# A Numerical Model using the Phase Field Method for Stress Induced Voiding in a Metal Line during Thermal Bake

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***Abstract*—We present a numerical model using the phase-field method (PFM) for stress-induced-voiding (SIV) in a metal line. The model was verified by comparison with the typical stress-migration (SM) analytical model. We investigated the effects of flaw location and density on time-to-failure (TTF). The model was applied to the failure analysis of the BEOL process of a 0.13um device for automobiles.**

***Keywords—SIV; SM;PFM;reliability;simulation***

## I. INTRODUCTION

Stress-induced-voiding (SIV) is a major reliability concern in modern electronic devices. A metal-line void arising from SIV can lead to device failure even without any electrical operation. Electro-migration caused by external electrical forces can be well measured and characterized. However, since stress-migration (SM) strongly depends on the stress distribution that sensitively varies with the layout design, as well as a three-dimensional structure, its characterization is not easy. To correctly estimate the metal lifetime for various layout patterns in a complicated 3D structure, it is necessary to use a 3D simulator having the proper physical models. For void evolution, a numerical model using the phase-field method (PFM) was implemented in a 3D interconnect simulator[1] that solves the coupled differential equations for mass transport, void growth and mechanics. The model was evaluated by the comparison with the typical SM analytical model[2][3]. The effects of flaw location and density at a metal surface on TTF were investigated. The model was evaluated with the serpentine pattern and the nose extension pattern in a 0.13um device.

## II. MODEL DESCRIPTION

The driving force to move the front of a void is induced by the imbalance between normal stress and surface energy density. The moving velocity of the outward-pointing normal direction at a void surface is modeled by

$$v_{norm} = \frac{DC\Omega^2}{lkT}(\sigma_n - \gamma\kappa) \quad (1)$$

where D, C and Ω are the vacancy diffusivity, concentration and the atomic volume respectively; $\sigma_n$, γ, and κ are the normal stress, metal surface tension and curvature respectively; l is the characteristic length for energy relaxation.

By introducing the phase field variable, ϕ, which describes whether a region is a metal (ϕ=1) or a void (ϕ=0), the governing equation of the front moving behavior can be derived from (1) by Beckermann's approach [4]:

$$\tau\frac{\partial\phi}{\partial t} = w^2\nabla^2\phi - \phi(1-\phi)(1-2\phi) - 5\frac{w\sigma_n}{\gamma}\phi^2(1-\phi)^2 \quad (2)$$

where $w$ is the phase transition width and τ is the energy relaxation time which is expressed as:

$$\tau \equiv \frac{w^2 lkT}{DC\Omega^2\gamma} \quad (3)$$

The vacancy diffusion is governed by

$$\frac{\partial C}{\partial t} = -\nabla\cdot\left(-\phi D\nabla C + (\Omega - \Omega_v)\frac{\phi DC}{kT}\nabla p\right) + \frac{a}{\Omega}\frac{\partial\phi}{\partial t} \quad (4)$$

where $\Omega_v$ and $p$ are the vacancy volume and the hydrostatic pressure respectively; $a$ is a parameter that controls the vacancy sink rate, which relies on the vacancy condensation in a void. The difference between the volume of atoms and vacancies causes volumetric strain so that the mechanical stress changes when vacancies migrate during mass transport [5], which is taken into account in the mechanics equation.

Void nucleation by vacancy condensation is not expected because it needs an unrealistically high vacancy supersaturation [6]. If the flaws or contaminants at an interface act as void nucleation sites, the energy barrier vanishes when the stress is above the critical value [7]

$$\sigma_c = 2\gamma\sin(\theta_c)/r_c \quad (5)$$

where $r_c$ is the contaminant or flaw size; $\theta_c$ is the equilibrium contact angle. The balance of forces leads to:

$$\theta_c = \cos^{-1}((\gamma_i - \gamma_{adj})/\gamma) \quad (6)$$

where $\gamma_i$ and $\gamma_{adj}$ are the surface tensions of an interface and the material adjacent to a metal, respectively. The initial voids are randomly located at places near an interface where the normal stress is larger than $\sigma_c$. For the barrier-less initial void formation, the phase field at an arbitrary location x on a metal surface is initialized by:

