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MODELING ELECTROMIGRATION AND MICROPORES FORMATION IN THIN-FILM IC INTERCONNECTS

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ABSTRACT

The modern tendency for increasing the productivity of microelectronic devices at the expense of the size shrinkage and the development of densely packed multilevel microelectronic structures stipulates the rising concern for the reliability of integrated circuits (IC). In this work the summary of general physical models of electromigration, the stress generation, and the void formation is given. On the basis of the models mentioned the simulation of the void nucleation in a triple point of the interconnect polycrystalline structure, as well as modeling the fracture of a two-level metallization in the plug region is performed. For both cases characteristic sizes of voids and times to their nucleation are calculated numerically.

KEYWORDS

Integrated circuits failure, electromigration, mechanical stresses, void nucleation.

INTRODUCTION

The IC failures are mainly caused by the fracture of interconnects. Interconnect is a thin-film metal line deposited on a silicon substrate and covered with a passivation layer. Its characteristic sizes in a cross-section vary from approximately 0.1 μm to several microns, while length lies within 10-1000 μm. In microelectronic devices of today interconnects are generally arranged in multilevel metallizations. The neighboring layers are connected by vertical plugs.

The fracture of interconnects is initiated by the nucleation of micropores in the regions supersaturated by vacancies. The rise of supersaturation is caused by the current-induced vacancy transfer (electromigration). The fundamental role of electromigration is stipulated by extremely high current densities ($\sim 10^{10}$-10^{12} A/m^2) used in modern microelectronics. Numerous experiments reveal that electromigration in thin films proceeds predominantly along grain boundaries. Therefore, the crystalline structure heterogeneities like triple points, inclusions, intersections of grain boundaries with the line lateral surface are preferable sites for the void nucleation, since they invoke strong vacancy flux divergence leading, in turn, to the supersaturation evolving. Subsequent growth of micropores, resulting from the vacancy inflow, causes the interconnect fracture. In multilevel metallization voids also form in the vicinity of a plug where the spatial distribution of the electric current is strongly non-uniform. In this case the void nucleation competes with the line edge depletion conditioned by intensive vacancy outflow.

Redistribution of vacancies under the electric current impact causes the rise of spatially non-uniform volume deformations in an interconnect, which, in turn, lead to the generation of the heterogeneous mechanical

stress field. Stresses influence both electromigration and the void nucleation. One of the main features of the interconnect deforming consists in the presence of a constraint from a substrate and a passivation cover, which are stiffer than a line.
Therefore, the goal of this study is the development of non-linear self-consistent models for the vacancy electromigration, the mechanical stress evolution, and the void nucleation. In the next section the model for the kinetics of electromigration-induced mechanical stresses is described briefly. In the third section a summary of the void nucleation kinetic model is given. In the fourth section results of calculations for the void formation in a triple point of the interconnect crystalline structure and for the damage of a two-level metallization in the plug region are presented.

MODELING THE VACANCY DIFFUSION AND THE MECHANICALSTRESSES RISE UNDER THE ELECTRIC CURRENT IMPACT

The spatio-temporal distribution of vacancies satisfies the following diffusion equation [1]

$$\dot{C} + q_{i,i} = -\tau_s^{-1}\left(C - C_e\right), \tag{1}$$

where $C(x_1, x_2, x_3, t)$ is the concentration of vacancies; $\dot{C} \equiv \partial C/\partial t$; $q_i(x_1, x_2, x_3, t)$ is the i-the component of the vacancy flux; $q_{i,i} \equiv \partial q_i/\partial x_i$, $i = 1, 2, 3$ (here and below repeated indices denote summation); τ_s is the characteristic time of the vacancy generation/annihilation; $C_e(x_1, x_2, x_3, t)$ is the equilibrium concentration of vacancies determined as [1]

