under a conserved void volume.

2. Modeling Method

The numerical scheme is divided into 2 parts. The first part treats the time evolution of the void shape by solving the forth-order partial differential equation for surface diffusion using finite-difference method. The method is well described in the previous shape evolution studies [22, 23]. The second part is essential to obtain the electrostatic potential along the Cu/void surface. The boundary element method has been shown to be quite efficient for this type of the electrostatic problem [12, 14].

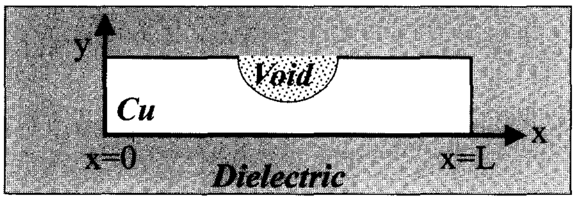

Fig. 2. A 2-dimensional model of a copper metallization with a void located at the Cu/dielectric interface.

A 2-dimensional model of a copper wire is illustrates in Fig. 2, with an interface void located on the copper/dielectric interface. The shape evolution of the void with an externally applied electric potential along the wire of length, L, is simulated, assuming that diffusion along the void surface dominates the atomic transport. The surface atomic flux takes the form [2, 11-14]:

$$J_s = M[\Omega\gamma_s(\partial\kappa/\partial s) - Z^* eE_s], \qquad (1)$$

where the first term is the capillary force, and the second term is the electron wind force. M refers to the surface atomic mobility and is given by $D_s\delta_s/[\Omega kT]$, where D_s is the surface diffusivity, δ_s is the thickness of the surface layer, Ω is the atomic volume, k is Boltzmann constant, and T is temperature. γ_s is the specific Cu surface free energy, κ is the surface curvature of the void, Z^* is the effective charge number, $e = 1.6\times10^{-19}$ joules, and E_s is the tangential component of the electric field along the void surface. The surface normal growth rate, v_n is expressed by equation (2),

$$v_n = -\Omega(\partial J_s/\partial s) \qquad (2)$$

Equation (2) is solved for the time evolution of the surface profile, y(x), using a finite-difference method. The void shape is assumed to have 2-fold symmetry (with Cu/dielectric interface as the mirror plane), in order to keep consistency with the earlier studies for Al metallization [11-14].

In the electrostatic problem, the E_s is obtained by solving the Laplace equation:

$$\partial^2\phi/\partial x^2 = 0,\ E_s = -\partial\phi/\partial s, \qquad (3)$$

where ϕ refers to the electric potential. The boundary conditions are given by,

$$\phi(0) = V_H,\ \phi(L) = V_L, \text{ and,}$$
$$\partial\phi/\partial n = 0 \text{ along the surface and interface} \qquad (4)$$

Where V_H and V_L are constants, and $V_H > V_L$. n refers to the unit surface normal. The boundary element method solves equation (3) by discretizing the surface

Table 2
Physical properties of Cu and Al. + denotes the values at high temperature, 600 K for Cu, and 500 K for Al, respectively [11]

Item	Cu	Al
Z^*	5	10~20
$\Omega(m^3)^+$	1.18×10^{-29}	1.66×10^{-29}
$\gamma(joules/m^2)^+$	1.7	1
$\rho(\Omega\text{-}m)$	1.67×10^{-8}	2.74×10^{-8}

alone. The computation length, L must be large enough to ensure that at $x = 0$, and $x = L$, E_s approaches E_o, the average electric field far from the void which is given by $E_o = -\Delta\phi/L$, where $\Delta\phi = V_L - V_H$. Following the study of Gungor and Maroudas [12], L is taken to be at least 40 times as large as the void size.