$$\phi(\vec{x}) = \prod_{i=1}^{m} \frac{1}{2}\left(1 + \tanh\left(\frac{\|\vec{x} - (\vec{x}_{s,i} + (r_c/\tan\theta_c)\vec{n}_{s,i})\| - r_c/\sin\theta_c}{w}\right)\right) \quad (7)$$

where $m$ is the number of initial voids; $\vec{x}_{s,i}$ is the position located on the metal surface for the i-th void; $\vec{n}_{s,i}$ is the unit vector along the normal direction to the surface at $\vec{x}_{s,i}$. The continuity equation for steady state is solved to calculate the resistance change due to void growth.

$$\nabla \cdot (\phi\sigma\nabla\psi) = 0 \quad (8)$$

where $\sigma$ and $\psi$ are the electrical conductivity and potential respectively.

## III. MODEL EVALUATION

### A. Comparison to Analytical Model

To compare the simulation results with the analytical model[2] , as in (9), based on the creep voiding rate model by McPherson and Dunn[3], a dual damascene process was simulated under different bake temperature conditions.

$$\text{MTTF(Mean-time-to-failure)} = A\,(T_0 - T)^{-N} \exp(E_a/kT) \quad (9)$$

As the temperature increases, the vacancies diffuse faster but the stress is reduced. The faster diffusion accelerates the void growth so that the lifetime is reduced. However, as the temperature becomes close to the stress-free temperature, a void can hardly grow and the lifetime drastically increases again. The analytical model in (9) describes such parabolic temperature-dependent behavior of MTTF. As shown in Fig.1, the simulation result correctly captures such typical temperature-dependent behavior of stress-migration. Fitting the analytical model to the simulation results gives 1.06 eV for $E_a$ which is very close to the diffusion activation energy 1.00 eV of vacancies used in the simulation.

Fig.2 and Fig.3 shows the simulation results for the void evolution and hydrostatic pressure distributions at 175°C bake for 1, 5, 10, and 15 hours. As time progresses, the void continues to grow and eventually covers the whole via area. However, it also shows that the void growth compresses the metal, which will eventually balance the forces and stop the growth.

### B. Standard Deviation due to Random Flaw Locations

To study the statistical variation of the life time with respect to a flaw location, the initial contaminant was randomly located at the metal surface where the normal stress is greater than the critical stress in (6). The flaw density is constant, by setting $m$=1 in (7) for all simulations. As shown in Fig.4, the standard deviation in lognormal distribution almost doesn't depend on the bake temperature since the activation energy for the vacancy diffusion is constant.

### C. Standard Deviation due to Different Flaw Densities

The quality of the metal surface can be represented by controlling the number of flaws, i.e. $m$ value in (7). Fig.5 shows the comparison between the simulation results with the different $m$ values ($m$=1 and 3). More flaws cause a wider TTF distribution. However, the standard deviation almost doesn't vary with the temperature because of the same diffusion activation energy.

## IV. APPLICATION

The model was applied to the BEOL process of a 0.13um device for automobiles. Al metal is deposited on the top of Ti-based layer that surrounds W-filled contacts. The metal line, on which a Ti-based layer is deposited, is formed and covered by FSG. We simulated two cases as follows.

### A. Serpentine pattern

The test pattern is serpentine. The thermal bake was performed for 1000 hours at 150°C. The model places the initial void in the bended region where the tensile stress is relatively larger as shown in Fig.6. Fig.7 shows the void evolution during the bake. Fig.8 shows the comparison with the simulation results for the resistance increase due to the void growth, which fits well within the measured range.