$$C_e = C_0 \exp\left(f_r'\Omega\sigma/k_B T\right), \tag{2}$$

where C_0 is the equilibrium concentration for lack of stresses; Ω is the atomic volume; $f_r' = 1 - f_r$, f_r is a parameter determining the relative contraction of an atomic cell on substituting an atom with a vacancy; $\sigma(x_1, x_2, x_3, t)$ is a spherical part of the mechanical stress tensor σ_{ij}; T is temperature; k_B is Boltzmann's constant. In general, when electromigration proceeds concurrently with the action of mechanical stresses, the vacancy flux has the following form [1]

$$q_i = D\left(-C_{,i} + Z^*\rho_0 j_i C/k_B T - f_r\Omega\sigma_{,i}C/k_B T\right), \tag{3}$$

where D is the vacancy diffusivity; $C_{,i} \equiv \partial C/\partial x_i$; $\sigma_{,i} \equiv \partial\sigma/\partial x_i$; Z^* is the effective charge of a vacancy; ρ_0 is the interconnect specific resistivity; $j_i(x_1, x_2, x_3)$ is the i-th component of the current density vector.
The rise of mechanical stresses in an interconnect is conditioned by heterogeneous volume deformations induced by electromigration of vacancies. As shown in [1,2], in the case considered the deformation rate $\dot{\varepsilon}_{ij}$ is determined as

$$\dot{\varepsilon}_{ij} = \dot{\varepsilon}_{ij}^{\sigma} + \dot{\varepsilon}_{ij}^{c} = C_{ijkl}\dot{\sigma}_{kl} + \Phi\delta_{ij}\,, \tag{4}$$

where $\dot{\varepsilon}_{ij}^{\sigma}$ is the deformation rate caused by mechanical stresses under fixed vacancy concentration; $\dot{\varepsilon}_{ij}^{c}$ is the deformation rate conditioned by the vacancy migration and the generation/annihilation processes for lack of stresses; C_{ijkl} is the compliance tensor; $\dot{\sigma}_{kl} \equiv \partial\sigma_{kl}/\partial t$; δ_{ij} is the Kronecker delta; $i, j, k, l = 1, 2, 3$;

$$\Phi = \Omega\left\{f_r q_{i,i} - f_r'\tau_s^{-1}\left(C - C_e\right)\right\}/3\,.$$

From Eqn. 4 it follows that

$$\dot{\sigma}_{kl} = C_{ijkl}^{-1}\left(\dot{\varepsilon}_{ij} - \Phi\delta_{ij}\right). \tag{5}$$

Applying the quasi-static approach, we may write [3]

$$\sigma_{kl,l} \equiv \partial\sigma_{kl}/\partial x_l = 0\,. \tag{6}$$

Lets assume the line isotropic. Differentiating Eqn. 5 with respect to x_l and taking Eqn. 6 into account we obtain an equation describing the electromigration-induced deformation of an interconnect [2]

$$V_{k,ki} + (1-2\nu)V_{i,kk} = 2(1+\nu)\Phi_{,i}\,, \tag{7}$$

where V_i is the i-th component of the displacement velocity vector; $V_{k,ki} \equiv \partial^2 V_k/\partial x_k \partial x_i$; $V_{i,kk} \equiv \partial^2 V_i/\partial x_k^2$; ν is the Poisson ratio; $\Phi_{,i} \equiv \partial\Phi/\partial x_i$; $i, k = 1, 2, 3$. Kinetics of the stress tensor components satisfies the following equation [2]

$$\dot{\sigma}_{ij} = \lambda V_{k,k}\delta_{ij} + \mu(V_{i,j} + V_{j,i}) - 3(3\lambda+\mu)\Phi\delta_{ij}\,, \tag{8}$$

where λ and μ are the Lame constants; $V_{i,j} \equiv \partial V_i/\partial x_j$; $i, j, k = 1, 2, 3$. Therefore, Eqns. 1-3 and Eqns. 7-8 form a system of 3D differential equations describing the vacancy transport and the stress field evolution under the electric current impact.

