REALISTIC MODELING OF ELECTROMIGRATION IN TODAY’S ULSI INTERCONNECTIONS

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Abstract

IC architecture makes extensively use of multiple interconnect levels with many vias that enable electrical current to flow between each level. A common failure mechanism in interconnections is the formation and the growth of voids and/or hillocks which may span across the line width and sever (or short) the electrical connections. The process of mass transportation is called Electromigration (EM). In contrast to a pure diffusion process due only to concentration gradients, the kinetic of EM in metal thin film is rather complicated and it is a mass transportation process controlled by various driving forces such as the electron wind, temperature gradients, stress gradients and the surface tension. Reliability evaluation and improvement of new interconnects require a more thorough understanding of the physics of EM, but experimental investigation can be too costly and too slow to cope with the changing interconnect systems. Physics-based modeling of the EM becomes necessary to complement the experimental investigation.

In the first part of this dissertation, a comprehensive review on the EM models for the interconnections and their evolution over the last three decades is presented. The different EM models are categorized according to their respective simulation methodologies. The primary objective of the review is to re-examine the different EM simulation methodologies and provide a good reference starting point for researchers who are new in the field of EM modeling.
In the subsequent parts of this dissertation, we present our study on physics-based numerical EM modeling. Our research methodology consists of both computer simulation and experimental study. In terms of computer simulation, Finite element analysis (FEA) and Monte Carlo method are adopted to model the process of EM statically or dynamically. Their application in EM simulation and its reliability evaluation is presented in details in subsequent chapters. In our study, we also propose a detail of EM process including the tiny void incubation, void nucleation and void growth. The importance of void nucleation in sub-micron and nano-interconnections is highlighted and the Median to failure (MTF) is derived theoretically. It reveals the detail physics of EM and how it is related to the MTF which is overlooked by industry for decades. Various package level accelerated EM testing under different accelerated conditions using both high current and temperature are performed to verify the assumptions, the theories and the prediction of computer simulation. The simulation is found to have a good agreement with the experimental observations and data.
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Dedication

I dedicate this work to my parents, whose love knows no bounds.
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Chapter 1: Introduction

1.1 History of Electromigration study

Electromigration (EM) describes the atomic motion in a metal under the influence of an applied electric field. It is basically a diffusion phenomenon under various driving forces. Investigation of this phenomenon can be traced back about a century with the first observation reported by Geradin (1861) in molten alloys of lead-tin and mercury-sodium. [1] However, systematic studies didn’t start until the 1950s. The concept of the ‘electron wind’ driving force was first formulated by Fiks (1959)[2] and Huntington and Grone (1961)[3]. Working independently, these authors employed a semi-classical ‘ballistic’ approach to treat the collision of the moving atom by the charge carriers. The formulation of the driving force was a major contribution to the study of EM, as it demonstrated the possibility of using EM to probe directly the interaction of mobile defects and charge carriers. It simulated considerable interest during the 1960s in experimental studies on EM in metals. During that period of time, the investigations were primarily basic studies and concentrated mostly on bulk materials. Until that time, the applied study of EM was rather limited[1].

The interest as well as the direction of EM study took a drastic turn in the late 1960s when EM was identified as the root cause of the failure of aluminum interconnecting lines in integrated circuit[4]. Since that time, the study of EM phenomenon has lasted for more than 40 years. In this duration, hundreds of papers were published to reveal
the EM behavior in metal interconnects and the corresponding theoretical models were developed.

1.2 Electromigration study in integrated circuit

An ordinary household extension cord conducts electricity without mass transport because the electric current density in the cord is low, about $10^2 \text{A/cm}^2$. The situation is different in the case of integrated circuit (IC) as IC use thin, narrow metal films for interconnection. Unlike the bulk conductor which will melt from the joule heating at about $10^4 \text{A/cm}^2$, the metallization in IC can sustain current densities greater than $10^7 \text{A/cm}^2$ due to the good thermal conductivity of the silicon substrate on which interconnects are built. On the other hand, in a device having a very dense integration of circuit, the heat management is a serious issue. Typically, a device is cooled by a fan or other means in order to maintain the operation temperature around 100°C.

For more than 40 years in the past, the EM issue in IC was greatly investigated in both academic and industry. It is found that EM is a rather complicated diffusion phenomenon which involves multiple physical processes, also named as failure mechanisms in the field of failure analysis. In these processes, the driving forces include not only electrical force, that is, the net force due to electron wind and direct field, but also the thermal gradient induced force, the concentration gradient induced force, and mechanical stress induced force[5]. If void are present, an additional factor, surface tension, is introduced and it will affect the shape of the voids[5]. In addition, healing effects, known as the mass backflow due to EM-induced concentration non-
uniformity and stress gradient, also play an important role in EM performance, which affect EM failure rate considerably, and as a result a threshold current density exists in metal line with cluster length greater than the Blech length[6].

Besides, thin films possess a small grain size and a high surface or interfacial area to volume ratio with many high mobility diffusion paths, allowing mass transport at low temperature along various diffusion paths, such as grain boundary diffusion, interface/surface diffusion and lattice diffusion[7]. When these diffusion paths intersect with one another, accumulation of atoms or voids nucleation starts at the intersection. This combination of driving forces of EM and availability of inhomogeneous high mobility diffusion paths network make thin film conductor susceptible to EM damage

1.3 Contribution of the dissertation

The main objective of our study is to explore the EM physics and the theory for EM modeling and the median time to failure (MTF) prediction. Its contribution covers the following aspects

1. A comprehensive review on the EM models of the interconnections and their evolution over the last three decades is presented. The different EM models are categorized according to their respective simulation methodologies. The primary contribution of this review is to re-examine the different EM simulation methodologies and provide a good reference starting point for researchers who are new in the field of EM modeling.
2. The alternative methodology using advance statistical analysis tools, 3-D physics-based EM simulation and experiments to develop the highly accelerated EM testing is presented in the dissertation. This methodology can be applied for Cu interconnects as well. Beside EM accelerated life test, this methodology could also be useful for other reliability accelerated life test to assess the change of physical mechanisms if the stress condition is changed.

3. We present the new 3-D physics-based EM simulation methodology combined both Monte Carlo method and Finite element analysis. The simulation is able to simulate the process of void nucleation and void growth and it considers both the effect of driving forces and diffusion paths of EM. It is a holistic EM simulation to study the whole physical process of EM degradation in the interconnect system.

4. In the dissertation, we also propose an alternative concept of EM modelling and present the derivation of physics-based MTF formula for void nucleation. The physical formulation of MTF reveals the key physical factors that are hidden in the Black’s equation. With the aid of the simulation, the effect of the key physical parameters on MTF can be studied and analyzed quantitatively. The Black’s equation has been known to be questionable for its application in today’s ULSI interconnect system through many reports in the literature. The study breaks new ground for the alternative solution for MTF prediction. We also perform comparison of this alternative model and the Black’s equation, and the superior performance of this alternative model in extrapolation over the Black’s equation is clearly seen.
1.4 Outline of Dissertation

The dissertation begins with a focused review on the physics-based EM modeling in Chapter 2, which covers the development of EM modeling in the past three decades. Chapter 3 discusses the EM simulation using multi-physics Finite Element analysis (FEA). The application of FEA in highly accelerated EM testing, reliability analysis in both Al and Cu interconnect system and the theory of FEA EM simulation in ULSI is explored. Chapter 4 focuses on the Monte Carlo methodology in EM simulation. Combined with various FEA techniques, we developed a powerful tool to explore the physics of EM in interconnect system holistically. In Chapter 5, we propose an alternative EM theory and a new physics-based model for the prediction of EM MTF. We also review the validity of the Black equation, especially its application in more advanced interconnect system. Chapter 6 concludes the theory and experiment studies, and its significance. The future work and research direction are also suggested in the last chapter.
Chapter 2: Physics of Electromigration and its modeling

2.1 Basic physics of Electromigration

Generally, electron movement in metal is random and the probability along any direction is statistically equivalent. Therefore, statistically, the force acted on metal atoms is uniform and equal to zero, and metal atoms in lattice structure appear to be relatively immobile. However, when a high current density is applied on metal, the presence of electrical field will drive the electrons to move from the cathode end to the anode end of metal line. From a statistical viewpoint, electron movement in metal exhibits unique directionality, namely electron wind. The collisions between electrons and metal atoms lead to the momentary exchange. The equilibrium between electrons and metal atoms is violated and the force acted on metal atoms is no longer uniform, causing atoms to move along the direction of electron wind. If a metal line is ideal without any defects, the divergence of mass transport of metal atoms doesn’t exist. However, various defects such as grain boundary, vacancies and poor adhesive interface are inevitably present in realistic metal line, and the divergence of mass flux may occur at these sites. With the divergence of mass flux, metal atoms will be redistributed close to these defects sites. Atom accumulation/depletion occurs in these sites which lead to the formation of the hillock/void. Once void/hillock is large enough to open/short the metal line, EM failure occurs.
As described above, EM behavior varies with different defects. Fig. 1 [8] gives the schematic illustration of these diffusions at the defect sites.

Figure 1: contributions to EM in polycrystalline Al. Considered is the monovacancy motion which is opposite to the material flux, (1) bulk diffusion (lattice diffusion), (2) grain boundary diffusion, (3) grain boundary to bulk diffusion, (4) defect diffusion, (5) surface diffusion, (6) interface diffusion[8]

As mentioned before, EM is a forced atomic diffusion due to various driving force. For example, Aluminum interconnects, the EM of aluminum requires the self diffusion of Al in an Al matrix. This is possible by having diffusing atom jump into a vacancy in an adjacent lattice site. Hence, the mathematical treatments of EM are usually cast in terms of vacancy diffusion[9]. The vacancy flux (J) due to the EM driving force is[10]:

\[ J = -D \overrightarrow{V} c + c \mu \overrightarrow{F} \]  

(2.1)
where $D$ is the diffusion coefficient, $c$ is the vacancy concentration, and $\mu$ is the atomic mobility. Applying the Nernst-Einstein relationship, $\mu = D/k_BT$, where $k_B$ is Blotzmann’s constant, and $T$ is the absolute temperature, we have

$$J = -D\nabla c + c\frac{D}{k_BT}\vec{F}$$

(2.2)

From the point of view of electrons, the atoms are heavy, slow-moving classical particles. And it has to break the bonding of surrounding atoms and overcome the binding energy to change its location in the lattice. When a high current density is applied to a metal thin film, the electrons exert a microscopic force on the atoms, and this force field provides the external energy and alters the energy barrier that the atoms must surmount to start its movement. In general, the microscopic force-field may depend on the position of the atoms along the diffusion jump-path[10]. However, it is customary to express the driving force in terms of an effective valence, $Z^*$, as follow:

$$\vec{F} = Z^*e\vec{E}$$

(2.3)

Various EM forces are possible in the interaction of electric current on atomic diffusion in the literatures. The most important one is the so-called “electron wind force”, which was identified as the sole EM driving force in the early days. This wind force arises from the interaction of a moving gas of free electrons with an atom. In the weak scattering by an atom modeled as a point charge in a free-electron gas, the force due to the electron wind is the average rate of momentum transfer from the electron current to the atom. The lumped parameter $Z^*$ associated with the wind-force is denoted as $Z^*_{wd}$. Another type of force is so-called “direct force” which is the force on an atom due to the long range electric field accompanying the electron transport.
process. The present of this force is under great controversy [3, 11-13]. In good
collectors, the wind-force dominates, and hence direct force is usually neglected.
Thus, $Z^* = Z^*_{wd}$. Since $E = \rho j$, where $j$ is the current density and $\rho$ is the resistivity of
the conductor, Eqn. 2.2 can be re-written as

$$J = -D \nabla c + \frac{Dc}{k_B T} Z^* e \rho \cdot j$$

(2.4)

Other driving forces, such as stress migration due to the hydrostatic stress gradient,
thermal migration due to the temperature gradient and the surface migration due to the
surface tension, are formulated and considered differently in various EM models.
They will be introduced in the next sections through the literature review of physics-
based EM modeling.

Consider a controlled volume as shown in Fig 2, three situations are possible:

Case one: $J_{in} > J_{out}$
In this case, metal atoms are accumulating in the controlled volume, and the hillock or
extrusion will lead to short circuit.

Case two: $J_{in} < J_{out}$
In this case, vacancies are accumulating in the controlled volume, and the void
nucleation/growth will lead to open circuit
Case three: \( J_{in} = J_{out} \)

Depending on the condition, void shape might change, hence causing open circuit. However, if void size is not significantly large, nothing will happen.

Therefore, EM failure happens only if there is a divergence of vacancy flux somewhere in the line that allow voids or extrusions to form. Hence, understand the physical factors that affect the vacancy flux will enable us to understand the failure mechanisms of EM. Physics-based EM model is adopted to study those physical factors and their role in the EM performance of an interconnect. A comprehensive review of the physics-based EM model will be present in the next section.

### 2.2 Physics-based EM modeling

#### 2.2.1 1-D continuum EM modeling

Like any physical modeling, physics-based EM modeling begins from 1-D analytical modeling by solving the following continuity equation\[14\] derived from the time evolution of the vacancy concentration along an interconnect line

\[
\frac{\partial C_v}{\partial t} + \frac{\partial J_v}{\partial x} + r = 0
\]  

(2.5)

Here \( C_v \) is the instantaneous vacancy concentration at position \( x \) and time \( t \), \( J_v \) is the vacancy flux due to EM driving forces and \( r \) is the sink/source term which allows for the recombination or generation of vacancies at sites such as grain boundary, dislocations, or surface\[14\].
In this category of simulation methodology, the focus is the simulation of kinetics of EM. The net vacancy flux along the length of an interconnect can be due to the electron wind force, vacancy diffusion as a result of concentration gradient (Fickian diffusion) and temperature gradient (Soret diffusion), hence the flux can be written as

\[ J_v = -D \frac{\partial C_v}{\partial x} + \frac{DC_vZ^*eE}{k_B T} + \frac{Q^*DC_v}{k_B T^2} \cdot \frac{\partial T}{\partial x} \]  

(2.6)

where \( D \) is the vacancy diffusivity \( (D=D_0\exp(-\Delta E_a/k_B T)) \), \( E_a \) is the activation energy for the vacancy diffusion, \( Z^*e \) is the effective charge of the diffusing species, \( E \) is the electric field and \( Q^* \) is the heat of transport.