### B. Nose extensions

The test patterns are two metal nose extensions from a power line. The extension lengths are 0.71um and 0.84um, but both extension widths are 0.24um. The 0.71um-long extension is connected to silicon thru one contact while the 0.84um-long extension is thru two contacts as shown in Fig.9. The test structure was subjected to thermal bake for 1200 hours at 200°C. The power line acts as a vacancy reservoir that supplies enough vacancies to form a big void in the metal. Fig.10 shows the comparison of the simulated void growth in 3D with the TEM picture. The 2D cut along the line shown in the picture matches the TEM picture. Fig.11 shows that a void in the 0.71um-long extension grows enough to block the current path thru Al metal to contact while a void in the 0.84um-long extension doesn't. Thus, the resistance of the 0.71um-long extension dramatically increases after 50 days bake while the resistance increase of the 0.84um-long extension is negligible even after 100 days bake as shown in Fig.12. The result matches well with the measured lifetime.

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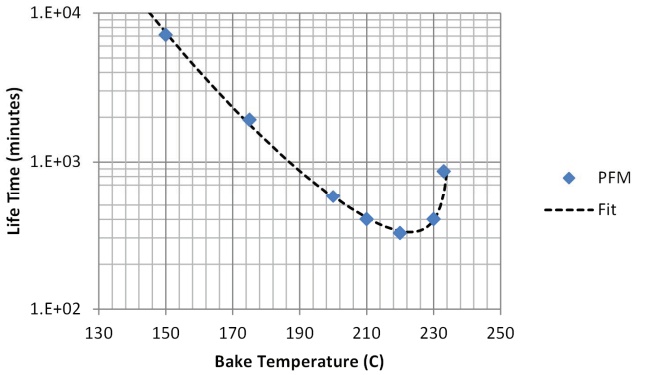


Fig. 1. Temperature vs. Life time. The symbol data are the simulation results using the PFM model. The dot line is the fitting curve to the analytical model of McPherson and Dunn.

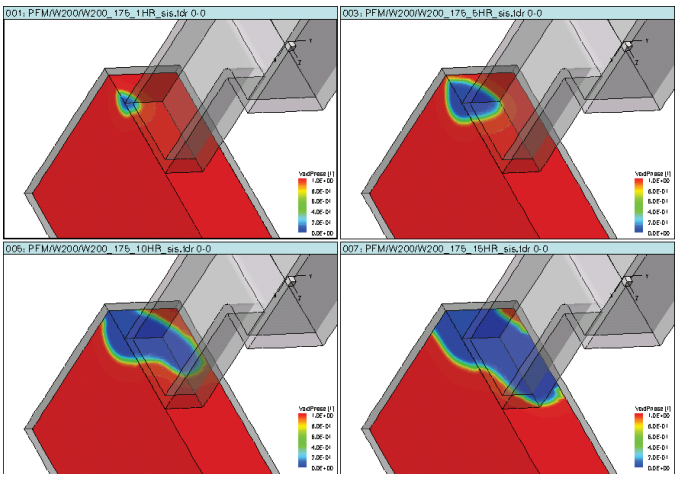

Fig. 2. Simulation results for void evolution during the thermal bake at 175°C. The layer drawn in transparent gray color The blue and red colors denote a void($\phi$=0) and a metal($\phi$=1) respectively. Void growth is shown after 1 hour (upper-left), 5 hours(upper-right), 10 hours(lower-left) and 15 hours(lower-right).

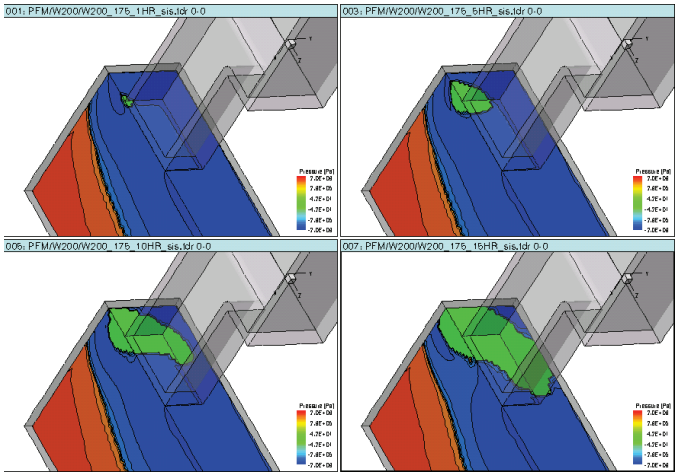

Fig. 3. Hydrostatic pressure distributions during the same bake conditions in Fig.2. Green color shows zero pressure region which is a void. Blue and orange colors for tensile and compressive regions respectively