In the present study, physical parameters appropriate for a quarter micron copper wire at 600 K are adopted. Table 2 shows the parameters for Cu and Al, where the high temperature measurements are for 600 K for Cu, and 500 K for Al, respectively [11, 12]. The results will be described with some important dimensionless parameters. The electron wind intensity, χ, refers to the relative strength of the electron wind force with respect to the capillary force, and is defined in equation (5),

$$\chi \equiv Z^*ew^2E_o/[\Omega\gamma_s], \tag{5}$$

where, w is the void-free thickness of the Cu wire. For Al metallization, w has been taken as the void-free width of the wire as the sidewall surface damages during reactive ion etching are considered to offer sites for void nucleation. For copper wires, the typical electromigration stress condition with an applied current density, $J = 3\times10^6$ A/cm^2 and $T = 600$ K gives χ~4. Numerical time τ is defined as $\tau = \delta tD_s\delta_s\Omega\gamma_s/[R^4kT]$, where δt is in real time unit. For a copper wire with thickness 0.4 μm and $D_s = 3.3\times10^{-14}$ m^2/s at 600 K, τ is approximately 10 hours.

According to the data of Cu listed in Table 2, the electrical resistivity is smaller by a factor 2, the effective charge is smaller by a factor 2~4, and the surface energy is larger by 70%, compared to those of Al cases. All these factors contribute to an order of magnitude smaller χ for Cu relative to that of Al when the wire dimension w, and the stress condition are identical for both cases. Obviously, the role of anisotropy in surface diffusivity for Cu metallization may be investigated by decreasing χ from its typical value of Al metallization. The anisotropic surface diffusion coefficient may take the following form [11, 12]:

$$D_s = D_o[\,1 + A\cos^2(m\theta)] \tag{6}$$

where D_o is a constant, A refers to the strength of the anisotropy, m is the grain symmetry, and θ is local surface orientation, and is given by, $\tan\theta = dy/dx$. In this study, the specific case of $A = 10$, and $m = 1$, in which case the evolution of a void is known to lead to a slit-like void, and cause open circuit failure for Al metallization, will be employed.

3. Results and Discussion

The case for an isotropic diffusion coefficient is analyzed first. Figure 3 displays the evolution of a wedge void when $\chi = 150$. The electric field direction is from left to right, where the electron flow, and thus the atomic flux takes the opposite direction. The evolution time, τ is expressed in the unit of 10^{-4}. As the stress time increases, the wedge void bends toward the electric field direction. The void translation in the direction parallel to the electric field is also observed. After a long time evolution ($\tau = 8.1\times10^{-4}$), the shape of the void becomes non-fatal compared to the initial wedge shape as the void dimension across the cross section decreases. The results are in agreement with Gungor and Maroudas [12], but certainly in disagreement with Kraft and Arzt [11], where the evolution of the wedge void results in open circuit failure. The subsequent modeling studies support the result of Gungor and Maroudas [14, 24].

In Fig. 4, the anisotropic diffusion coefficient, $D_s/D_o = 1 + A\cos^2\theta$ where $A = 10$, is employed in the evolution of initially semi-circular voids with radius, $r_i = 0.6w$. For each case, the intensity of the electron wind force is given by (a) $\chi = 20$, (b) $\chi = 12$, (c) $\chi = 5$, (d) $\chi = 2$, and (e) $\chi = 1$, respectively. When χ is large such as (a) and (b), the slit-like void tip quickly develops across the cross section, and leads to the open circuit in relatively a short time, τ~7.5×10^{-4}. When χ decreases to 5 in (c), the slit-like shape still develops and leads to the open circuit, but time to reach the failure is delayed consider-

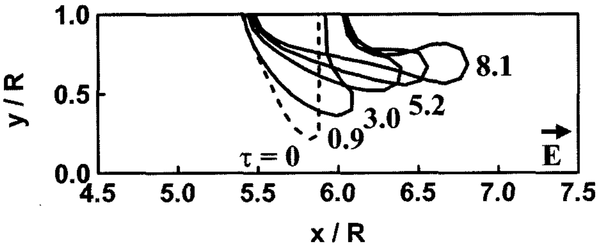

Fig. 3. Evolution of a wedge void. Isotropic diffusion coefficient and $\chi = 150$ are used in the computation. The evolution time, τ is in the unit of 10^{-4}.