The sink/source term \( r \) can be expressed as

\[ r = \frac{C_v - C_{ve}}{\tau} \]  

(2.7)

where \( C_{ve} \) is the equilibrium concentration of vacancies within the grain, and \( \tau \) is the average lifetime of a vacancy.

Eqn. 2.5 is a basic EM equation from the first principle, and it is adopted by many 1-D analytic EM models reported in literature. With certain assumptions, various EM models are proposed based on different boundary conditions. With these boundary conditions, the phenomenon of EM can be simulated by analyzing the evolution of the vacancy concentration in an interconnect metal line using the aforementioned EM equation.
2.2.1.1. Without the consideration of stress migration due to stress gradient

In one of the pioneer works on 1-D continuum EM modeling, the work of Rosenberg and Ohring[15], all the aforementioned EM driving forces, namely the electron wind force, concentration gradients (Fickian diffusion) and temperature gradients (Soret diffusion) are taken into consideration with the presence of the vacancy sink/source. As shown in Fig. 3, they proposed a model from the appropriate solution of Eqn. 2.5 where it was assumed that two grains intersect at \( x=0 \) and that each grain can be characterized by their respective vacancy diffusion parameters \( D, C_{\text{ve}}, \tau, \) and field strength \( E \). The vacancy behavior as expressed by Eqn. 2.5 can be written separately for the two grains if the diffusion parameters are assumed to be constant within each grain.

\[ S = \frac{C_v}{C_{\text{ve}}} - 1 \]

**Figure 3: Model of two grain boundaries intersecting at \( x=0 \). Variations in flux \( J_1 \) and \( J_2 \) give rise to vacancy saturation \( S \) \((S = C_v/C_{\text{ve}} - 1) \) [15]**

In order for vacancy accumulation to take place, it is necessary that the vacancy flux induced by the electron flow is different in the two grain regions. The boundary conditions for this calculation are the vacancy concentration and flux at \( x=0 \) are continuous, and all diffusion parameters are the same in the two grains except that the
activation energies are 0.6 ev for \( x > 0 \) and 0.8 ev for \( x < 0 \). Using Laplace transform method, both transient time dependent solution and steady state solution of \( C_v(t) \) are obtained.

The model simulates the vacancy saturation due to the divergence of vacancy flux at the grain boundary with the consideration of multiple EM driving forces. Although the thermal migration due to temperature gradient is taken into consideration during the initial modeling of EM, it is dropped for the sake of simplicity during the actual calculation. It is a reasonable simplification because interconnect length is the only dimension considered for 1-D EM model, and with the current density evenly distributed throughout the length, the temperature along the length is a constant as Al or Cu is a very good heat conductor. However, in actual interconnect, 3D modeling is necessary as will be discussed in the following sections, and the effect of the temperature gradient can no longer be ignored. Also, the choice of the boundary condition with infinite ends renders the model incapable of catering the length effect of a confined metal thin film which was discovered by Blech few years later [6, 16]. Due to this incapability, this type of boundary condition was not chosen for the subsequent 1-D continuum EM modeling.

A more realistic boundary condition was proposed by Shatzkes and Lloyd [17]. In their study, the case of vacancy flow in the region of a purely blocking boundary was examined. Fig. 4 shows the semi-infinite grain boundary considered by Shatzkes and Lloyd.
This condition can occur in real conductors, for instance, at the boundary of a “bamboo” grain, and has been found experimentally to be related to failure. Mathematically, the boundary condition can be expressed as

\[ C(-\infty, t) = C_0 \quad \text{(2.8)} \]

\[ J_v(0, t) = 0 \quad \text{(2.9)} \]

Although this solution treats a special case of a perfectly blocking boundary, it may also be useful in the understanding of other conditions where the boundary conditions allow a reduced vacancy flow as pointed out by the authors. In general, there will be a flux through any given region, but a divergence may still exist. By treating this “residual” mass flux as a background, one can then treat the accumulation of vacancies above the background in the present manner. The trends and general features of atom or vacancy accumulation predicted here for the perfectly blocking boundary will still hold true for other more commonly encountered conditions. In their study, the vacancy flux due to thermal migration was not considered as well, and the vacancy sink/source term was also dropped in their EM equation. The justification of this modification of EM was addressed by Kirchheim and Kaeber in their report[18].
Based on the same EM equation, Kirchheim and Kaeber[18] in 1991 reported their EM modeling and solved the EM equation based on different boundary conditions. As shown in Fig. 5, the EM equation is solved for a case of a single grain boundary structure.

\[ J_v(x=0) = J_v(x=L) = 0 \]  

Figure 5: Grain boundary between two triple points at \( x=0 \) and \( x=L \). The angle between the grain boundary and the current density \( j \) is labeled \( \theta \)[18]

Compared with the infinite boundary condition proposed by Rosenberg and Ohring[15] and the semi-infinite boundary condition proposed by Shatzkes and Lloyd[17], Fig. 5 shows a special case of finite boundary that the fluxes at both ends are zero (i.e., due to very low vacancy mobility in the adjacent grain boundaries), that is,

\[ J_v(x=0) = J_v(x=L) = 0 \]  

In the work of Kirchheim and Kaeber, both the solutions with and without consideration of vacancy sink/source were analyzed and discussed. The authors argued that the formation and annihilation of vacancies in the grains require volume diffusion between grain boundaries and sinks/sources within the grains will play a role at elevated temperatures only. With this justification, their study focused on the steady-state concentration profile without vacancy sinks/sources which was also adopted in the previously work of Shatzkes and Lloyd[17]. Moreover, in the
calculation of vacancy flux, the grain boundary component of the electric field or current density is used for the calculation of vacancy flux due to electron wind force, i.e., the total current density has to be multiplied by \( \cos \theta \) (refer to Fig. 5).

With this finite boundary condition, the mass backflow during EM can be simulated. However, contrary to the generally accepted interpretation[6, 16], as a flow of matter is caused by a stress gradient within the Al line, the interpretation of the backflow is based on the diffusional backflow of vacancies with respect to the vacancy concentration profile. The authors argued that the vacancy fluxes and internal stress gradients are coupled since production and annihilation of vacancies is often accompanied by plastic deformation. This interpretation of the backflow is only a different way of approaching the problem in comparison with the usual way of consideration of stress gradient.

A more completed study on the boundary conditions of the EM equation was reported by Clement and Lloyd[19]. Similar to the previous studies, both the electron wind force and vacancy concentration gradient are taken into the consideration as driving forces of EM. In their report, the physical meanings of the three boundary conditions used are described and the solutions are compared at the blocking barrier. The first boundary condition corresponds to a situation of a semi-infinite metal line which is the same as the one proposed by Shatzkes and Lloyd[17]. The other two boundary conditions are for the cases of the finite interconnect length. The first case corresponds to a situation where the number of vacancies is conserved. An example of such case is
an interconnect line with a thick and strong passivation layer that precludes volume
change of the conductor. The above-mentioned boundary conditions and their solution
have been reported by Kirchheim and Kaeber[18]. The second case corresponds to a
situation where the passivation or adherent oxide layer on the metal line is not so
strong and stiff as to preclude the creation of vacancies. This is what one might expect
in an Al conductor covered only by its native oxide. Refer to Fig. 5, this new perfectly
blocking boundary condition can be expressed as:

\[ J_v(L, t) = 0 \quad (2.11) \]
\[ C(0, t) = C_0 \quad (2.12) \]

Solutions to the above-mentioned three reasonable boundary conditions for the EM
equation were investigated numerically. It was shown that regardless of the boundary
condition chosen, the time to failure would approximate the semi-infinite solution of
Shatzkes and Lloyd as long as the critical failure vacancy concentration is significant
different from its steady-state value.

A more complete review on the 1-D EM modeling was contributed by Clement in his
review paper[14]. He reviewed all the 1-D EM models before 2001 from the
perspectives of the consideration of driving forces of EM, choices of the boundary
conditions and the corresponding numerical solutions. In his report, the 1-D EM
models with consideration of vacancy sink/source were compared with those without
it. Although the numerical solutions of the EM equation for both cases are quite
similar, there is one critical difference. The effect of the consideration of vacancy
sink/source is the shift in time scale for the buildup of vacancies. Hence, the calculated
time-to-failure will be on the order of several days, rather than a few seconds as obtained from those models without the consideration. This highlights the importance of including the sink/source term in the 1-D EM model. For more details of investigation on the effects of vacancy sink/source term on the solutions of the EM equations, one can refer to the review paper by Clement[14].

2.2.1.2. With the consideration of stress migration due to back stress

With the shrinking metal line dimension, it is found that, in the confined metal interconnects deposited on an oxidized silicon substrate and covered by a dielectric passivation layer, EM gives rise to back stresses that can retard EM itself[20]. A few reports on the modeling of EM incorporating the effect of the transient back stress buildup can be found, such as Ross[21], Kirchheim[22], Korhonen et al.[23]. The modeling of the EM driving forces was modified to account for the effect of the migration due to the back stress.

For example, in the work by Kirchheim[22], additional EM driving force, the stress gradient, is taken into consideration. Moving an atom from the grain boundaries to the surface changes the volume by one atomic volume, $\Omega$. Allowing relaxation of the neighboring atoms leads to a contraction in volume of $f\Omega$ (0<$f$<1), and hence the total volume change is $(1-f)\Omega'=f'\Omega$. Therefore, due to the strain caused by the lattice relaxation, a vacancy experiences a driving force in a stress gradient and the corresponding flux is given by

$$J_v = -\frac{DC_v}{kT} j\sigma \frac{\partial \sigma}{\partial x}$$  \hspace{1cm} (2.13)
With this additional driving force, Eqn. 2.6 was modified as

\[ J_v = -D \frac{\partial C_v}{\partial x} + \frac{D C_v Z' e E}{k_b T} + \frac{Q' D C_v}{k_b T^2} \frac{\partial T}{\partial x} - \frac{D C_v}{k_b T} \beta \Theta \frac{\partial \sigma}{\partial x} \]  

(2.14)

For the same reason stated above, the atomic migration due to the temperature gradient is neglected in the modeling. Vacancy sink/source is considered in a similar way as in previous studies of the Eqn. 2.7. To account for the effect of the back stress, the vacancy concentration change due to both the vacancy flux and the vacancy sink/source is coupled with stress evolution by the Hook’s Law as given below

\[ f \left( \frac{\delta}{d} \frac{\partial C_v}{V} = \frac{\partial V}{V} = \frac{\partial \sigma}{B} \right) \]  

(2.15)

Here \( \delta/d \) accounts for the fact that the concentrations are related to the grain boundary volume whereas the stresses are induced within the volume of a grain. Using the two coupled differential Eqn. 2.14 and Eqn. 2.15, a continuity equation for the vacancy concentration as in Eqn. 2.5 and a rate equation for sink and source reactions Eqn. 2.7, the EM phenomenon is simulated in a finite line blocked at both ends \( J_v (x = 0) = J_v (x = l) = 0 \) as shown in Fig. 5.

In the model developed by Korhonen et al. [23], the driving forces of EM include only the electron wind force and the stress gradient, and both of them are formulated based on the atomic flux instead of the vacancy flux. The vacancy sink/source term was dropped in their consideration with the assumption that the net number of atoms entering a volume element was large enough to include vacancy sources and sinks. In
their modeling, the change in atomic concentration was also coupled with the stress evolution in a similar manner as in the work by Kirchheim[22]. The solutions of the EM equations with the consideration of stress evolution was presented by Korhonen et al[23] for several representative cases, such as the semi-infinite metal line where the flux is blocked at the end x=0, and the confined finite metal line where the flux is blocked at the both ends. Besides the investigation of the EM equation’s solutions with different boundary conditions, Korhonen et al also studied the influence of the stress evolution on the diffusivity of atoms and its impact on the solutions of the EM equation. More details can be found in their report[23].

Although the EM equation formulated by Korhonen et al[23] as discussed above is very similar to those by Rosenberg and Ohring[15], Shatzkes and Lloyd[17], Kirchheim and Kaeber[18] and Clement and Lloyd[19], there are differences. With the consideration of the stress evolution, the current induced flux creates a stress-directed counter flux, which retards EM damage. On the other hand, the counter flux arises due to the vacancy concentration gradient does not retard EM damage. Furthermore, significant vacancy concentration gradients can be created in a matter of seconds because of the almost negligibly small material transport involved. However, the stress evolution in the interconnect lines during EM can last hundreds of hours as predicted by Korhonen et al[23].

With the development of the analytical modeling and interconnect technology, Korhonen’s model received further review and continuous development in order to
explain the physics of EM in the new advanced interconnect systems. Clement and Thompson[24] reported a complete review on the Korhonen’s model and found that the analytic solution for a semi-infinite line with a blocking boundary given by Korhonen et al is a good approximation only when the stress buildup is small, and this is usually not the case for narrow, encapsulated interconnect lines in which the EM-induced stress can be very high prior to failure. They proposed a complete model description and a more accurate analytic solution to the differential equations describing the EM-induced stress buildup at a blocking boundary[24].

Based on the improved model, Park, Andleigh and Thompson reported another EM model to simulate the reliability of Al and Al-Cu interconnects[25]. In their work, the effect of the impurity Cu atoms in Al interconnects on stress evolution and lifetime was investigated in various structures. In addition, the significance of the effect of the mechanical stress on the diffusivity of both the Al and Cu was determined. Current density exponents of both $n=2$ for void nucleation and $n=1$ for void growth failure modes were found in both pure Al and Al-Cu lines. More importantly, the application of the model can be further extended to the investigation of other interconnection materials such as Cu and its alloys by modifying the input material properties. The detail mathematical formulation used in the analysis can be found their report and earlier study[26]. Their analytic EM model was developed into an EM simulation package, MIT/EmSim[27] which was extensively employed in their other EM studies [28-30] and provided theoretical support to various experimental observation successfully.
Although the stress migration due to back stress has been well addressed by the models we discussed above, the other important source of the stress is neglected in their theoretical consideration which is the thermo-mechanical stress due to the thermal mismatch between the metal stack and its surrounding materials. The thermo-mechanical stress depends on the thermal expansion coefficient of the materials and the shape of the metal line itself, and the 1-D EM models are incapable of simulating the above aspects. However, as will be discussed in Section 2.2.3.1, this thermo-mechanical stress is found to be dominant as the line width decreases.