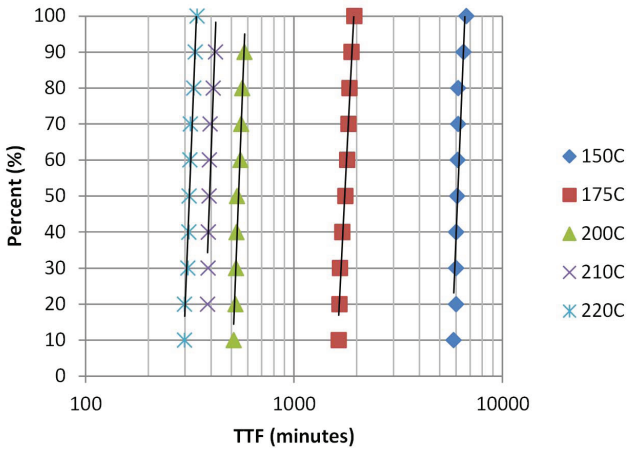


Fig. 4. Statistical SM lifetime simulation results for random flaw locations.

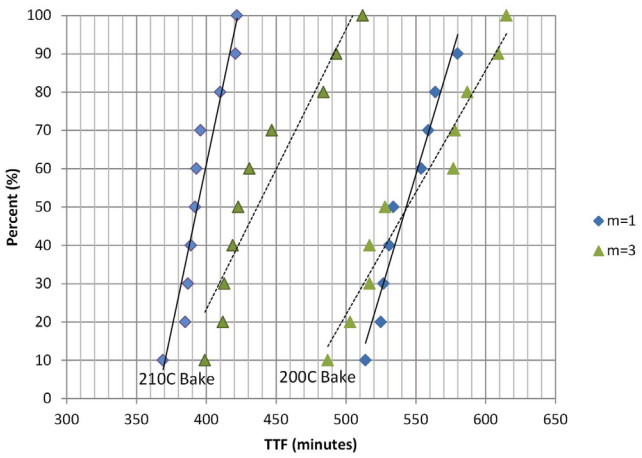


Fig. 5. The effect of flaw density on the TTF standard deviation

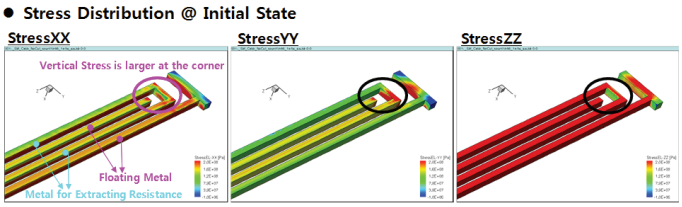


Fig. 6. Initial stress distribution in the serpentine metal structure

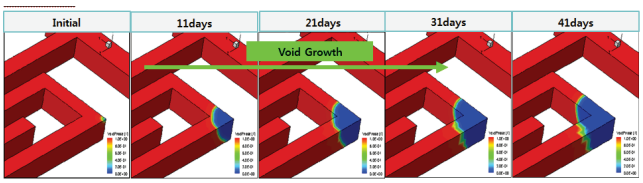


Fig. 7. Void growth in the serpentine metal structure

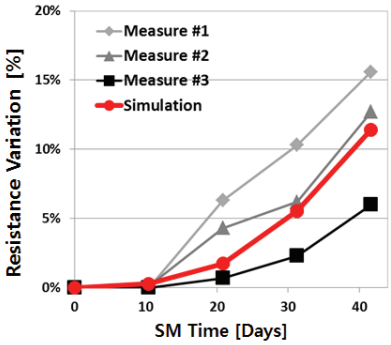


Fig. 8. Resistance change due to a void formation in the serpentine structure

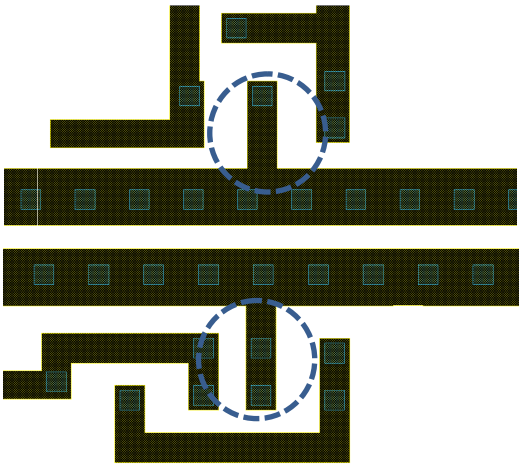

Fig. 9. Two metal extensions (dotted circles) from a power line. The extension dimensions of the top and bottom patterns are 0.24um x 0.71um and 0.24um x 0.84um respectively.

