Finite Difference Time Domain Analysis of Stress Evolution and Void Growth for General Interconnect Wires

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***Abstract*—Electromigration (EM) has become a dominate long term failure mechanism leading to reduced reliability in nanometer VLSI chips. Existing compact EM models do not work well for complicated interconnect structures and stressed conditions. This paper presents a numerical technique using the Finite Difference Time Domain (FDTD) method to solve stress diffusion equation governing the EM kinetics for the void nucleation and growth phases. The new method can be applied for general interconnect structures under various stressed conditions. These equations are then discretized and a system of linear equations is formed and solved. Transient void size is then generated using the stress calculated from the FDTD method. The FDTD method proposed in this paper is validated against the finite element based COMSOL software, the gold standard in PDE solving, and shows good agreement with the results.**

***Index Terms*—Electromigration, finite difference, interconnect, reliability**

x

I. Introduction

Electromigration (EM) has become a major reliability problem in nanometer VLSI chips. Traditional methods for EM reliability signoff include the use of compact EM models such as Black's equation [1] and Blech limit [2]. However, these can lead to over-design and 2x-3x larger guard bands [3]. Such conservative over-design rules, while already negatively affecting chip designs, will prove increasingly detrimental as chip timing requirements will be more difficult to meet with excessively large guard bands. Thus, a worst-case design methodology results in inefficiency and considerable penalties in chip area, performance, power, and reliability budgets. Consequently, more accurate EM modeling and analysis methods are necessary for efficient chip design.

These traditional EM models are incapable of providing accurate dynamic stress evolution for complicated interconnects and stress conditions. Additionally, individual wires within the interconnects are not independently affected by EM [4] [5]. These models are analyzed empirically and not based on physics, this presents a major drawback of these models as they become less accurate when applied to complicated structures and stress conditions.

A Recently proposed compact physics-based EM model for full-chip reliability analysis [6] [7] based on the hydrostatic stress diffusion equation presents an accurate model for dynamic stress evolution. This model has been extended to deal with multi-branch interconnects using a new analytical model which gives accurate transient stress evolution [8]. However, this model is sometimes unable to handle general interconnect trees, or has extreme difficulty doing so, arranged in arbitrary configurations as these structures are difficult to find analytical solutions for. Additionally, these models cannot generally accommodate existing residual stress, due to stress migration for instance, which significantly impacts the effect EM has on the interconnects.

In this paper, we propose a numerically based EM analysis method utilizing physics based modeling of the dynamic stress evolution for general interconnects. We apply the Finite Difference Time Domain (FDTD) method to solve fundamental hydrostatic stress evolution Partial Differential Equations (PDEs) for the void nucleation and void growth phases of the EM failure process. We apply this method to both one and two dimensional structures commonly found in IC interconnects. We show the results for a single wire and the three-wire T-shape interconnect. This new method has the advantage of being easily scalable with the introduction of any new physical variables such as transient thermal and time-varying current effects, which cannot be done in existing compact EM models. Furthermore, this numerical method has the capability to facilitate the acceleration of the EM validation process in future work by employing advanced model order reduction and hardware acceleration techniques. The FDTD method proposed in this paper is validated against the finite element based COMSOL software, the gold standard in PDE solving, and shows good agreement with the results.

II. EM Physics and modeling

EM is the physical phenomenon of the migration of metal atoms along the direction of an applied electrical field. Atoms (either lattice atoms or defects/impurities) migrate toward the anode end of the metal wire along the trajectory of conducting electrons. During the migration process, hydrostatic stress will be generated inside the embedded metal wire due to momentum exchange between lattice atoms and conduction electrons and is a prime cause of void and hillock formations at either end of the wire. Indeed, when a metal wire is embedded into a rigid confinement, which is the case with interconnect metallization, the wire volume changes (induced by the atom depletion and accumulation due to migration) create tension at the cathode end and compression at the anode end of the line. Over time, the lasting unidirectional electrical load will increase hydrostatic stress, as well as the stress gradient which acts as counter-forces for atom migration along the metal line. In some cases, usually when a line is long, this stress can reach a critical level, resulting in a void nucleation at the cathode and/or hillock formation at the anode end of the line. Existing Black's model [1] is a semi-empirical model with