2.2.1.3. Summary

From the above discussion, all the 1-D continuum EM models were based on the so called "EM equation". The kinetics of EM, such as the EM driving forces due to electron wind force and vacancy concentration as well as stress gradients, was simulated through the calculation of vacancy concentration change along the metal line. With properly boundary condition setup, the 1-D continuum EM equation is solved along the length of a metal line. The evolution of the vacancy concentration is simulated in the EM model, through which the critical location of the metal line can be identified. Moreover, the time to failure can be extracted if a reasonable criterion of failure is given.

In the development of the 1-D continuum EM models, there are a few critical aspects need to be considered and integrated into the model as follows

-22-
• Boundary conditions: infinite, semi-infinite or finite
• The vacancy sink/source
• The consideration of EM driving forces: electron wind force, concentration gradient and temperature gradient
• The consideration of stress development during the EM
• The choice of solutions: transient or steady-state solution

The 1-D continuum EM modeling is capable of integrating the multiple driving forces to simulate the kinetic of EM process and evaluating the impact of the properties of the metal line on the EM performance, such as the length, the passivation and the various boundary conditions that represent the interconnect structures and the microstructures in a simplified manner. However, the real EM process in a metal line is rather complicated. 1-D continuum EM modeling is only capable of simulating the simplified scenarios of EM due to its limitation on dimensionality. The influence of the triple points of the multiple grain textures, the surrounding materials and the induced thermal-mechanical stress, the shape of the metal line or the metal stack structure in the interconnect system is poorly addressed in the 1-D modeling. The consideration of the EM from thermodynamics aspect, such as the various diffusion paths, is inevitably simplified in the 1-D model.

The development of the 2-D continuum EM model, or even 3-D, is necessary. However, the difficulties and complexities in the mathematical implementation increase dramatically as the coupled partial differential equations have to be solved in
multiple dimensions. Different approaches have been proposed to simulate the EM process in a 2-D or 3-D dimensions as will be discussed later.

2.2.2 Void surface evolution model

Besides studying the evolution of the vacancy concentration along a metal thin film in 1-D EM model as presented in previous section, another class of model for EM is developed primarily focus on the kinetics of EM on the void surface, namely the size evolution and stability of a void due to the atomic migration along its surface under the various driving forces.

The simulation methodology for this class of model begins in the mid 1990’s, and there are two different models developed. One is the *sharp interface model* that attempts to model the void surface as a sharp interface between the conductor material and empty space in the void. This requires a tracking and accurate book-keeping of the surface elements and their geometry. The method is cumbersome but able to explain some experimental observations quite well.

The other method is the *phase field model*. This model defined the level of the presence of the conductor material based on a phase field scalar variable. The value of the variable defines the phase of the material at any point on a fixed grid that defining the simulated specimen. The transaction from metal material to an empty void is not sharp as modeled by the first approach, but gradual in terms of the presence of the
material. It requires less book-keeping and seems to be more computational efficiency.
Both models are 2-D models.

2.2.2.1 Sharp interface model

In 1994, Arzt and Kraft et al.[31] published their work on the investigation of the behavior of EM-induced voids in narrow, unpassivated aluminum interconnects. Experimentally, it was found that the fatal voids have a specific asymmetric shape with respect to the electron flow direction. They proposed, to our best knowledge, the first model which attempted to simulate the void shape changes on the basis of atomic diffusion along the void surface. In their model, they considered an isolated two-dimensional void which extends through the thickness of the line, and atomic diffusion on the void surface was assumed to be the primary transport mechanism. Depending on the balance of the arriving and departing atoms at each point on the surface, the movement and the shape change of a void relative to a fixed coordinated system in the line are tracked as shown in Fig. 6.

![Figure 6: The finite element analysis for a sharp interface model[31]]
The driving forces for such a behavior are modeled using the surface mass flux through a surface element, and they considered two types of mass fluxes due to the electron wind force and the curvature of the surface respectively as follows

\[ I_s^j = - \frac{\delta D_s}{\Omega kT} e Z^* \rho j, \quad (2.16) \]

\[ I_s^k = \frac{\delta D_s \gamma}{kT} \frac{\partial \kappa}{\partial s}, \quad (2.17) \]

where \( I_s^j \) and \( I_s^k \) are the mass flux along the surface due to the electron wind force and the curvature of the surface respectively, \( \delta \) is the film thickness, \( D_s \) is the surface diffusivity, \( \Omega \) is the atomic volume, \( k \) is the Boltzmann constant, \( T \) is the absolute temperature, \( e \) is the charge of an electron, \( Z^* \) is the effective valence, \( \rho \) is the resistivity, \( j_s \) is the current density along the surface. \( \gamma \) is the surface tension, \( \kappa \) is the curvature, and \( s \) is the arc length along the surface.

In their model, the current density distribution was calculated based on the assumption of a steady flow of an incompressible, non-viscous, circulation-free liquid, of which the expressions are mathematically identical to the equations of electrostatics. With the knowledge of current density and mass fluxes, the normal velocity at each point of the surface can be computed and the resulting equation of motion for the void surface can be obtained as

\[ v_s = \Omega \frac{\partial}{\partial s} \left( I_s^j + I_s^k \right). \quad (2.18) \]

However, with their methodology, the inhomogeneous current distribution in the interconnect around the void is not considered in their model. This non-uniform
current density distribution will produce temperature gradients, and thus result in local changes in the resistivity and the diffusivity. These effects are believed to be potentially important for the failure mechanism.

The simulation methodology was further elaborated in their subsequent report[32]. A finite element method was used in the calculation of the current density and the temperature distribution. A finite difference method was employed for the void motion and the shape changes computation. Fig. 7 shows some of their simulation results of the void motion and the shape changes in an Al metal line.

The commercial finite element software ANSYS was used in their modeling. The consideration of the crystallographic orientation leading to a surface diffusivity change for different angles of the surface with respect to the crystal is also included in their

Figure 7: Simulation of the development of initially semi-circular voids with radii of a)0.8um b)0.6um in a 1um wide Al metal line. The applied current density was 2MA/cm2 and the time is given in units of 100s[32]
work. To model this effect, they considered the surface diffusivity to be no longer constant and the anisotropy can be incorporated in the FEA by describing the surface diffusivity as a function of the angle $\theta$ between the surface tangent and the conductor line length direction.

In their study, they found that slit voids that form within grains are likely to be caused by EM induced surface diffusion. Under sufficiently high current density, a rounded void is unstable and will spontaneously collapse into a slit. The procedure used by Kraft et al. is shown in Fig. 8 where an initial void shape is defined, followed by the computation of the current density and temperature due to joule heating, then the calculation on the shape changes of the void surface. Thereafter, a re-meshing is needed for the modified structure, and the process repeated itself. With this procedure, void shape evolution and shape stability with different void geometries can be studied, and the model has the potential of predicting the lifetime of metal line with certain void shape.
Another similar model was proposed by Wang et. al.[33]. In their early studies [34, 35], they showed that atomic diffusion on the void surface, driven by the electrical current, can cause a circular void to translate into a slit void. During this translation process, two forces compete in determining the void shape, one is the surface tension force and the other is the electron wind force due to the electrical current. Surface tension force favors the formation of a rounded void, while electrical current favors a slit void; a rounded void will collapses and becomes a slit when the electron wind force dominates.

In their later published work[33], they reviewed the experimental and theoretical findings, and provided a numerical simulation of the void shape change. Similar to the Kraft’s model, they adopted the sharp interface approach and assumed that the void shape change is due to the surface diffusion only, considering all other transport
processes as negligibly slow during the void shape change. This approach utilizes the same equations as in Kraft’s model[31] to model the mass transport. By approximating the void perimeter by many short straight segments, they formulated a finite element procedure for the shape evolution, as had been done by Kraft[31].

The difference between the above-mentioned two models lies in the implementation of the physical system analysis. Wang et al. uses a conformal mapping technique to determine the electric field around the circular void. After that, the electric potential and the curvature of the void surface are determined, and then the Galerkin method[36] is used to determine the EM kinetic system. As a result, their model is capable of modeling void and surface evolutions, and their results are similar to that obtained by Kraft et al. Compared with the finite element method by Kraft, Wang’s approach, while mathematically elegant, is not versatile and is hard to yield more complex geometry evolutions[37]. Other similar works are reported by Gungor et al.[38, 39] and Schimschak et al.[40].

In the sharp interface models, the common assumption is that the atomic surface diffusion is the dominant diffusion mechanism, and the surface diffusion is driven by the electron wind force and the surface tension force due to the curvature of the void surface only. The anisotropy of the void surface diffusivity is emphasized, and slit voids will only form in grains with certain crystallographic orientations. They studied moving boundary problems entail explicit tracking of the boundary. The interface is described by specifying a large number of points on it. The same equations are used
by them to model the atomic surface diffusion and the motion of the void surface at each interface point.

2.2.2.2 Phase field model

In the Sharp interface model, a lot of interface points are required to accurately describe the void surface when the void shape is evolving, and the changing boundary conditions must be implemented at this increasingly numerous set of points. Thus, the sharp interface model can get very complicated and also tends to have rather poor numerical stability[41, 42].

On the other hand, if the entire domain is described by a continuously varying scalar order parameter $\phi$ which has a value of +1 for region well within the metal “phase” and -1 for region well within the void “phase”, and $\phi$ has a value between +1 to -1 for the metal-void interface as shown in Fig. 9, we have the phase field model[42].

![Figure 9: The void simulation in a phase field model](image)
This model was introduced independently by Fix[43] and Collins & Levine[44], and it received considerable attention in the context of phenomena associated with evolving interface. The earliest attempt to use the phase field model for the line interconnect failure simulation was reported by Mahadevan and Bradley[42]. In their study, they simulated the time evolution of a perturbation to the edge of a current carrying, single-crystal, unpassivated metal line. Surface electron wind force migration, surface self-diffusion due to the current crowding, and the curvature of the void surface are all taken into account. They adopted the same formula that model the diffusion mechanisms along the void surface used by Kraft[31], but the idea of a sharp interface between metal and void is abandoned. The inclusion of the phase field model results in two coupled partial differential equation with the first one describing the dynamics of the phase field, and the second one describing the electric field as given below.

\[-\varepsilon \frac{\partial \phi}{\partial t} = \nabla \cdot \left\{ \alpha_0 \left[ 1 + \lambda_1 \varepsilon \left( \nabla \phi \right)^2 \right] \nabla \psi - \left[ \varepsilon^2 \beta_0 (\phi + 1) \left( \nabla \phi \right)^2 \nabla \Phi_E \right] \right\} \quad (2.19)\]

\[\phi_t = a_0 = \frac{3M_0 \lambda_1 \Omega}{D_s L}, \quad \lambda_1 = 3D_s h \frac{M_0 L k_B T}{a_0}, \quad \beta_0 = \frac{3Z_s eE_s h}{k_B T} \quad (2.20)\]

\[v = \varepsilon^2 \nabla^2 \phi + g(\phi), \quad g(\phi) = (\phi - \phi^3)/2 \quad (2.21)\]

and

\[\nabla \cdot \left[ \sigma(\phi) \nabla \Phi_E \right] = 0 \quad (2.22)\]

where $D_s$ is the surface diffusivity, and $L$ is a characteristic length describing the void which can be taken to be the square root of the void surface area. $\Phi_E$ is the electrical potential, $\varepsilon$ is a dimensionless constant proportional to the interface width, $M_0$ is the
lattice diffusivity of the phase field, \( k_B \) is the Boltzmann constant, \( \lambda_s \) is the surface tension, \( T \) is the temperature, and \( \sigma \) is the conductivity.

The phase field model was used for an isolated void in an infinite thin film, and this method can be easily extended so that it applies to the time evolution of an edge perturbation in a metal line of finite extent. By solving the phase field equations and electric field equations numerically, the model provides the time evolution of a small notch at the edge of a current-carrying single crystal metal line. The model is able to predict a threshold value of the applied current so that the edge perturbation will grow into a slit-shaped void that spans the wire. They also explained the physical origin of this instability and pointed out the importance of the crystalline anisotropy and mass transport along the edge of the line.

At nearly the same time as Mahadevan and Bradley, Bhate et al.[45] reported their own version of the phase field model for simulating the process of electron wind force migration, curvature driven surface migration, and the stress driven migration. In their work, Bhate et al.[45] briefly discussed the theory of the sharp interface model and its limitations or disadvantages, and hence they proposed their own phase field model. Their approach is based on the introduction of an order parameter field to characterize the damaged state of an interconnect. The order parameter takes on distinct uniform values within the material and the void, varying rapidly from one to the other over narrow interfacial layers associated with the void surface. They derived the field
equations for the order parameters based on the micro-force balance principle of Gurtin[46].