A KINETIC MODEL FOR THE VOID NUCLEATION

Owing to electromigration the distribution of vacancies in a line deviates from equilibrium. In the sites where their concentration exceeds equilibrium (supersaturation) the fluctuational clusterization of vacancies becomes thermodynamically advantageous. This process can be described by the classical nucleation theory [4]. According to its fundamentals, only the clusters, which size (the number n of vacancies forming a cluster) exceeds a certain critical value n^*, are thermodynamically stable and, therefore, able for subsequent growth. The critical cluster size is determined from the condition of maximum for the Gibbs free energy change on clusterization ΔG_n:

$$\left(\partial\Delta G_n/\partial n\right)_{n=n^*} = 0\,.$$

Hereinafter the void nucleation is treated as the formation of a vacancy cluster of the critical size.
Using equations of the classical nucleation theory, we derive an equation for the time to the void nucleation $t_i(t')$ under fixed values of the vacancy concentration and stresses attained by the time moment t' [5]:

$$\int_{t'}^{t_i(t')} \exp\left(-\frac{\tau(t')}{\tilde{t}-t'}\right) d\tilde{t} = \frac{1}{V_N J_S^*(t')}\,, \tag{9}$$

where V_N is the characteristic volume of the region where the void formation takes place; J_S^* is a steady-state value of the nucleation rate (the net number of voids forming per unit volume and time); τ is the incubation time characterizing the time interval, during which the nucleation rate attains by order of magnitude its steady-state value. Expressions for J_S^* and τ are given in [5,6].
Since the current time of electromigration satisfies $0 \le t' < \infty$ and the probability of nucleation exists at any time moment, the probability of nucleation per unit time equals $[t_i(t') - t']^{-1}$. Then, the value

$$dP(t') = dt'/[t_i(t') - t']$$

is the probability of the void formation within the time interval $[t'; t' + dt']$. Hence, the time t_n to the void nucleation with regard to contributions $dP(t')$ from $t' = 0$ is determined as the time for which the net probability becomes equal to unity, i.e. from the integral equation

$$\int dP = \int_0^{t_n} \frac{dt'}{t_i(t') - t'} = 1 . \qquad (10)$$

The time t_n is calculated by solving the integral Eqns. 9-10, determining the void nucleation kinetics, jointly with the differential Eqns. 1-3 and 7-8, describing electromigration and the stress field evolution.

RESULTS OF CALCULATIONS FOR THE VOID NUCLEATION IN A TRIPLE POINT AND FOR THE DAMAGE OF A TWO-LEVEL METALLIZATION

Within the framework of the models developed we have performed numerical calculations for the void nucleation in a triple point of the interconnect crystalline structure [6] and in the plug region of a two-level metallization [7]. Since in the latter case the void formation competes with the line edge depletion [7], we have also taken that fracture mechanism into account. The results for a triple point are presented in Figures 1-2 and for a two-level metallization – in Figures 3-5.