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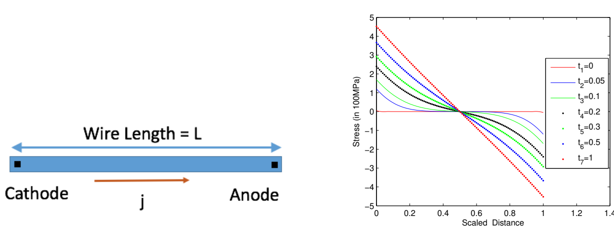
consideration of physics. For instance, it does not consider the impact that residual stress or wire length have on the Mean Time to Failure (MTTF) of the wire. Also, when the wire reaches the MTTF, the wire is treated as an open circuit, which will over-estimate the EM-impacts in circuit reliability. Because of this, a new physics-based EM analysis method is used in this paper.

A. Void nucleation phase

Development of analytical formulation for electronic migration was proposed by Korhonen [9]. The failure process consists of two phases, nucleation and growth. In the first phase, void nucleation happens near the cathode edge of the line. Stress field $\sigma(x,t)$ is calculated by equation:

$$\begin{aligned} PDE &: \frac{\partial \sigma}{\partial t} = \frac{\partial}{\partial x}\left[\kappa\left(\frac{\partial \sigma}{\partial x} + G\right)\right], \text{ at } 0 < t < t_{nuc} \\ BC &: \frac{\partial \sigma}{\partial x}(0,t) = G, \text{ at } 0 < t < t_{nuc} \\ BC &: \frac{\partial \sigma}{\partial x}(L,t) = -G, \text{ at } 0 < t < t_{nuc} \end{aligned} \quad (1)$$

Here, $\kappa = D_a B\Omega/kT$, where $D_a = D_0 exp(Ea/kT)$ is the effective atomic diffusivity, E_a is the activation energy of the failure process, T is the absolute temperature and k is the Boltzmann constant. B is the effective bulk elasticity modulus, Ω is the atomic lattice volume, and $G = \frac{eZ\rho j}{\Omega}$, where e is the electron charge, eZ is the effective charge of the migrating atoms, ρ is the wire electrical resistivity, j is current density, x is the coordinate along the line, and t is time. The initial condition (IC) is the stress on the wire at time $t = 0$. For the boundary condition (BC), since the flux is blocked at both ends $x = 0$ and $x = L$ so $J(0,t) = J(L,t) = 0$ where $J(x,t) = \frac{D_a}{kT}(\frac{d\sigma(x,t)}{dx} + G)$



(a) (b)

Fig. 1. (a) Single wire with wire length L (b) EM-stress distribution change over time in a simple metal wire.

Fig. 1(a) shows a single wire with normalized length. Fig. 1(b) shows the EM-induced transient stress development for a single metal wire from the finite element analysis for a given current density and temperature setting. During this process, tensile stress (positive stress) will be developed at the cathode side (the left node), while compressive stress (negative stress) will be generated at the anode side of the wire (right node). When the tensile stress reaches a critical level(σ_{crit}), a void will be generated at the cathode edge of line ($x = 0$). The time at which stress reaches σ_{crit} is called nucleation time(t_{nuc}).

B. Void growth phase

Void size growth begins in the second phase. After the nucleation phase, resistance of the wires will be increased as the void grows until void growth saturates. The effective thickness of the void interface (δ) which is infinitely small in comparison with all other involved lengths is introduced. It allows us to introduce a stress gradient between the zero stress void surface and the surrounding metal as $\nabla\sigma = \sigma(\delta,t)/\delta$, where $\sigma(\delta,t) \approx \sigma(0,t)$ is the time dependent stress in the metal near the void surface. The differential condition is written as, [10]:

$$\begin{aligned} PDE &: \frac{\partial \sigma}{\partial t} = \kappa\frac{\partial^2 \sigma}{\partial x^2}, \text{ at } 0 < t < \infty \\ BC &: \frac{\partial \sigma}{\partial x}(0,t) = \frac{\sigma(0,t)}{\delta}, \text{ at } 0 < t < \infty \\ BC &: \frac{\partial \sigma}{\partial x}(L,t) = -G, \text{ at } 0 < t < \infty \end{aligned} \quad (2)$$