Accordingly, they express the free energy of the line as

\[
\mathbb{F}(\phi, \varphi) = \int_R F(\phi, \nabla \phi, \varphi) dV = \int_R \left\{ \frac{2\gamma_s}{\varphi \pi} \left( f(\phi) + \frac{1}{2} \varphi^2 |\nabla \phi|^2 \right) + W(\varphi, \phi) \right\} dV, \quad (2.23)
\]

where \( f(\phi) \) is the bulk free energy, \( \gamma_s \) is the isotropic surface energy, and \( \varphi \) is a parameter that controls the thickness of the interfacial layer associated with the void surfaces, and \( W \) is the elastic strain energy. The field equation for the electrical potential in the line has the identical form as in Eqn. 2.22. The atomic diffusion paths through the bulk and grain boundary are assumed to be negligible, and the only mode of transport for atoms is the diffusion along the void surfaces in their model. This is the same assumption as in most sharp interface models except the surface diffusivity in their model is treated as isotropic. However, this assumption is not justifiable since it has been proved that the anisotropic diffusivity of atoms along the void surface has a strong effect on the evolution of void during EM[31]

2.2.2.3 Summary

This category of EM modeling technique focuses on the evolution and the stability of the void shape though the simulation of the EM kinetics on the void surface, and the impact of the different void shapes on the EM performance of the metal line is also studied. All the models in this category are based on 2-D simulation.
Unlike the 1-D continuum EM models, the driving forces in the 2-D void surface evolution models are essentially electron wind forces and the surface migration due to the void surface curvature. Other driving forces, such as the temperature and stress gradients are not taken into the consideration, and the void surface is assumed to be the only diffusion path in the EM model during the void shape change.

However, ignoring the temperature and stress gradients in the 2-D void surface evolution models is not justifiable in a narrow interconnect. This is because the formation of the void can severely change the temperature distribution around the void[32], rendering difference in the diffusivity of the atoms and vacancies in these areas. The local unbalance of the diffusion will influence the evolution of the void shape and its stability. This effect is more severe as the dimension of the metal line shrinks. The local stress due to the thermal mismatch can also alter the atom/vacancy flux around the voiding region The importance of the temperature and stress gradients in the EM simulation of both Al and Cu interconnect has been highlighted in our previous studies[47, 48]

Furthermore, like in the 1-D continuum EM model, the consideration of EM from the thermodynamics aspect in these void surface evolution models is inadequate. The assumption of the sole void surface path is unsuitable in the new Cu interconnect technology. The fast diffusion path along the interface of the capping layer and Cu can dramatically change the behavior of the void during the EM. Experimental observations found that the void can migrate, coalescent and interact with grain
boundaries under the influence of the various driving forces[49]. In fact, the consideration of both the EM kinetics (multiple driving forces) and its thermodynamic (multiple diffusion paths) are imperative for the EM simulation in the interconnect systems. In the subsequent sections, other simulation techniques will be introduced that overcome the difficulties encountered in the 1-D continuum EM models and 2-D void surface evolution models and they will make the study of the EM physics more realistically in an actual 3-D system.

2.2.3 Other physics-based EM modeling

2.2.3.1 EM modeling using atomic flux divergence (AFD) and Finite element analysis (FEA)

The lifetime of a metal line is closely related with the void and hillock formation in the line[50]. Divergence of the atomic flux due to EM gives rise to the formation of the void and hillock. In the presence of the inhomogeneity in the microstructure and texture, the atomic diffusivity is altered along a diffusion path, thus producing Atomic Flux Divergence (AFD). AFD occurs at the triple point of grain boundaries[51], the intersection of cap layer/grain boundary/barrier layer and grain boundary itself[52]. Besides, the distributions of the current density, the temperature and the hydrostatic stress along the metal line are also key affecting factors on the AFD[5]. In this category of the models, AFD is the basis for the EM simulation, but their mathematical implementation and theoretical derivation can be different among the models.
Sasagawa et al. reported their detailed study on AFD in 1998[53, 54]. They proposed a calculation method of AFD due to EM by considering all the factors on void formation for both cases of unpassivated polycrystalline line and bamboo line. Later on, the calculation method of AFD was also applied to passivated polycrystalline line including the effect of the back flow stress in their subsequent work[55]. In their study, the AFD is identified as a parameter governing the void formation, and the distributions of the current density, the temperature and the material properties of the metal thin film are considered in the computation of the AFD. Lifetime and failure site in a passivated/unpassivated metal line are predicted by means of the numerical simulation of the processes of the void initiation and void growth based on the AFD, and the change in the distributions of the current density and temperature with void growth is taken into account.

For the case of unpassivated metal lines[54], they adopted the basic atomic flux formula as follows[3]:

\[
|J| = \frac{ND_0}{k_BT} \exp\left(-\frac{E_{a,gb}}{k_BT}\right) Z^* e \rho^* f, \quad (2.24)
\]

where \(J\) is the atomic flux vector along the direction of the dominant grain boundary, \(N\) denotes the atomic density, \(D_0\) is a prefactor for diffusion, \(k_B\) is the Boltzmann’s constant, \(T\) is the absolute temperature, \(E_{a,gb}\) is the activation energy for grain boundary diffusion, \(Z^*\) is the effective valence, \(e\) is the electronic charge, \(\rho\) denotes the temperature-dependent resistivity expressed as \(\rho = \rho_0 \left[1 + \alpha (T - T_e)\right]\), \(\rho_0\) and \(\alpha\) are the
resistivity and its temperature coefficient at the substrate temperature $T_s$, respectively. $j^*$ is the component of the current density vector in the direction of $J$.

For the case of passivated metal line[55], they adopted the basic atomic flux formula as[56]

$$|J| = \frac{ND_0}{k_B T} \exp \left( -\frac{E_{a,gb} - \sigma \Omega}{k_B T} \right) \left( Z^* e \rho j^* + \Omega \frac{\partial \sigma}{\partial l} \right), \quad (2.25)$$

where $\sigma$ is the hydrostatic stress, $\Omega$ is the atomic volume, and $\frac{\partial \sigma}{\partial l}$ is the component of the stress gradient in the direction of $J$. By introducing a two-dimensional model of the polycrystalline microstructure, the derivation of the AFD for unpassivated and passivated metal line are obtained and presented in detail in their published work[54, 55]. The proposed AFD formula is also used in their simulation model in the prediction of the failure site and the lifetime of the metal line. The lifetime of a metal line is closely related with the void and hillock formation in the line[50]. Divergence of the atomic flux due to EM gives rise to the formation of the void and hillock. In the presence of the inhomogeneity in the microstructure and texture, the atomic diffusivity is altered along a diffusion path, thus producing AFD. AFD occurs at the triple point of grain boundaries[51], the intersection of cap layer/grain boundary/barrier layer and grain boundary itself[52]. Besides, the distributions of the current density, the temperature and the hydrostatic stress along the metal line are also key affecting factors on the AFD[5]. In this category of the models, AFD is the basis for the EM simulation, but their mathematical implementation and theoretical derivation can be different among the models.
In 1999, Rzepka et al. presented their three-dimensional finite element simulator of EM in interconnect metal lines[57]. Their model simulates the migration of matter due to various driving forces, namely the concentration gradients, the mechanical stress gradient, the electrical field, the temperature gradients, and the surface tension due to the changes in surface curvature. Their work is the pioneer study on 3-D model for EM simulation and various driving forces of EM.

In their work, they creatively used the thermal analysis routine to model the diffusion phenomena. As the basic mechanism that allows matter to move in solid is diffusion with the following fundamental relations

\begin{equation}
J = -D \nabla c, \quad (2.26)
\end{equation}

\begin{equation}
\frac{\partial c}{\partial t} = -\nabla \cdot J, \quad (2.27)
\end{equation}

where \( J, D, c \) and \( t \) denote the diffusion flux, the diffusion coefficient, the concentration and the time respectively, they found that these fundamental formulae are analogous to the heat flux equation in thermal analysis which was found by Adolf Fick in 1855[58]. Because of this similarity, the atomic concentration change and atomic flux due to the various driving forces can be generalized to be expressed as follows

\begin{equation}
\frac{\partial c}{\partial t} = -\sum_i \nabla \cdot J_i = -\sum_i \nabla \left[ -\frac{Dc_0}{k_B T} \nabla (V_i) \right] = \sum_i \nabla (M_{c_0} F_i), \quad (2.28)
\end{equation}
where \( c_0 \) is the initial concentration, \( M \) is the mobility of that particular matter, \( J_i \) is the individual diffusion flux (\( \nabla \cdot J_i \) is AFD) that results from the driving force \( F_i \), which itself is caused by the gradient of the corresponding potential, \( V_i \), such as

Concentration, \( c \)

\[ V_c = \Omega k_b T c \] (2.29)

Mechanical stress, \( \sigma \)

\[ V_{\sigma} = -\Omega \sigma \] (2.30)

Electrical potential, \( \phi \)

\[ V_{\phi} = Z^* e \phi \] (2.31)

Temperature, \( T \)

\[ V_T = Q^* \ln T \] (2.32)

Surface curvature, \( \kappa \)

\[ V_{\kappa} = \gamma \Omega \kappa \] (2.33)

By applying the thermal routine of ANSYS multiply, the individual fluxes and AFD can be sequentially calculated, thus obtained the change in the total atomic concentration.

In 2001, Dalleau and Weide-Zaage published their study on 3-D voids simulation in chip metallization structures[59]. In their study, the different mass flow such as the electron wind force migration, the thermo-migration due to temperature gradients and the stress-migration due to thermal induced stress gradients are modeled respectively as

\[
\bar{J}_{\text{EWM}} = \frac{N}{k_b T} e Z^* j \rho D_0 \exp\left(\frac{E_A}{k_b T}\right), \quad (2.34)
\]

\[
\bar{J}_{\text{th}} = -\frac{N Q' D_0}{K_b T} \exp\left(-\frac{E_A}{K_b T}\right) \nabla T, \quad (2.35)
\]

\[
\bar{J}_{\text{str}} = \frac{N \Omega D_0}{K_b T} \exp\left(-\frac{E_A}{K_b T}\right) \nabla \sigma_H, \quad (2.36)
\]
where $E_a$ is the measured activation energy, $Q^*$ is the heat of transport, $\sigma_H$ is the local hydrostatic stress value ($\sigma_H=\frac{1}{3}(\sigma_{xx}+\sigma_{yy}+\sigma_{zz})$). Based on the above atomic flux equations, they derived the approximated AFD for the respective driving forces as follows

\[
div(\vec{J}_{EWM}) = \left(\frac{E_a}{k_B T} - \frac{1}{T} + \frac{\rho_0}{\rho}\right) \cdot \vec{J}_{EWM} \cdot \nabla T, \quad (2.37)
\]

\[
div(\vec{J}_{th}) = \left(\frac{E_a}{k_B T} - \frac{3}{T} + \frac{\rho_0}{\rho}\right) \cdot \vec{J}_{th} \cdot \nabla T + \frac{NQ^D_0}{3k_B^3 T^3} J^2 \rho^2 e^2 \exp\left(-\frac{E_a}{k_B T}\right), \quad (2.38)
\]

\[
div(\vec{J}_{
u}) = \left(\frac{E_a}{k_B T} - \frac{1}{T} \right) \vec{J}_{
u} \nabla T + \frac{2EN\Omega D_0 \nu}{3(1-\nu)k_B T} \exp\left(-\frac{E_a}{k_B T}\right) \left(\frac{1}{T} - \frac{\rho_0}{\rho}\right) \nabla T^2 + \frac{2EN\Omega D_0 \nu}{3(1-\nu)k_B T} \left(-\frac{E_a}{k_B T}\right) \frac{J^2 \rho^2 e^2}{3k_B^2 T}, \quad (2.39)
\]

The coupled field analysis, namely electrical-thermal analysis and thermal-mechanical analysis, is performed using a commercial FEA package ANSYS. Based on their analysis results, the distributions of the current density, the temperature, the hydrostatic stress and their respective gradients are obtained and the value of AFD due to these three driving forces are calculated according to the formula above. Both the failure site of the test structure and the lifetime of the test structure are predicted by their method.

Figure 10: Simulated destruction of testing structure under EM using Finite element modeling[59]
In their subsequent work, the formula were also applied to different test structures, such as meander structure, pad structure[59], and dual-damascene structure[60] for both the Al and Cu technologies[61].

*Summary of AFD and FEA models*

3-D simulation of EM had been realized in this category of EM simulation. The EM kinetic due to various driving forces, such as electron wind force, thermal gradients, stress gradients and concentration gradients, is quantitatively modeled through the calculation of the corresponding AFD. Instead of solving the EM equation in a 3-D model, the necessary physical parameters are firstly calculated using FEA. The AFD due to different EM driving forces is then calculated locally. With the knowledge of AFD at every point in the model, the formation and evolution of the void can be simulated. Using this simulation methodology, the EM kinetic can be evaluated not only in the voiding region but also within the entire EM testing structure.

Due to the capability of the simulation in 3-D structure, the effect of surrounding material, the shape of the metal line or the metal stack structure in the interconnect system and even the microstructure of metal can be simulated in a single model. Furthermore, compared with the previous categories of EM simulation techniques, the EM simulator using AFD and FEA is capable of studying the EM kinetics locally around the region of voiding, and addressing the EM performance and potential reliability weakness of a metal interconnect from a macroscopic point of view.
One of the drawbacks of this category is its incapability of simulating the activity of vacancies/atoms during EM from a thermodynamics aspect. The redistribution of vacancies/atoms through various diffusion paths during the void nucleation at the early stage of EM failure is essential for the narrow interconnect system in the future. This is because of the small dimension and the high current density in the narrow interconnect system, and the process of EM failure after the void is nucleated can be very abrupt[62]. Under such circumstance, the method to retard the void nucleation at the early stage of EM failure will be a primary concern as this period of time could be almost the entire EM lifetime for narrow interconnections.

However, the redistribution of vacancies/atoms will not disturb much the physical environment of the entire EM testing structure, and the process is nearly impossible to be simulated using EM AFD simulator since the calculation of AFD is based on the FEA on the physical environment of the entire EM model for the interconnect. Including the simulation of EM void nucleation from the thermodynamic aspect in the EM simulation is therefore imperative. In the following section, a promising simulation methodology for the void nucleation will be introduced and how it can be incorporated into current EM AFD simulator is also described.

2.2.3.2 Monte Carlo simulation of EM

Monte Carlo method is a class of non-deterministic computational algorithms for simulating the behavior of various physical and mathematical systems. There are only
a few publications on the simulation of EM using Monte Carlo method. They are different from other simulation methods by being stochastic as opposed to deterministic algorithms introduced in the above sections. In this section, we present a brief review on a few applications of Monte Carlo method in the simulation of the physical process of EM.