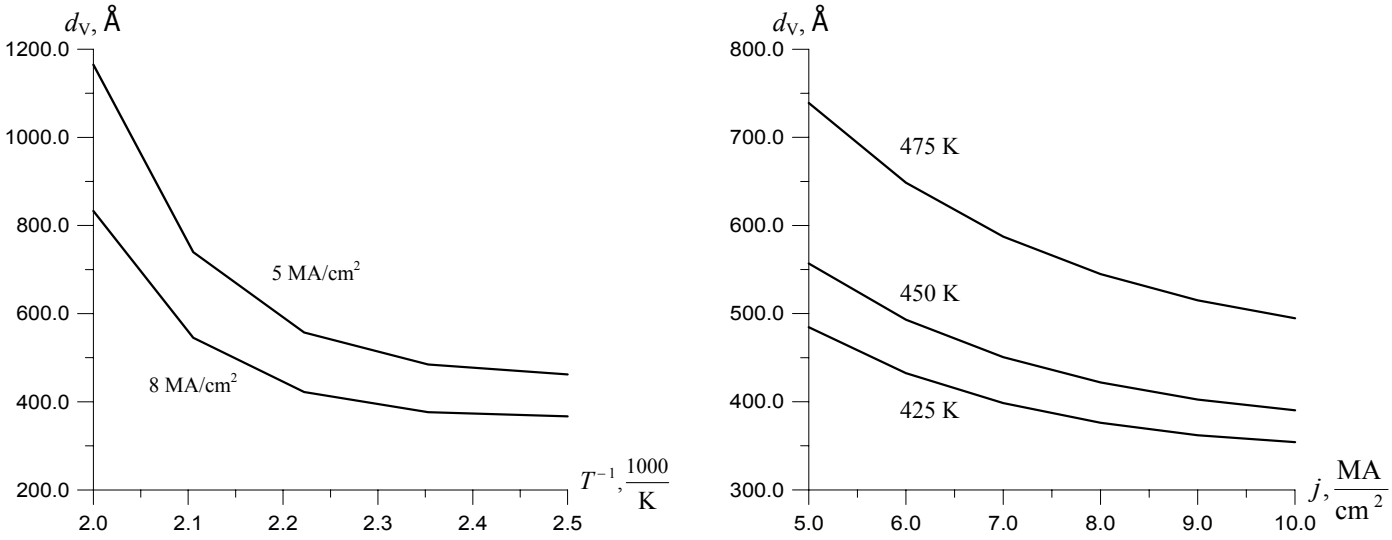

Figure 1: The void characteristic size as a function of temperature and current density

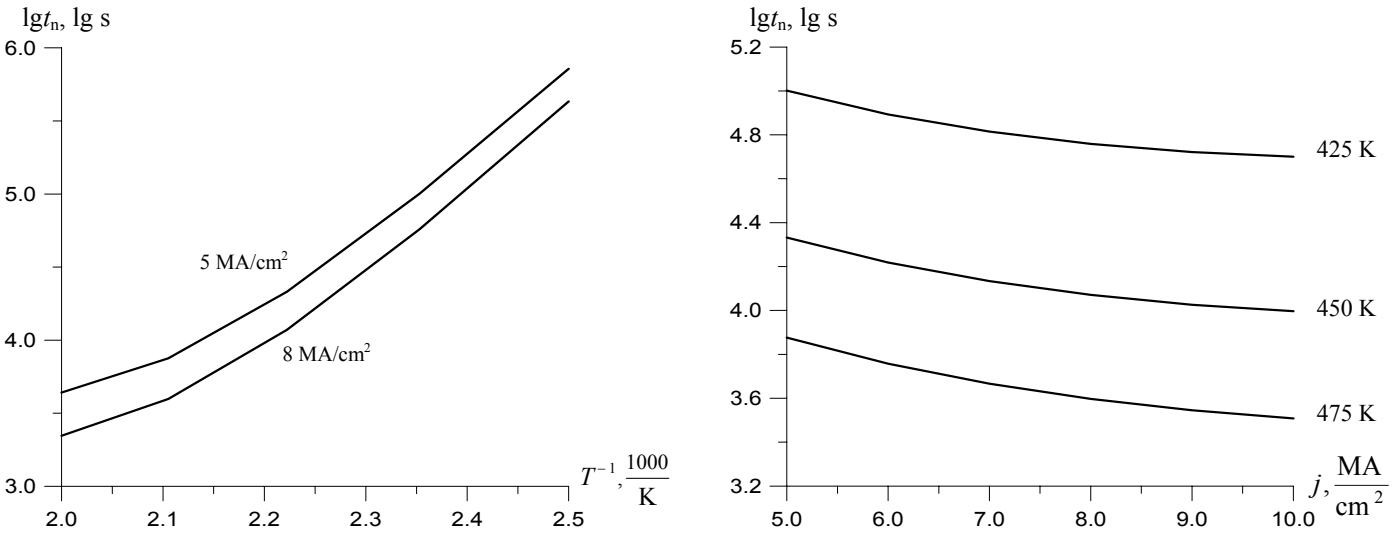

Figure 2: The time to the void nucleation as a function of temperature and current density