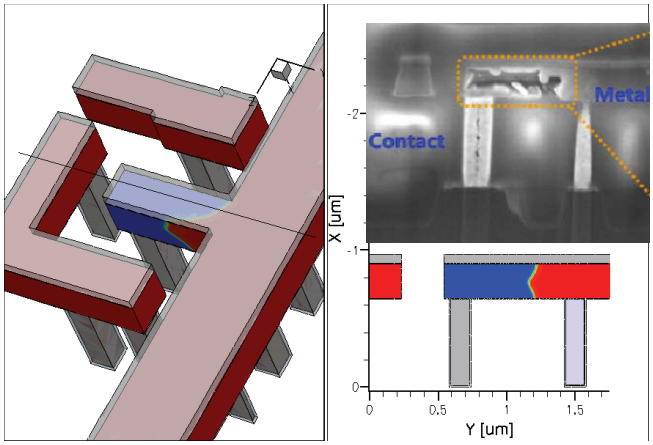


Fig. 10. Comparison of the simulated void growth with the TEM picture. 2D cut along the line matches with the TEM picture.

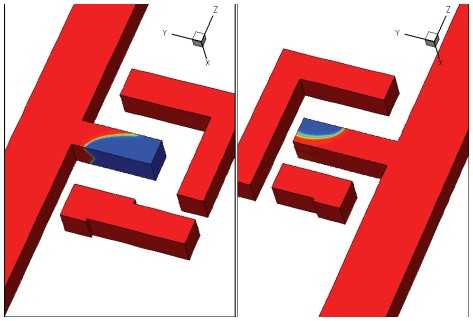

Fig. 11. Comparison of the void growth between 0.71um-long(left) and 0.84um-long(right) metal extensions after 1200 hours bake at 200ºC.

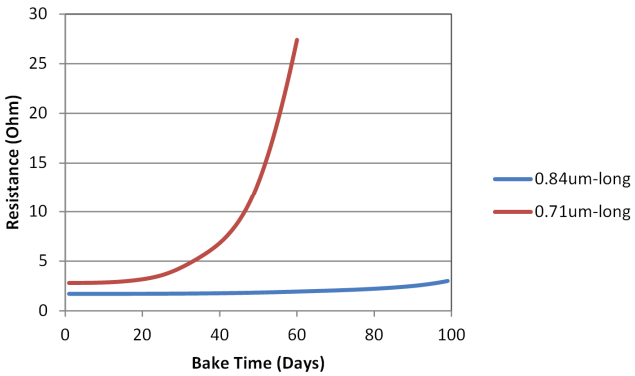


Fig. 12. Simulated Resistance vs. Bake Time. The resistance of the 0.71um-long extension (red curve) increases dramatically because of a big void formation. However, the 0.84um-long extension (blue curve) doesn't show a noticeable resistance increase even after 100 days.