Monte Carlo EM models

Smy et al published their work on a Monte Carlo computer simulation of EM in 1993 [63]. In the model, the motion of atoms are simulated according to two processes during EM, a drift of activated atoms in response to the electron wind force and the annealing due to the atoms movement to minimize the curvature of the grain boundaries. The grain structure is modeled by disks, each comprising some 2000 atoms. This is an attempt to describe events at the atomic level limited by the restrictions on computer memory. However, the physical laws used are not those obeyed by an individual atom, but rather are those appropriate to describe the average behavior of the atoms. The simulation of the electron wind force migration consists of two steps, selection of disks at random and drifting under electron wind force. The number of disks selected is proportional to the number of activated atoms given below

\[ N_i \approx e^{-E_{gb}/2kT} N_{gb} \]  

(2.40)

where \( N_{gb} \) is the number of grain boundary disks, and \( E_{gb} \) is the activation energy of activated atom formation and its motion. They are drifted under electron wind force according to the following equation
\[ v = \frac{Z^* e}{k_B T} \exp\left(-\frac{E_{gb}}{2k_B T}\right)J \cos \phi \sin \left(\frac{\theta}{2}\right), \quad (2.41) \]

where \( \theta \) is the mis-orientations of grains and \( \phi \) is the angle between the grain boundary and the prevailing current density as indicated in Fig. 11.

Annealing is a motion of disks to minimize surface curvature, and is carried out at a fraction of the rate at which disks are migrated. The disks are also selected at random along the line, and are moved from sites of positive curvature to sites of negative curvature for reducing the surface energy. The motion of disks during the EM and the annealing events is illustrated in Fig. 11.

This disk manipulation routines are collectively referred to as SIMBAD code reported in their previous reports, which have been applied to the studies in areas such as the microstructure of deposited metals[64, 65], dielectrics[66] and the formation of hailstones[67].
Another atomic Monte Carlo simulation of EM in polycrystalline thin films was reported by Bruschi[68]. In their study, they proposed an atomic Monte Carlo EM simulations based on a model of atom diffusion that includes the effect of electron wind force on the activation barrier. The samples are represented by a 3-D array of cubic cell. Each cell is a data structure which includes the following objects: i) a list of sites, ii) a list of atoms and iii) an electron wind force. The electron wind force is calculated by simulating the injection of a constant current and solving an equivalent resistor network extracted from the sample. The atomic Monte Carlo simulator calculates the interatomic interactions and seeking the possible destination for atom hopping which can be either a substrate site or an induced site.

![Diagram of atoms and sites in two grains with different orientation](image)

**Figure 12: Atoms and Sites in the two grains with different orientation[68]**

Substrate sites simulate the vacancies in a grain, and induce sites simulate the vacancies along the grain boundary. Incorporation of atoms into the induced sites results in grain growth. The sample then evolves through a series of transitions, each one consists of an atom jump from the initial position to an empty site (substrate site or induced site) providing that the site lies within a maximum jump length from the
initial position, and the model can simulate the void growth, the hillock formation and the grain growth on the sample.

Basically, the atomistic Monte Carlo simulation is a promising approach that can be applied to various problems related to diffusion and nucleation of atoms on a surface[69, 70].

As the interconnect technology shifting to Cu, there are new experimental observations of EM reported in the literature, such as void migration at the interface between thin metallic film and dielectric[71]. Zaporozhets et al.[49] proposed an atomistic Monte Carlo methodology to simulate the void migration in a Cu interconnect as observed in the experiments of their research group. The simulator models the shape evolution, atomic displacements in the frame of a stochastic Monte Carlo method, with probability of displacement depending exponentially on the change of the energy as a result of the displacement. The electron wind force energy and the pair interaction energy are taken into consideration. The metallic film material is modeled at an atomic level, and the electrical field is solved by using finite difference method with a time-dependent boundary condition. The interaction of bulk, grain boundary, dielectric and vacancy with the moving atoms is described by a matrix of interaction coefficients for the different pair interaction energy.

Based on their model, they simulated the behavior of the void under several conditions, namely i) Surface void migration along the interface metal/dielectric in the absence of
grain boundary; ii) void migration along grain boundaries of different orientations with respect to current; and iii) behavior of the voids at triple junctions of grain boundaries.

Figure 13: Evolution of void detachment from GBs that are perpendicular to the current direction: (a) 0 MCs (b) 466 MCs (c) 701 MCs (d) 944 MCs[49]

Summary of Monte Carlo EM modeling

The use of Monte Carlo method to model physical problems allows us to examine more complex systems than we otherwise can. Different from those EM simulation techniques introduced in the previous sections, in this category of EM simulation, the EM theory formulation is based on a single atom or a single vacancy. With the basic theory of EM physics, Monte Carlo method randomly generates numbers of scenarios for each atom/vacancy to simulate its behavior. The EM process is modeled by tracking the behavior of all atoms, vacancies or their clusters. In fact, the accuracy of a
Monte Carlo simulation is proportional to the square root of the number of scenarios used. Unfortunately, this also means that it is computing intensive and should be avoided if simpler solutions are possible. While solving equations which describe the interactions between two atoms is fairly simple, solving the same equations for hundreds and thousands of atoms is nearly impossible for a standard computer system. For this reason, Monte Carlo method does not become the main stream of EM simulation.

However, in the following chapters, an alternative EM simulation methodology combining FEA and Monte Carlo method will be presented in this work. Monte Carlo methodology can be modified to simulate the behavior of vacancy clusters without compromising the accuracy of the simulation. The Monte Carlo simulation can actually be incorporated with FEA to simulate the void nucleation from the thermodynamics perspective during EM process. As mentioned above, both the EM kinetics (driving forces) and its thermodynamics aspect (diffusion paths) are essential in the study of the underlying physics of EM process. In the application of nano-interconnect system in integrated circuit in the very near future, the understanding and the simulation of void nucleation is becoming more and more important, and such void nucleation is best studied using Monte Carlo simulation from the thermodynamics aspects. The attempt of combining the simulation of EM kinetics and its thermodynamics aspect will overcome the incapabilities of other EM models discussed previous and produce a more realistic EM model. It will give us an
insightful analysis of EM physics and help us understand the physical phenomenon of EM better.
Chapter 3: The application of finite element analysis in Electromigration study

3.1 Introduction

FEA is a powerful and popular tool in mechanical engineering. However, in the area of Integrated Circuit, its capability of reliability and failure analysis is not fully recognized in both the academic and industry. By combining with the theory of Electromigration (EM), we demonstrate how FEA can help us understand the physics of EM and improve the productivity in the industry.

3.2 Development of highly accelerated EM test using finite element modeling

EM is an important reliability issues in ULSI, and as interconnect technology becomes more reliable, the MTF of devices get longer. As various mechanisms are involved in an EM process occurring in metal thin film[5], simply increasing the stress condition of EM test could render different physical mechanism governing the EM failures, thus making the prediction of EM performance through extrapolation of the test results invalid. On the other hand, manufacturing plant is constantly striving to shorten accelerated life testing without compromising the accuracy of the result. Various highly accelerated stress methods are developed, however most of them have resulted in different mechanisms of EM as compared to that in their corresponding standard
reliability tests, rendering invalidity of the test data for reliability evaluation of products[72]. For other highly accelerated stress methods, the situation of maintaining the same mechanism of EM are not clear[73].

In this section, a highly accelerated EM test is developed to reduce the test time while keeping the same physical mechanism of EM. A systematic methodology is developed to ensure the mechanism of EM remains the same when stress conditions are varied.

3.2.1 Methodology description

This method is a combination of the simulation using FEA of EM and statistical analysis of test data. Using the physics-based FEA EM simulation developed in this work, we firstly determine the accelerated stress conditions. The actual reliability tests at the computed stress conditions and failure analysis on failed samples are performed for the verification. The test data is analyzed using statistical means such that any difference in mechanisms of EM can be detected, and thus a highly accelerated stress condition without any change in physical mechanism of EM can be derived.

3.2.2 Finite element modeling

The schematic of the Al test structure is shown in Fig. 14. The test line thickness is 0.45 μm and via diameter is 0.288 μm.
Multi-physics FEA software ANSYS™ is used to create a 3-dimensional Finite Element Model (FEM) of the via-line structure. Only half of the structure is modeled due to the mirror symmetrical nature of the structure, as shown in Fig 15.

The material properties for the simulation are taken from reference[5] and shown in the table below.
Table 1: Material properties used in simulation

<table>
<thead>
<tr>
<th>Physical parameter</th>
<th>Symbol</th>
<th>Value (Al)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Atom Concentration</td>
<td>$N$</td>
<td>$6.03 \times 10^{10}/\mu m^3$</td>
</tr>
<tr>
<td>Effective valence charge</td>
<td>$Z^*$</td>
<td>10</td>
</tr>
<tr>
<td>Pre-exponential factor</td>
<td>$D_0$</td>
<td>$2.3 \times 10^8 \mu m^2/s$</td>
</tr>
<tr>
<td>Resistivity</td>
<td>$\rho_0$</td>
<td>$2.65 \times 10^{-14} \Omega \mu m$</td>
</tr>
<tr>
<td>Temperature coefficient of resistivity</td>
<td>$\alpha$</td>
<td>0.0043</td>
</tr>
<tr>
<td>Heat of transfer</td>
<td>$Q^*$</td>
<td>$1.22 \times 10^8 \text{pJ}$</td>
</tr>
<tr>
<td>Poisson ratio</td>
<td>$\nu$</td>
<td>0.34</td>
</tr>
<tr>
<td>Young’s modulus</td>
<td>$E$</td>
<td>$7 \times 10^4 \text{MPa}$</td>
</tr>
<tr>
<td>Coefficient of thermal expansion</td>
<td>$\alpha_l$</td>
<td>$23.1 \times 10^6/\text{K}$</td>
</tr>
<tr>
<td>Activation energy for surface diffusivity</td>
<td>$E_a$</td>
<td>0.9 ev</td>
</tr>
</tbody>
</table>

Since the analysis involves complex electrical-thermal-mechanical interaction, two couple-field analyses were employed in the study, namely the electrical-thermal couple and thermal-mechanical couple field analyses. In the procedure of generating the element, element solid 69 with tetrahedral shape constructed by four nodes is used for electrical-thermal analysis; an equivalent element type solid 45 is used for thermal-mechanical analysis. In the simulation, the electrical-thermal and thermal-mechanical analysis results are combined and the AFD due to different mechanisms of EM, namely the temperature gradient induced atomic migration (TM), the stress gradient induced migration (SM) and electron wind force induced migration (EWM) are calculated at various stress conditions. The mathematical implementation for the
computation are described in details by Dalleau et al.[59]. The value of the activation energy $E_a$ is experimental found to be $0.9\text{eV}$, and the stress free temperature is set at the final annealing temperature of wafers.

The stress current is applied from metal 1, through via, and then to metal 2. The stress temperature is applied at the bottom of structure, the silicon substrate. The standard EM test condition used is $200^{\circ}\text{C}$ at $3.5\text{MA/cm}^2$. Various stress temperatures are simulated while keeping the stress current density, and stress temperature of $250^{\circ}\text{C}$ (split 1 in Table 2) is found to accelerate the testing without changing the dominant mechanism of EM. Similarly, various stress currents are simulated, and stress current density of $6\text{MA/cm}^2$ at $200^{\circ}\text{C}$ (split 2 in Table 2) is found to be able to shorten the testing time while keeping the dominate physical mechanism of EM unchanged.

Subjected to the direction of electron flow, metal 1 under via is the most vulnerable part in the entire structure since W via exhibits negligible diffusion or transport and Al is depleted due to EM without replacement. Fig 16a, 16b, 16c is the contour plot of total AFD value in metal 1 under via. The solid line outlines the position of the Tungsten via. The figures show the potential void starting locations at the three stress conditions based on the value of the maximum total AFD. In all three test conditions, the void tends to form at the via-line interface and the outer corners which are Al and SiO$_2$ interface surfaces.
Higher AFD value under via is mainly due to EWM. This is because of the current crowding effect results in an extremely high current density when current enters the metal 1 at the corner.

<table>
<thead>
<tr>
<th>Table 2: Contribution of different physical mechanisms of the EM (simulation)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Temperature</strong></td>
</tr>
<tr>
<td>Std</td>
</tr>
<tr>
<td>Split 1</td>
</tr>
<tr>
<td>Split 2</td>
</tr>
</tbody>
</table>

SM has a much larger contribution at the outer corner of via-line interface. This is because of the thermal mismatch of Al and SiO₂ at their interface results in a large stress induced migration which causes an extremely high AFD due to localized SM. Table 2 summarizes the contribution from the various mechanisms of EM at the three stress conditions. In all three cases, the dominant mechanism found is SM, which is consistent with the reports from other works[47, 74].
3.2.3 Experimental result and analysis

Experimental verification of the simulated results was performed using package level EM tests. The failure criterion is set as 10% of the relative resistance change.

An in-house developed reliability data analysis software REDAS™ [75, 76] is used to analyze the test data. Firstly, outlier point in the data must be identified before the statistical analysis. Outlier point in a data set is an observation which deviates so much from other observations as to arouse suspicions that it was generated by a different mechanism. Curve fitting without taking consideration of the presence of outlier point can render the analysis conclusion inaccurate and misleading. In REDAS™, outlier detection is based on the Rank Limit method [77]. In our analysis, one outlier point is detected in the data from the standard and split 1 test conditions respectively. For the split 2 test condition, 2 outlier points are detected. Then, Expectation and Maximization algorithm [78, 79] is used to examine the possibility of the presence of more than one mechanisms of EM, and all of the test data from the three stress conditions has only one mechanism of EM which is believed to be the SM based on the FEA as shown in Table 2.