IC is the stress at t_{nuc} in the nucleation phase since the growth phase starts immediately after nucleation which means $\sigma(x=0,t=0) = \sigma_{crit}$

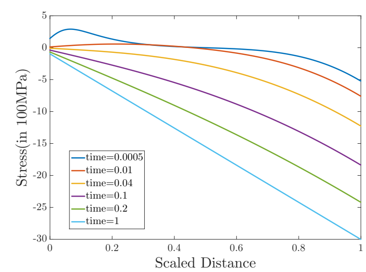


Fig. 2. EM-stress distribution change over time in simple metal wire for void growth.

Fig. 2 the evolution of stress starting from the void nucleation time $t = 0$ till the steady state is achieved.

III. Void Volume Calculation

During the void growth phase, a void has actually nucleated in the wire and begins to grow. This void causes changes to the electrical properties of the wire, resistance for example, and leads to the eventual failure of the interconnect. For this reason, being able to measure the void volume growth is critical to the proper analysis of the interconnect. Using the dynamic stress evolution of the wire, which will be calculated by the FDTD method in this paper, we can also calculate the volume of the void as it grows. This is accomplished by calculating the atom drift volume in the wire [11]. Essentially, the stress σ over bulk elasticity modulus B is integrated over the length L of the wire and multiplied by the wire's cross-sectional area A.

$$V(t) = A\int_0^L \frac{\sigma(t)}{B}dx \quad (3)$$

From this equation we can then begin to make inferences about the effect the growth will have on the interconnect's electrical properties.

IV. Finite Difference Method for EM Analysis

The Finite Difference Time Domain (FDTD) method is a numerical method of solving a Partial Differential Equation (PDE) [12]. A Numerical method finds an approximate solution by iteratively obtaining values as apposed to analytically finding a solution to a PDE. FDTD gives us the ability to quickly and easily find a solution for complicated PDEs that would otherwise be difficult to solve using analytical methods. Furthermore, it has the ability to handle complex structures and scale with larger problem domains.

FDTD works by discretizing both the time and spatial variables in a PDE. This discretization is accomplished by employing the local taylor expansion to PDE, in conjunction with the structure being analyzed, which yields a system of linear equations which are solved for the discrete values within the structure. While there are several discretization schemes, this work uses the central difference method to discretize the spatial variable x and the first order backward method to discretize time t.

$$\frac{\sigma_i^{n+1} - \sigma_i^n}{\Delta t} = \kappa \frac{\sigma_{i+1}^{n+1} - 2\sigma_i^{n+1} + \sigma_{i-1}^{n+1}}{\Delta x^2} \tag{4}$$

In (4), the superscript n indicates the time step and subscript i is the space index, x.

$$-S\sigma_{i+1}^{n+1} + (1-2S)\sigma_i^{n+1} - S\sigma_{i-1}^{n+1} = \sigma_i^n \tag{5}$$

where $S = \kappa \frac{\Delta t}{\Delta x^2}$. This discretization method gives us an implicit scheme for solving the PDE numerically. This Implicit scheme allows us more freedom on how large the time step Δt can be as we don't need to worry about stability, which is a problem in explicit methods [12].

For the boundary conditions, stress is dependent on the derivative of the stress function. Thus, Neumann boundaries are used and discretized [13].

$$\sigma_x(0,t) = G = \frac{\partial \sigma_i^n}{\partial x} \tag{6}$$

$$\sigma_x(0,t) = \frac{\partial \sigma_i^n}{\partial x} = \frac{\sigma_i^{n+1} - \sigma_{i-1}^{n+1}}{\Delta x} = G \tag{7}$$

We can now use this discretization scheme and plug it into (5) to obtain the following.

$$(S+1)\sigma_i^{n+1} - S\sigma_{i+1}^{n+1} = \sigma_i^n - SG\Delta x \tag{8}$$

Note that we omit the derivation for the second boundary condition $\sigma_x(L,t)$. The resulting system of equations can be mapped to an equation in the form of $A\sigma^{n+1} = \sigma^n$. A is a tri-diagonal coefficient matrix with the diagonal elements equal to $(1-2S)$ and the lower and upper diagonal elements equal to $(-S)$. The vector σ^{n+1} is a vector of unknown stress along the wire and σ^n is a vector of previously solved for stress. The first element in σ^n is $\sigma_{left}^n + \beta$ and the last element is $\sigma_{right}^n - \beta$. These correspond to the boundary conditions at each end of the wire where β is equal to $SG\Delta x$.