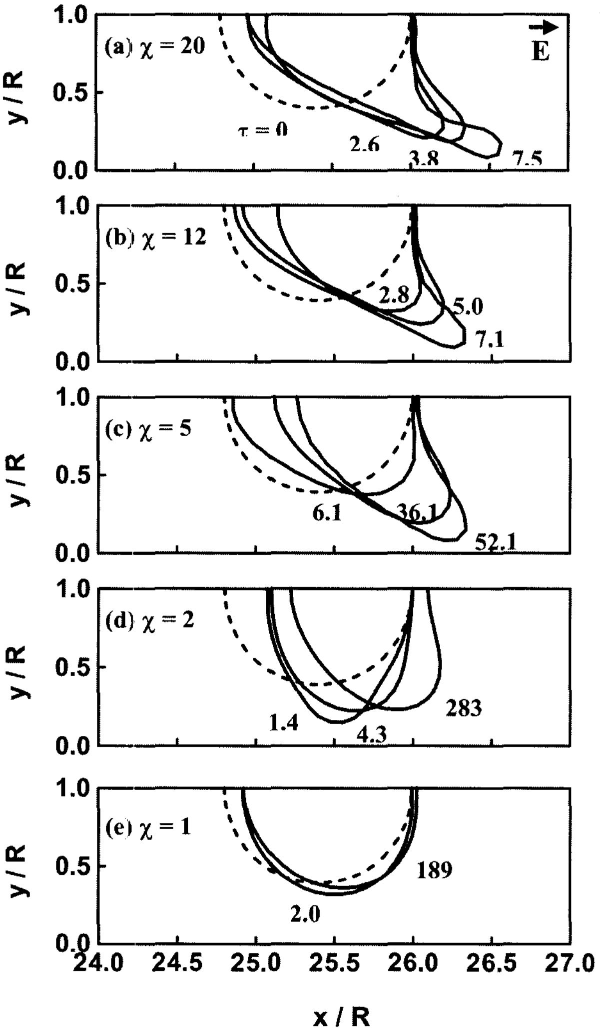

Fig. 4. Evolution of semi-circular voids with radius, r_i = 0.6w and an anisotropic diffusion coefficient with two-fold crystal symmetry (m = 1). The normalized diffusion coefficient is given by $D_s/D_0 = 1 + A\cos^2\theta$, where A = 10, and θ is local surface orientation. The intensity of the electron wind force is given by (a) $\chi = 20$, (b) $\chi = 12$, (c) $\chi = 5$, (d) $\chi = 2$, and (e) $\chi = 1$. The evolution time, τ is in the unit of 10^{-4}.

ably at, $\tau = 52\times10^{-4}$. For (d) and (e), where $\chi = 2$, and $\chi = 1$, respectively, the failure never occurs even for a longer time period. The increasing contribution of the capillary force over the electron wind force suppresses the development of the slit-like void tip, and makes the final shape more circular. The results show that under a typical electromigration test condition for Cu metallization where χ is smaller by an order of magnitude compared to that of Al metallization, a void may not develop a slit-like shape in its evolution process. Compared to Al metallization, the physical properties, mainly smaller electrical resistivity and effective charge of Cu decrease the electron wind force relative to capillary force on the shape evolution process.

4. Conclusions

A 2-dimensional finite-difference numerical method combined with a boundary element method is employed to study the effect of anisotropic surface duffision coefficient on the shape evolution of the interface void of copper metallization under electromigration stress. The numerical results show that the initially circular void evolves to become a fatal slit-like shape when the electron wind force is large, while the shape becomes nonfatal and circular as the electron wind force decreases. Therefore, under a normal electromigration stress condition of Cu where χ smaller by an order of magnitude compared to that of Al metallization, the open circuit failure induced by slit-like void shape is far less probable to be observed.

Acknowledgement

The author thanks Advanced Systems Institute for research support.

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