Treating the outlier points as censored data points, the lognormal CDF plots for the three set of test data are constructed as shown in Fig. 17.
From the plots, it is observed that the slopes of the plots for the standard and split 1 are parallel, indicating similar physical mechanism. This result is further confirmed by the TEM analysis. The TEM micrographs in Fig. 18 shows the cross-sections of the failed via from the standard and split 1 test. The black circles show the possible void starting location. It is believed that the void start from the outer corners of the via-line interface, and as the voids grow, they merge and eventually form the big void as shown. The void starting location is as simulated by the FEM developed in this work.
On the other hand, Fig. 17 shows that the physical mechanism of EM for the split 2 might be different from that of the standard as their slopes are different. This is believed to be due to the Blech back stress effect as the current density used in split 2 is very high. This Blech effect is not considered in the FEM developed in this work, and hence such a deviation is possible.

In summary, split 1 has the same physical mechanism of EM as the standard EM test used. Although similar mechanism is expected through simulation for split 2, it is later proved though experiments and reliability data analysis that it actually possesses a totally different physical mechanism of EM due to the Blech back stress effect which is not considered in the FEM. Therefore, the highly accelerated stress condition chosen is 250°C at 3.5mA/cm². As compared to the standard EM test used in the plant, the test time is reduced by more than 80% with the mechanism of EM kept unchanged.
3.2.4 Summary

In this part of study, it is found that a stress condition of 250°C at 3.5mA/cm² can accelerate the test with a reduction of the average test time by more than 80% while keeping the physical mechanism of EM the same as the original standard EM test. This work combines the use of FEA, statistical analysis, actual reliability test and failure analysis. A rigorous and systematic method of developing a highly accelerated stress condition for EM is thus presented and verified experimentally in Aluminum interconnect, and this methodology can be applied for other metallic interconnect as well. Beside EM accelerated life test, this methodology could also be useful for other reliability accelerated life test. Different physical mechanisms might be introduced into the accelerated reliability test if the stress condition is increased without such assessment and it can make the conclusion misleading.

3.3 Enhanced Finite Element Modeling of Cu Electromigration using ANSYS and Matlab

In the section 3.2, we have demonstrated how FEA can help us understand the failure mechanism and develop a highly accelerated lifetime testing in the industry. In this section, we adopt FEA to study the EM in a more advanced interconnect system and demonstrate how we can overcome its limitation by combing it with advanced mathematic software. To predict the potential void starting locations in
interconnections, FEA using ANSYS is commonly employed[5, 57, 59]. However, due to the computational limitation of ANSYS post-processing module, the formulae of AFD are needed for its computation, and Dalleau et. al. has provided the approximated AFD formulae[59].

While the approximated AFD formulae have been successfully in explaining many EM experimental observations, some EM failures observed experimentally cannot be explained. This is believed to be due to the use of the approximated formulae for the AFD calculation. The inaccuracy of conventional approximated AFD formulae in advanced interconnect system is reported in another study from our research group. This inaccuracy arises from the fact that as line becomes extremely narrow, the assumptions made in the derivations for the conventional AFD formulation are no longer valid as will be detailed in our report[80]. In the present study, we propose a new simulation methodology by combining the commercial software ANSYS and Matlab, so that the computational limitation of ANSYS can be complemented by Matlab, thus enable us to compute the AFD directly.

With the extension of the capability of ANSYS static thermal analysis algorithm by linking with Matlab, and taking into account the effect of microstructure inhomogeneities of Cu thin film, surrounding materials of the test structure and their thermal mechanical mismatches in the new model, we successfully identify a potential EM reliability hazard in the state of arts ULSI Cu interconnections.
3.3.1 Finite element model

The finite element model of the Cu thin film with its surrounding materials is created using ANSYS Multi-physics as shown in Fig. 19. The barrier layer is Ta, the capping layer is SiN and the entire metallization stack is embedded in SiO₂.

![Finite element model of Cu thin film and its surrounding materials](image)

Figure 19: Finite element model of Cu thin film and its surrounding materials

In the simulation, SiO₂, SiN and Ta are taken as isotropic linear elastic solids, and Cu is characterized as an isotropic elastic-perfectly plastic solid[81]. Their material properties are summarized in Table 3.

<table>
<thead>
<tr>
<th>Material</th>
<th>Young’s modulus (GPa)</th>
<th>Poisson ratio</th>
<th>Yield stress (MPa)</th>
<th>Thermal conductivity (W/mK)</th>
<th>Coefficient of thermal expansion(°C)</th>
<th>Ref</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu</td>
<td>129.8</td>
<td>0.339</td>
<td>676(20°C) 165 (350°C)</td>
<td>379</td>
<td>16.5×10⁻⁶</td>
<td>[5, 81]</td>
</tr>
<tr>
<td>Ta</td>
<td>186.2</td>
<td>0.35</td>
<td>-</td>
<td>53.65</td>
<td>6.48×10⁻⁶</td>
<td>[82]</td>
</tr>
<tr>
<td>SiN</td>
<td>265</td>
<td>0.27</td>
<td>-</td>
<td>0.8</td>
<td>1.5×10⁻⁶</td>
<td>[82]</td>
</tr>
<tr>
<td>SiO₂</td>
<td>71.4</td>
<td>0.16</td>
<td>-</td>
<td>1.75</td>
<td>0.68×10⁻⁶</td>
<td>[82]</td>
</tr>
</tbody>
</table>

Table 3: Material properties used in finite element model (Cu interconnect)
The Cu thin film has a height of 0.4μm and a width of 0.25μm. The thickness of the capping layer SiN and the barrier layer Ta are 0.05μm and 0.025μm, respectively. Fig. 20 shows the hypothetical grain structure of the Cu thin film. The arrow shows the direction of the electron flow.

![Figure 20: Different grains in the finite element model (surrounding materials are not shown for the sake of clarity)](image)

Since the simulation involves complex electrical-thermal-mechanical interaction, two couple-field analyses are employed in the study, namely the electrical-thermal couple field analysis and thermal-mechanical couple field analysis.

In the procedure of generating the element, element type solid 69 with tetrahedral shape is used for the electrical-thermal analysis; an equivalent element type solid 45 was used for the thermal-mechanical analysis. The stress free temperature in the
model is set at 350 °C which is the final annealing temperature of the wafers. The simulated test condition is 300°C and 3MA/cm².

3.3.2 Simulation methodology

The physical environment of the Cu thin film during EM test is obtained through the aforementioned electrical-thermal couple field analysis and thermal-mechanical couple field analysis. The mathematical expressions for atomic fluxes due to electron wind force, thermo-mechanical stress gradient and temperature gradient were reported by Valeriy Sukharev et. al.[83] and D. Dalleau et. al.[59] as follow

\[
\dot{J}_{ew} = \frac{N}{k_B T} e Z^* \overline{E} D_0 \exp\left( -\frac{E_A}{k_B T} \right) 
\]

\[
\dot{J}_{str} = -\frac{N \Omega D_0}{K_B T} \exp\left( -\frac{E_A}{K_B T} \right) \overline{\nabla \sigma_H} 
\]

\[
\dot{J}_{th} = -\frac{N Q^* D_0}{K_B T^2} \exp\left( -\frac{E_A}{K_B T} \right) \overline{\nabla T} 
\]

Where \( J_{ew}, J_{str}, \) and \( J_{th} \) are the atomic fluxes due to the electron wind force, stress gradients and temperature gradients respectively. \( N \) is the atomic concentration, \( E \) is the electrical field, \( T \) is the temperature, \( \sigma H \) is the hydrostatic stress, \( \Omega \) is the atomic volume, \( Z^* \) is the effective valence charge, \( Q^* \) is the heat of transfer and \( E_a \) is the activation energy. The physical parameters are summarized in Table 4 below.

<table>
<thead>
<tr>
<th>Physical parameter</th>
<th>Symbol</th>
<th>Value (Cu)</th>
</tr>
</thead>
</table>

-64-
The fundamental formulae of the atomic flux are analogous to the heat flux equation in thermal analysis which was found by Adolf Fick in 1855[58] after studying the thermodynamic analogy between the transport of heat and matter[57].

In ANSYS static thermal analysis, the heat flux is calculated as:

\[ J_{heat} = -K \nabla \nu \quad (3.4) \]

where \( K \) is the thermal conductivity and \( \nu \) is the temperature. Although ANSYS is not able to model the diffusion under various EM driving forces, we can calculate the atomic flux using its static thermal analysis by replacing the value of \( K \) and \( \nu \) according to Eqn. 3.1 ~ 3.3 respectively based on the results from the aforementioned two coupled field analyses. Therefore, by solving the finite element model for thermal
analysis in ANSYS, we can obtain the heat flux which has the same numerical value as EM atomic fluxes under various driving forces.

To examine the effect of the different driving forces of EM, their respective corresponding AFD needs to be calculated. However, ANSYS post-processing module has the limitation to calculate the divergence of a flux vector field obtained from its solution. In this work, a link between ANSYS and Matlab is developed to transfer the data and the system control between these two commercial software, i.e. the EM atomic fluxes are calculated in ANSYS as mentioned earlier and the atomic flux results are sent to Matlab for the computation of the AFD due to various EM driving forces. After that, the AFD result is transferred back to ANSYS for the further analysis. The flowchart of the simulation and the mathematical implementation is illustrated in Fig. 21.
The transfer is performed automatically according to a pre-coded command flow without user intervention. Using the ANSYS command “*VWRITE”, the value of the respective atomic flux is written into a file in a formatted sequence. Please note that “*VWRITE” command must be contained in an externally prepared file and read into ANSYS (i.e., *USE, /INPUT, etc.). After the data is extracted from ANSYS and stored in a txt file, the string /SYS, C:\MATLAB7\bin\win32\MATLAB.exe /r filename.m is executed. By executing the string, the system control will be passed to Matlab environment without quitting ANSYS and the filename.m is the Matlab m file used to extract the ANSYS data from the txt file. In the m file, the Matlab command “load” and a few nested “for” loops are used to read and sort the ANSYS data into Matlab from the txt file to calculate the flux divergence in a 3-D matrix. To quit Matlab, the
command “exit” is executed, and the system control will then return to ANSYS and continue with the ANSYS commands before the control was passed to Matlab. The data and system control exchange method can be applied to other simulation involved FEA using ANSYS to enhance the data processing capability.

3.3.3 Simulation and experimental result

In recent Cu interconnect technology, special treatment of the interface between the capping layer and Cu thin film has successfully retarded the atomic diffusion along the fast interface diffusion path by increasing the bonding strength of the capping layer to Cu. With the absence of the fastest diffusion path, the second fastest diffusion path, the grain boundaries become dominant[84-86] and this could introduce new EM failure mechanism.

In this work, the EM phenomenon of a Cu interconnect thin film is simulated assuming the interface diffusion in Cu interconnections is retarded by the processing technology improvement. The activation energies for diffusion along important mass transport pathways in the simulation are listed in Table 5.

<table>
<thead>
<tr>
<th>Diffusion path</th>
<th>Activation energy Ea (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lattice</td>
<td>2.1</td>
</tr>
<tr>
<td>Grain boundary</td>
<td>1.2</td>
</tr>
<tr>
<td>Interface</td>
<td>1.2</td>
</tr>
</tbody>
</table>

Table 5: Activation energy used in Cu interconnect EM simulation
By virtue of our assumption in interface improvement, the activation energy of the interface diffusion is chosen to be the highest in the reported value (typical value is 0.9~1.2eV[87])

![Figure 22: Maximum AFD value in Cu thin film using enhanced ANSYS simulation](image)

Fig. 22 shows the plot of the AFD distribution in the Cu thin film using the new proposed ANSYS+Matlab simulation. The potential void nucleation location is found to be at the cap layer-grain boundary intersection due to its high AFD value.

The simulation result is consistent with the experimental observation as shown in Fig. 23. The Cu EM sample is fabricated with SiH₄ surface treatment at the capping layer interface. Failure analysis found that the EM induced void occurs at the cap layer-grain boundary intersection of Copper line after EM test, which agrees with the predicted void nucleation location in the simulation.
On the other hand, using the approximated AFD formulae, the observed failure location is not accurately predicted in the AFD plot as shown in Fig. 24. The simulation fails to predict the potential void initiation location in this circumstance.

Figure 23: Experimental observation of void at the intersection of grain boundary and cap layer in Cu interconnect after EM (courtesy from Prof Subodh Mhaisalkar, NTU MSE)

Figure 24: Maximum AFD value in Cu thin film using approximated AFD formula
3.3.4 Summary

An enhanced EM simulation methodology is developed by linking the ANSYS data post-processing module and Matlab. Various EM driving forces, such as electron wind force, stress migration due to stress gradient and thermal migration due to temperature gradient, Cu thin film microstructures and surrounding materials of the test structure are taken into account in the simulation.

With the assumption of improved cap layer/Cu interface, our simulation identify that the intersections of barrier layers and grain boundaries provides a new potential EM reliability hazard in the Cu interconnect technology. The result is found to agree well with experimental observation.

3.4 Conclusion

In this chapter, the capability of FEA in the microelectronic is demonstrated and applied to two different areas by integrated it with the theory of EM. In the section 3.2, the FEA successfully identifies the failure mechanism in an accelerated EM lifetime testing. With the support of EM simulation, the highly accelerated EM lifetime testing is developed. The study greatly improves the productivity in a reliability testing lab of a wafer fab. In the section 3.3, we focus on the physics of EM in a more advanced interconnect technology, the EM FEA and its traditional EM theory is revised. The limitation of FEA of EM in nano-interconnect is observed. A new simulation
methodology by combing FEA and MatLab is demonstrated. The simulation result shows a good agreement with experimental observation.
Chapter 4: Monte Carlo method in Electromigration simulation

4.1 Introduction

In previous chapter, the theory of EM is integrated in FEA to study the physics of EM in the advanced interconnect system of integrated circuit. The application of this simulation method in the development of a highly accelerated EM lifetime testing is demonstrated. However, the development of our understanding of EM and its simulation need not only the powerful analysis software, but also new physics theory and critical simulation methodology. In the following two chapters, we will present the breakthrough in both of the areas from our research. In this chapter, we are going to introduce an alternative EM simulation concept to simulate void nucleation and void growth using both Monte Carlo method and advanced FEA.