Each solution of the system of equations results in a vector containing the stress of the wire at a single time step. Subsequent solution of this system, using previous time step solution as the σ^n vector, can produce a vector containing the stress at the respective time steps. By iteratively solving the system of equations, we obtain the transient stress evolution for the entire wire length.

This previous section shows the basic FDTD scheme for a one dimensional wire, however; this can be easily expanded to the two or three dimensional case. The discretization for the two dimensional case used in this work is presented below, albeit without derivation.

$$-S_y\sigma_{i+1,j}^{n+1} + (1 + 2S_y + 2S_x)\sigma_{i,j}^{n+1} - S_y\sigma_{i-1,j}^{n+1} - S_x\sigma_{i,j+1}^{n+1} - S_x\sigma_{i,j-1}^{n+1} = \sigma_{i,j}^n \tag{9}$$

In this equation, i is the discrete variable in the $x-axis$ and j is the discrete variable in the $y-axis$. The value S also is specified as S_x or S_y to differentiate discretization steps used in either direction.

The void growth phase follows the void nucleation phase. For void growth phase, the A matrices are similar (with different boundary and initial conditions). The analyzer can take an arbitrary vector of initial conditions or the output stress distribution from the previous void nucleation phase can be used. Once this has been determined by the user, the growth phase portion of the framework operates the same as the void nucleation phase. That is, the new growth phase discretized equation $A\sigma^{n+1} = \sigma^n$ is formed and is then solved iteratively to generate transient data for the wire stress.

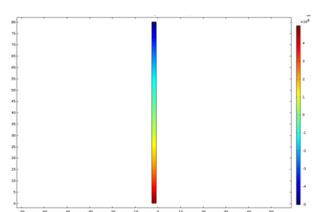
TABLE I
NOTATIONS AND TYPICAL VALUE IN OUR TRANSIENT SIMULATION

Term	Typical value	Description
ρ	3.00e-8Ω· m	Electrical resistivity
e	1.60e-19C	Electric charge
Z^*	10	Effective valence charge
Ω	1.18e-29 m^3	Atomic volume
k	1.38e-23J/K	Boltzmann constant
B	1.10e11Pa	Back flow stress modular
D_0	7.56e-5m^2/ s	Self-diffusion coefficient
E_a	1.76e-19J	Activation energy
σ_{crit}	500MPa	Critical stress
T	373K	Absolute temperature
δ	3e-7m	Effective thickness of the void interface

V. NUMERICAL RESULT AND DISCUSSIONS

The proposed FDM-based EM analyzer was prototyped in MATLAB. COMSOL multiphysics [14] is used to validate our proposed analyzer.

In order to validate our result, a FEA tool, COMSOL [14] is used. In the nucleation phase, the initial conditions are set to be zero and default zero flux boundary conditions are used. In the growth phase, initial conditions come from the time at which the cathode in the nucleation phase reaches critical stress. We summarize the major notations and typical parameter values in Table I.


(a)

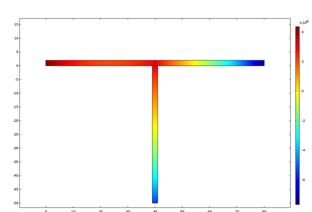
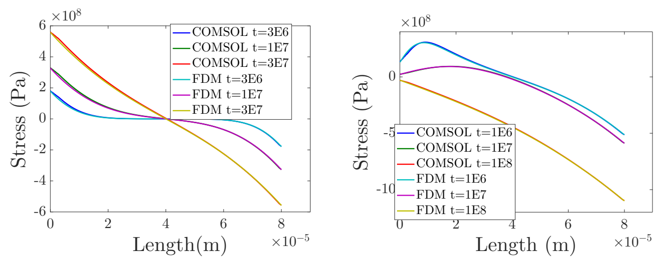

(b)

Fig. 3. The testing interconnect structures: (a) 1-wire (b) 2 connected wires

A. Validation for single 2-terminal wire

For the 2-terminal single wire as shown in Fig 3(a), tensile stress was generated in the cathode (left node) while the anode node experiences compressive stress. This agrees with our expectations which say that a void should be nucleated at the cathode end of the single wire. Root Mean Squared Error(RMSE) when compared to COMSOL for the void nucleation phase, seen in Fig 4(a), and void growth phase, seen in Fig 4(b), are 0.8033% and 0.4435% respectively.