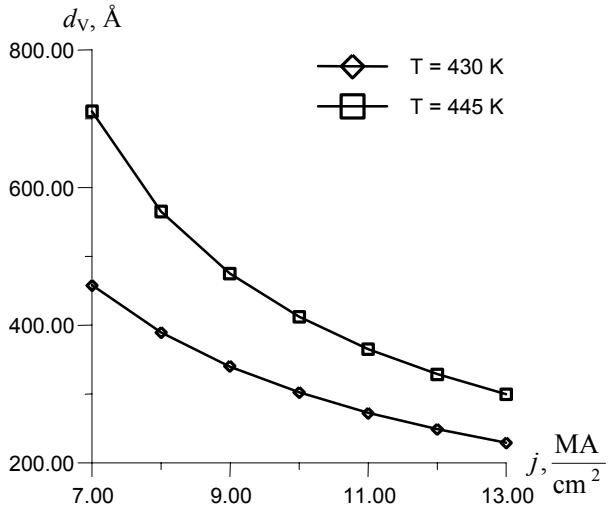

Figure 3: The void characteristic size as a function of current density

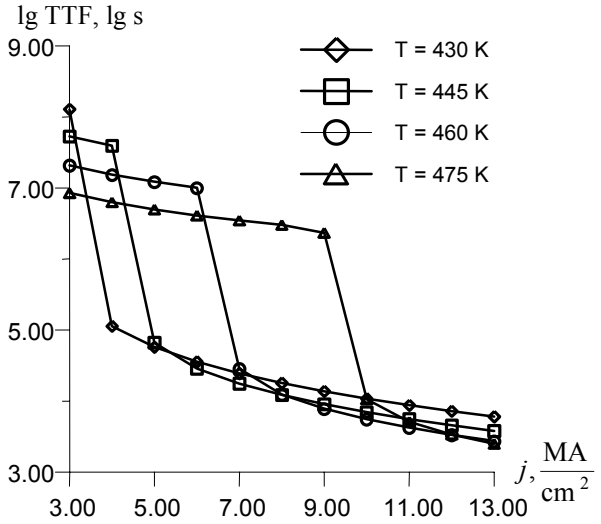

Figure 4: TTF as a function of current density

In Figure 4 the time to fracture (TTF) of a two-level metallization is presented, at that the line is considered to be damaged if a void nucleates or the edge erosion (see Figure 5) exceeds a certain critical value [7]. A bimodal character of the metallization fracture is seen: for low current densities the edge depletion takes place, while for high currents the void nucleation occurs. The results obtained agree well with experimental data [5-7].

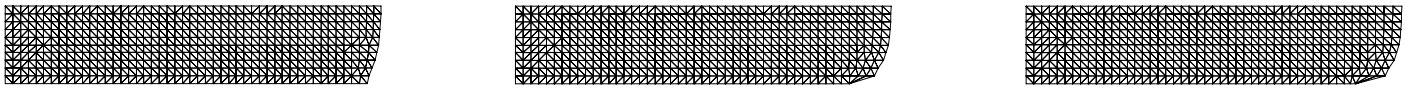

Figure 5: Evolution of the line edge depletion (T = 445 K, j = 4 MA/cm^2)

CONCLUSION

In this study we give a summary of non-linear self-consistent models for the vacancy electromigration, the mechanical stress evolution, and the void nucleation in thin-film IC interconnects. Within the framework of the models developed we have performed numerical calculations for the void formation in a triple point of the interconnect crystalline structure and for the damage of a two-level metallization in the plug region. In

the latter case fracture is caused either by the void nucleation, or by the line edge depletion. The results obtained agree well with experimental data.

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