4.2 A holistic EM modeling using Monte Carlo method and Finite element analysis

Electromigration (EM) in Ultra-Large-Scale Integration (ULSI) interconnections has been studied extensively since the 1950’s and the electron wind force is usually considered to be the sole driving force for atomic migration in EM. Under the driving force, metal atoms diffuse along various diffusion paths in interconnection due to the presence of its microstructure and texture. In the presence of the inhomogeneity of the
microstructure/texture, the atomic diffusivity is altered along a diffusion path, and Atomic Flux Divergences (AFD) is produced. This AFD renders void and hillock formations in interconnections. The presence of the surrounding materials, such as the barrier metals and the oxide, will cause non-uniform temperature/stress distributions along an interconnect. This non-uniformity enhances the disparity of the atomic diffusivity along a diffusion path which in turn increases the AFD.

As line width becomes narrow, the effect of the surrounding materials on EM can no longer be accounted for by the modification of the atomic diffusivity alone as was described in the above-mentioned diffusion path approach. In fact, the effects of the non-uniformity in temperature and stress distributions are so strong that they can counteract the electron wind force, and thus create different types of driving forces during EM in interconnections as will be elaborated in the subsequent section. Consequently, the driving force approach for the study of EM was developed recently. Rzepka et al. presented a pioneer work to combine the various driving forces using FEA. Subsequently, Dalleau and Weide-Zaage developed a FEA model to study EM simulation from the perspective of the driving force and the void growth dynamics. The driving force approach is also adopted by Tan et al. to explain the intrinsic EM characteristics of Al and Cu.

While the surrounding materials can induce different driving forces for the diffusion of metal atoms in interconnections, the presence of the various diffusion paths in interconnections also determines the metal atom diffusion rate. Hence, both the
driving forces and diffusion paths should be considered in the modeling of EM. However, such an EM model is presently lacking.

Also, the void nucleation is not found in any reported EM models. In fact, the physics of void nucleation is best studied using Monte Carlo simulation. Smy et al.\textsuperscript{7} and Bruschi et al.\textsuperscript{8} have reported Monte Carlo algorithms to study the motion of atoms along the grain boundary during EM. Monte Carlo simulation is also reported by Zaporozhets et al.\textsuperscript{9} to investigate void migration at the interface between the thin metallic film and the dielectric.

Therefore, a more realistic EM model should include both the diffusion and the driving force approaches with Monte Carlo simulation for the initial void nucleation process. It is the purpose of the present work to develop such a model for EM simulation in interconnections. With such a model, the entire EM failure process beginning from void nucleation to its growth can be modeled and hopefully, our present understanding of EM physics can be enhanced so that the key material properties that influence the reliability of ULSI interconnections can be identified.

4.2.1 Description of simulation methodology

4.2.1.1 Test structure description

To demonstrate the simulation methodology developed in the present study, Al interconnect test structure is chosen as an illustration. The same principle and methodology can be applied to other metallic interconnect. The test structure is an Al
metal line sandwiched between two TiN layers and the entire metallization stack is embedded in SiO₂ dielectric as shown in Fig. 25. The stress free temperature in the model is set at 410 °C which is the final annealing temperature of the wafers.[88]

![Finite element model of Al test structure](image)

Figure 25: Finite element model of Al test structure

As a common practice, SiO₂ and TiN are taken as isotropic linear elastic solids, and Al is characterized as an isotropic elastic-perfectly plastic solid.[89] These assumptions are justified by Greenabaum et al.[89] in their experiments and calculations. The properties of the materials involved in our study are summarized in TABLE 6 and 7.

<table>
<thead>
<tr>
<th>Physical parameter</th>
<th>Symbol</th>
<th>Value (Al)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Atom Concentration</td>
<td>( N )</td>
<td>( 6.03 \times 10^{10}/\mu m^3 )</td>
</tr>
<tr>
<td>Effective valence charge</td>
<td>( Z^* )</td>
<td>10</td>
</tr>
<tr>
<td>Pre-exponential factor</td>
<td>( D_0 )</td>
<td>( 2.3 \times 10^8 \mu m^2/s )</td>
</tr>
<tr>
<td>Resistivity</td>
<td>( \rho_0 )</td>
<td>( 2.65 \times 10^{-14} \Omega \mu m )</td>
</tr>
<tr>
<td>Property</td>
<td>Value</td>
<td></td>
</tr>
<tr>
<td>----------------------------------------------</td>
<td>----------------</td>
<td></td>
</tr>
<tr>
<td>Temperature coefficient of resistivity (\alpha)</td>
<td>0.0043</td>
<td></td>
</tr>
<tr>
<td>Heat of transfer (Q^*)</td>
<td>(1.22 \times 10^8) pJ</td>
<td></td>
</tr>
<tr>
<td>Poisson ratio (\nu)</td>
<td>0.34</td>
<td></td>
</tr>
<tr>
<td>Young’s modulus (E)</td>
<td>(7 \times 10^4) MPa</td>
<td></td>
</tr>
<tr>
<td>Coefficient of thermal expansion (\alpha_l)</td>
<td>(23.1 \times 10^{-6}) K</td>
<td></td>
</tr>
<tr>
<td>Activation energy for lattice diffusivity (E_{a,lattic})</td>
<td>1.41 ev</td>
<td></td>
</tr>
<tr>
<td>Activation energy for grain boundary diffusivity (E_{a,GB})</td>
<td>0.48 ev</td>
<td></td>
</tr>
<tr>
<td>Activation energy for surface diffusivity (E_{a,surf})</td>
<td>0.84 ev</td>
<td></td>
</tr>
</tbody>
</table>

**Table 7: Mechanical properties of Al and its surrounding materials**

<table>
<thead>
<tr>
<th>Property</th>
<th>Al (^a)</th>
<th>TiN (^b)</th>
<th>SiO(_2) (^c)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coefficient of thermal expansion (K(^{-1}))</td>
<td>(23.1 \times 10^{-6})</td>
<td>(9.4 \times 10^{-6})</td>
<td>(0.68 \times 10^{-6})</td>
</tr>
<tr>
<td>Young’s modulus (MPa)</td>
<td>(7 \times 10^4)</td>
<td>(2.7 \times 10^5)</td>
<td>(7.1 \times 10^4)</td>
</tr>
<tr>
<td>Yield strength (MPa)</td>
<td>67.4</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>((400^\circ C))</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Poisson ratio</td>
<td>0.35</td>
<td>0.25</td>
<td>0.16</td>
</tr>
<tr>
<td>Thermal conductivity (pW/(\mu)m.K)</td>
<td>(2.32 \times 10^8)</td>
<td>(2.61 \times 10^7)</td>
<td>(1.75 \times 10^6)</td>
</tr>
<tr>
<td>Resistivity (T(\Omega)(\mu)m)</td>
<td>(2.65 \times 10^{-14})</td>
<td>(1.24 \times 10^{-12})</td>
<td>(1 \times 10^{\text{26}})</td>
</tr>
</tbody>
</table>

\(^a\) Reference [5], [90]

\(^b\) Reference [91], [59] and [92]
The dimension of the metal line in our model is 0.475μm×0.3μm×1.875μm. Since the analysis involves complex electrical-thermal-mechanical interactions, two couple-field analyses are employed in the study, namely the electrical-thermal coupled field analysis and the thermal-mechanical coupled field analysis. Element *solid 69* with tetrahedral shape is used in the electrical-thermal analysis, and *solid 45* is used for the thermal-mechanical analysis. All the elements have an identical size of 0.025μm×0.025μm×0.025μm. Different grains in the thin film are created in a random manner as shown in Fig. 26. The elements along grain boundary possess different atomic diffusivity and adhesion energy from those elements inside the grain. The details of the energy calculation are presented in the next section.

The stress current density is 3 MA/cm² and the stress temperature is 200°C. The temperature distribution including the joule heating effect obtained from the electrical-thermal analysis is applied as the load to the *solid 45* model for the thermal-mechanical analysis.
4.2.1.2 Monte Carlo simulation of void nucleation

Void nucleation is a process of motion of vacancies and atoms in order to minimize the system energy. To model the process of void nucleation qualitatively, Monte Carlo method is employed. Three factors are considered in the simulation as follows:

\textit{a. Energy calculation}

In the presence of the driving forces during EM, the total energy of an element consists of the electron wind force energy, the strain energy, the thermal energy and the pairing energy between the element and its nearest neighboring elements.

The pairing energy represents the initial cohesion between one element and its surrounding elements without any external excitations such as elevated temperature and stress. In the absence of any external excitations, an element is at its lowest energy
The pairing energy is the amount of the energy required to bring the element from its lowest energy state and free it out of its surrounding elements. It is estimated by using the relation \( E_{pair} = -zE_f \).[37] where \( z \) is the number of the nearest neighbor elements, \( E_f \) is the adhesion energy between two elements. Within an Al grain, \( E_f \) is estimated from the sublimation energy of Al and its value is approximately \( 2.487 \times 10^{-4} \) pJ.[49]

The adhesion energy between TiN and Al is \( E_{f, TiN} \approx 3 \times E_f \).[93] Due to the formation of an ultra-thin alumina between SiO\(_2\) and Al,[93] the adhesive energy of Al and SiO\(_2\), \( E_{f, SiO} \) is given by the adhesive energy of Al/Al\(_2\)O\(_3\) and estimated as \( E_{f, SiO} \approx E_f \).[94] For the elements in the different Al grains, the adhesion energy is estimated as \( E_{f, GB} \approx 0.4 \times E_f \).[49] The minus sign in the expression of the pairing energy indicates that if \( E_f \) or \( z \) is higher, the pairing energy state of an element will be more negative, and higher excitation energy is required to free the element from its surrounding elements. In other words, the element will be more stable in its position.

By using different pairing energies for the elements along the grain boundaries and inside the grains, we simulate the effect of inhomogeneity due to the interconnect microstructure and texture on EM.

The strain energy and the thermal energy are two external excitations on an element. They both raise the energy state of the element from its initial state which is defined by the pairing energy described previously. Explicitly, the probability of movement of
the element is higher due to these two external excitations, since the minimum energy required for the movement of the element is lowered. In other words, the pairing energy, the strain energy and the thermal energy simulate the stability of an element, and the summation of these three energies represents the cohesion of the element with its surrounding elements.

The strain energy is given as,[95]

\[ E_{str} = E_e^{el} + E_e^{pl} = \frac{1}{2} \{ \sigma \}^T \{ \varepsilon_e^{el} \} vol_e + \{ \sigma \}^T \{ \Delta \varepsilon_e^{pl} \} vol_e. \] (4.1)

Here \( E_e^{el} \) and \( E_e^{pl} \) are the elastic and plastic strain energy, respectively. \( \{ \sigma \} \) is the stress vector, \( \{ \varepsilon_e^{el} \} \) is the elastic strain vector, \( \{ \Delta \varepsilon_e^{pl} \} \) is the plastic strain increment, \( vol_e \) is the volume of the element.

The thermal energy is given as

\[ E_{th} = N \times \frac{3}{2} k_B T, \] (4.2)

where \( N \) is the number of the atoms in one element, \( T \) is the temperature of the element in Kelvin and \( k_B \) is the Boltzmann’s constant.

The third external excitation is the electron current flow. The electron wind force energy is equal to the work done by the electron wind force during an element displacement, and it is given as \( E_{ew} = Z' e U. \) [49] where \( Z' e \) is the effective charge of Al atom, \( U \) is the electrical potential.

\[ b. \ Element \ movement \]
At stated temperature and current density used in the present work, the strain energy and the thermal energy are not high enough to balance or exceed the pairing energy of an element (a case of de-cohesion), but the energy required to free an element is reduced under these excitations, and hence the probability of an element movement increases. Together with the excitation from the electron wind force, the probability of the movement of an element becomes higher along a particular direction. Based on the statistical mechanics, the probability of an element displacement is exponentially dependent on the change of the total energy between the target position and the original position of the element. The probability is given as

\[
\text{probability} = \exp\left( -\frac{\Delta E_{ew} + \Delta E_{str} + \Delta E_{th} + \Delta E_{pair}}{N \times k_B T} \right)
\]  

(4.3)

c. Monte Carlo subroutine

Monte Carlo method is used to simulate the movement of an element from one lattice location to another. To begin, groups of vacancy sites, which are empty sites without elements in the finite element model, are randomly generated along the grain boundaries. Since the grain boundary is the main diffusion path of EM in Al polycrystalline thin film, we focus our study on the movement of the vacancies that reside along these grain boundaries. The reported average vacancy concentration in Al is found to be 0.01-0.1%,[96][97] and the vacancy concentration of 0.1% is chosen in this study because the concentration is expected to be higher along the grain boundaries at the elevated test temperature of 200°C.
A Monte Carlo subroutine randomly selects one vacancy site, and the total energy change for each of its nearest neighbor elements to move and fill this vacancy site is computed individually. The movement of an element is accepted if its probability as computed using Eqn. 4.3 is the highest among other surrounding elements and above 50%.[37] The particular element and vacancy site will then swap their original positions, and a new Monte Carlo loop begins with another random selection of the vacancy site. After a number of Monte Carlo loops, the movement of vacancies in the structure can be observed, and the void nucleation as a result of the vacancies clustering can be identified

4.2.1.3 Dynamic simulation of void evolution

After the void nucleation, the values of AFD at the nucleation sites due to the various driving forces are calculated, and the voids begin to grow due to the continuous removal of material from the nucleation sites with the rate of the mass transport given by the value of the total AFD. The numerical implementation of the AFD computation due to the driving forces of EM is described in details by Dalleau et al.[59] Different diffusion paths are taken into account by considering the different diffusivities of metal atoms along the grain boundaries, the interfaces and inside the grains. The activation energies of the diffusivities for the different diffusion paths are included in the AFD computation as listed in TABLE 6.

Fig. 27 shows the flowchart of the dynamic simulation of the void growth. Starting with the electrical-thermal coupled field analysis and the thermal-mechanical coupled
field analysis, the value of the total AFD due to the driving forces of EM is calculated. Thirty elements with the highest total AFD value are selected and physically deleted in every iteration to simulate the growth of the void. The geometry of the finite element model is thus modified and the two coupled field analyses are performed again. The new values of AFD for the remaining elements are computed and the same deletion procedure continues until the resistance of the metal line is increased above the pre-selected criterion which is 10% in the present work.