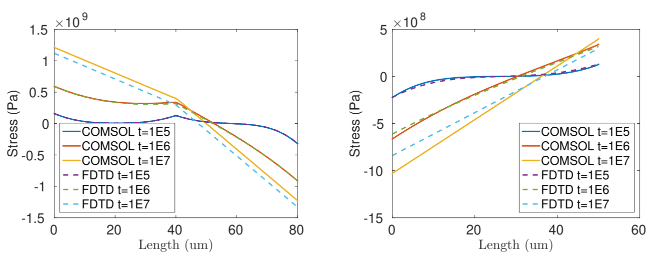


(a) (b)

Fig. 4. EM-stress distribution change over time with $j = 5 \times 10^9 A/m^2$ in single 2-terminal wire for (a) void nucleation and (b) void growth

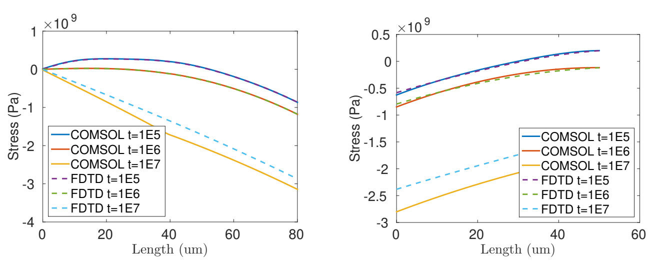
B. Validation for three wire T-shape intersection

In the three wire T-shaped interconnect shown in Fig 3(b), currents were applied as: $j_1 = 5 \times 10^9 A/m^2$, $j_2 = -6 \times 10^9 A/^2$, $j_3 = -7 \times 10^9$. With current flowing in through wire one, we expect the void to nucleate here. Results, show that our expectations are met and the numerical data agrees with the COMSOL results for both nucleation, seen in Fig 5(a) and Fig 5(b) and growth phases, Fig 6(a) and Fig 6(b). RSME for the nucleation phase is 2.011% and 2.23% for the growth phase. Results for other current configurations are omitted for space but produce similar results.



(a) (b)

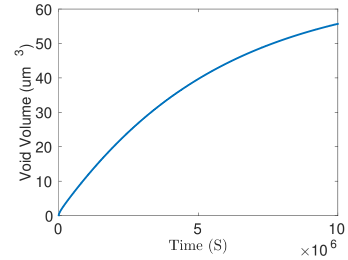
Fig. 5. T-shape nucleation phase for (a) horizontal wire (b) vertical wire



(a) (b)

Fig. 6. T-shape growth phase for (a) horizontal wire (b) vertical wire

Once the dynamic stress evolution data has been collected from the FDTD analysis, we can apply the void volume calculation to see the transient void volume growth. These results are shown in Fig 7(a).



(a)

Fig. 7. Growth of void volume over time (t=1E7)

VI. Conclusion

In this paper, we proposed an accurate EM analysis model by performing FDTD for EM effects in multi-branch interconnects based on the kinetics of the first principle of EM physics. We started with the fundamental hydrostatic stress evolution diffusion equation for both void growth and nucleation phases with proper boundary and initial conditions for typical multi-branch wires: the single 2-terminal wire, and the three wire T-shaped interconnect. The void size was then calculated based on the transient stress data provided from the FDTD analysis. The new FDTD EM analysis easily accommodated existing nonuniform residual stress distribution which is not considered in existing EM models. Furthermore, it can considered transient temperature and time-varying current densitie, both of which are difficult for existing models. Numerical results showed that the proposed method agrees with the COMSOL based finite element method in terms of accuracy.

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