**Figure 27: Flowchart of the dynamic simulation of the void growth process**

4.2.2 Result and discussion

Figs. 28-30 show the initial and final profiles of the vacancies in the metal line in four different viewing angles. As shown in Figs.28-30, the vacancies move through the grain boundaries from the anode to the cathode, and ultimately become immobilized at
the intersection of the barrier layer and the grain boundary. The immobilization occur because the intersection has higher strain energy due to thermal mismatch of the different materials at the intersection. Vacancies tend to move and nucleate there so that the strain energy can be reduced.

Figure 28: Randomly generated vacancies along the grain boundaries
Figure 29: Vacancy movement along the grain boundaries.

Figure 30: Nucleation of the voids inside the metal line.
Vacancies also nucleate at other locations inside the structure as shown in Fig. 30, such as the grain boundaries or sidewalls as these are also weak points in the metal line; however, the size of the nucleated voids is relatively small at these weak points. This is in agreement with the experimental observations reported by Smith et al.[94], where they found that some of the nucleated voids cannot grow and form fatal voids across the metal line eventually. As shown in Fig. 31, the nucleated voids located at the barrier layer-grain boundary intersection grow at a faster rate due to higher AFD as compared to the voids at other weak points in the interconnect. These nucleated voids grow, merge and finally form a fatal void which covers almost the entire metal cross-section and causes the interconnect resistance to increase sharply.

![Figure 31: Void growth in the metal line](image-url)
Figs. 31 and 32 show the void growth process, and the growth process is similar to the observation reported by Prybyla \textit{et al.}[98] In their experiment, they used an in-situ transmission electron microscopy (TEM) to record the process of the mini void migration and they observed the trapping of the voids at the barrier layer-grain boundary intersection. These trapped voids then began to grow along the grain boundary. Our Monte Carlo simulation agrees well with their experimental observation.

The capping layer-grain boundary intersection is also found to be the weak point in Cu interconnections during EM test.[99] In recent Cu interconnect technology, special treatment of the interface between the capping layer and Cu thin film is employed to
retard the Cu atoms migration along the fast interface diffusion path effectively. However, due to the thermal mismatch of the two materials at the capping layer-grain boundary intersection, the intersection poses a potential reliability hazard. Fig. 33 shows a Cu EM sample which is fabricated with SiH₄ surface treatment at the Cu/capping layer interface. The SiH₄ treatment increases the bonding strength of the top interface and consequently reduces the mass transport along the Cu/Capping layer interface. Upon failure analysis on the EM failed sample, it is found that the EM induced voids occur at the capping layer-grain boundary intersection of Cu metal line. Such a failure phenomena could be due to the thermal mismatch of different materials at the intersection, similar to our simulation result in an Al metal line.

In short, the high defect density at grain boundaries and the thermal mismatch of different materials at the intersections of barrier layers and grain boundaries make the intersections to be vulnerable weak points in both Al and Cu interconnections.
4.2.3 Summary

A methodology that combines Monte Carlo algorithm and FEA is presented to study the dynamic physical process of EM. The inhomogeneity of the interconnect microstructure and the resulting different atomic diffusivities along the various diffusion paths are considered in the model. The presence of the various driving forces of EM is also included in the analysis. From the modeling, we found that the barrier layer-grain boundary intersections are the weakest points for the void formation in the metallization due to the high stress resulting from the thermal mismatch of different materials at the intersection. Our model demonstrates the vacancy trapping, void nucleation and void growth during EM, and the results are found to agree well with the experimental observations reported in literatures.

4.3 A Monte Carlo simulation of void nucleation using Finite element submodeling

Implementation of Monte Carlo simulation of EM to the testing structure with more complicated geometry property is a great challenge. In previous section, the methodology is developed and verified using a testing structure with a simple geometry, a straight metal line. However, in the real situation, the geometry of the testing structure is rather complicated. It involves various different interfaces, corners and shapes, which could be a potential critical region of EM due to the current crowding effect or high stress due to sharp corners. In our Monte Carlo simulation, the
meshed elements need to be identical so that the same energy calculation method can be used for all of them without consideration of the effect of size. It is almost impossible to mesh certain geometry with identical elements, such as cylinders or the interface between different shapes. In this part of work, an advance FEA technique, submodeling, is used to study the critical region of testing structure during EM test. In our study, a via-line EM testing structure is used and it is shown that the Monte Carlo method is able to be implemented to the more complicated EM models.

4.3.1 Understanding finite element submodeling

Submodeling is a finite element technique that you can use to obtain more accurate results in a particular region of a model. A finite element mesh may be too coarse to produce satisfactory results in a given region of interest. The results away from this region, however, may be satisfactory. Reanalyzing the entire model using a greater mesh refinement in order to obtain more accurate results in one particular region is time-consuming and costly. Instead, we can use submodeling to generate an independent, more finely meshed model of only the region (submodel) of interest and then analyze it. The figure illustrates how to deal with the problem by using submodeling to create a finer mesh on the region (submodel) of interest.
Submodeling is also known as the cut-boundary displacement method or the specified boundary displacement method. The cut boundary is the boundary of the submodel which represents a cut through the coarse model. Displacements calculated on the cut boundary of the coarse model are specified as boundary conditions for the submodel. Submodeling is based on St. Venant's principle, which states that if an actual distribution of forces is replaced by a statically equivalent system, the distribution of stress and strain is altered only near the regions of load application. The principle implies that stress concentration effects are localized around the concentration; therefore, if the boundaries of the submodel are far enough away from the stress concentration, reasonably accurate results can be calculated in the submodel.

We can achieve more accurate FEA result on the critical region of the testing structure and we are also able to re-mesh the region with identical element size so that the implementation of Monte Carlo method is possible.
4.3.2 Testing structure description

Multi-physics FEA software ANSYS is used to create a 3-dimensional finite element model (FEM) of the via-line structure. The materials of metal stacks, via, and the inter-metal dielectric are indicated in Fig. 35. Only half of the structure is modeled due to the mirror symmetrical nature of the structure. In order for experimental comparison, Al interconnect is employed in the simulation, and the metal stack thickness is 0.45 µm with the via diameter of 0.288 µm. The stress free temperature in the model is set at 410 °C which is the final annealing temperature of the wafers.

![Coarse finite element model of the test structure and its submodel](image)

**Figure 35: Coarse finite element model of the test structure and its submodel**

In order to obtain more accurate results in the critical region which is along the via-line interface, a submodel with a much higher mesh density is created. Its position is
highlighted in the coarse finite element model shown in Fig. 35. Since the analysis of EM involves complex electrical-thermal-mechanical interactions, two couple-field analyses are employed in the study, namely the electrical-thermal coupled field analysis and the thermal-mechanical coupled field analysis[100]. Element solid 69 with tetrahedral shape is used in the electrical-thermal analysis, and solid 45 is used for the thermal-mechanical analysis.

All the elements in the submodel have an identical size of 0.008μm×0.008μm×0.008μm. Groups of tiny voids, which are empty sites without elements in the finite element model, are randomly generated inside the submodel and they represent tiny voids after small groups of vacancy aggregation at any inhomogeneity sites inside the structure. The reported average vacancy concentration in Al is found to be 0.01-0.1%[96, 97], and the vacancy concentration of 0.05% is chosen in this study.

4.3.3. Monte Carlo simulation of void nucleation simulation

Void nucleation is a process of movement of tiny voids, vacancies and atoms in order to minimize the system energy. Following the FEA of the physical environment of the test structure, Monte Carlo method is employed to simulate the process of the void nucleation. In the presence of the various EM driving forces, the total energy of an element consists of the potential energy resulting from electron wind force, stress gradients and temperature gradients.
Also, the element has the pairing energy between the element and its nearest neighboring elements. The pairing energy represents the initial cohesion between one element and its surrounding elements without any external excitations. It is the amount of energy required to bring the element from its lowest energy state and free it out of its surrounding elements when there is no other external excitation. The strain energy and the thermal energy are two external excitations on an element. The pairing energy, the strain energy and the thermal energy simulate the stability of an element, and the summation of these three energies represents the cohesion of the element with its surrounding elements.

Monte Carlo methodology is employed to simulate the tiny void movement with the consideration of the aforementioned energy redistribution. Every single movement of tiny void is associated with the redistribution of the system energy. The energies of the initial location of the elements and all its possible moving locations are calculated, and the probability of the moving location is exponentially depended on the energy difference between the initial and final location. The movement is accepted if the calculated probability is the highest among other scenarios and over 50%. At the same time, the energy reduced due to this movement is recorded and accumulated in the following next Monte Carlo simulation loops. The detailed implementation of the Monte Carlo methodology can be found in the previous section[48].
4.3.4 Experiment and simulation Result

In this section, both the simulation and experimental result will be presented. The experimental EM failure data was obtained by performing an accelerated package level EM tests on an aluminum Via-line structure where the via-filling material is Tungsten (W), the barrier metal is TiN/Ti composition and the TARC layer is Ti. Fig.36 a) shows the initial randomized locations of the tiny voids in the finite element submodel. The testing condition is 200°C and 3.5MA/cm². The simulation stops till a 1% change in resistance of the metal interconnect. The same failure criterion is chosen in the experiment to ensure that the testing sample does not go into the rapid resistance increasing stage of void growth. The final simulation result in shown in Fig. 36 b) which indicates the void nucleation site is under the W plug and it is slightly closed to the edge of the metal line.

Figure 36: The Monte Carlo simulation of the void nucleation
Fig. 36 is the experimental observation of the EM testing sample after 1% resistance change is recorded. 1% resistance change criterion is chosen because the size of the nucleated void up to 1% resistance change does not alter the distribution of various EM driving forces in the model as verified by our simulation work, and we consider this period of the EM process as the phase of void nucleation. As indicated in the figure, a small void nucleation site is observed under the W plug and closer to the outer counter of the via-line interface as predicted by the simulation.

![Void nucleation site in testing structure](image)

**Figure 37: Void nucleation site in testing structure**

### 4.3.5 Summary

The implementation of Monte Carlo simulation in a more realistic EM testing structure by using finite element submodeling is demonstrated in this section. It is shown that the submodeling technique can extend the application of Monte Carlo simulation of EM to the testing structure with more general geometry without
compromising its accuracy in prediction of void nucleation location. Highly accelerated EM testing on via-line structure is performed. The failed sample is investigated using TEM and its shows a good agreement with our simulation prediction.

4.4 Conclusion

In this chapter, we present an alternative simulation methodology using both Monte Carlo method and advanced FEA. From the physics of EM and FEA, we developed the Monte Carlo simulation algorithm to simulate the holistic EM process including the void nucleation based on the diffusion path approach and the void growth based on the driving force approach. The inhomogeneity of the interconnect microstructure and the resulting different atomic diffusivities along the various diffusion paths are also considered in the model. In the section 4.3, we reveal the limitation of our Monte Carlo method in simulating a testing structure with complicated geometry. However, we have also find the solution and demonstrated an advanced FEA technique, submodeling, to overcome its disadvantage. With submodelling technique, the Monte Carlo method can be applied to the EM simulation of any testing structures with different sharp theoretically. In our study, the advanced simulation and experiments will not only help us assess the reliability concern in particular structure, but also improve our understanding on the EM physics. In the next chapter, we will present a alternative EM physics theory and how the theory help us to understand and predict the time to failure of EM in the interconnect system of advanced integrated circuit
Chapter 5: The predictive simulation and modeling of Median Time to Failure of Electromigration

5.1 Introduction

In the area of both academic and industry, great effort has been made in understanding and predicting the degradation process of interconnections due to this phenomenon. Introduced by Black in 1967[101], the Black’s equation is a simple empirical EM model, which is widely accepted in the industry as the most common method to extrapolate the median time to failure (MTF) from the accelerated testing condition to the normal operating condition. Although the empirical model of the Black’s equation is simple in implementation, it fails to consider many physical factors which can seriously affect the accuracy of its prediction. In this chapter, we reveal the problems in the application of the Black equation on EM study and explore the physics of EM and its acceleration during highly stress testing. An alternative concept of EM and its acceleration physics is proposed and formularized in our study. Integrating with the simulation methodology presented in previous chapters, a new method of predictive simulation of EM is developed and MTF formula is derived. In the second part of this chapter, we review the validity of inherent implications of the Black equation. Based on our study and previous academic reports in the literature, we found that the application of the Black’s equation in today ULSI interconnects fails evidently due to neglecting of additional stress factor in ULSI interconnects. In contrast, our proposed
MTF formula has a much better prediction result than the black equation based on the experimental data.

5.2 Predictive dynamic simulation for void nucleation during Electromigration in ULSI interconnects

As mentioned earlier, the Black’s equation fails to consider many physical factors which can seriously affect the accuracy of its prediction. These physical factors are the microstructure of the metal thin film, the surrounding material and the presence of the various driving forces of EM, etc[48]. Moreover, it has been a great controversy on the choice of the current density exponent and the activation energy in its basic formula, which brings with it a large potential error[102, 103]. The understanding and inclusion of these physical factors for the interconnects EM lifetime prediction requires a physics-based modeling.

In this work, an alternative concept of EM modeling is proposed, and the EM MTF of an interconnect during void nucleation is derived theoretically. A physics-based predictive Monte Carlo simulation methodology is used to model the void nucleation process during EM. It is shown that the model can successfully predict the voiding location in the interconnects and it has a good agreement with the experimental observations on the MTF and activation energy of the EM process.
5.2.1 Alternative concept in EM modeling

In this work, the entire EM process is divided into three different physical stages as follows. Firstly, it is the tiny void (nucleus) incubation due to vacancy aggregation. Next, void nucleation due to the movement and coalescence of the tiny voids. Then a rapid void growth due to atomic flux divergence around the nucleated voids at weak locations, which is an inevitable runaway mechanism. Fig. 38 illustrates the process of formation of the tiny void and its coalescence.
Figure 38: The formation of the tiny void and its coalescence

The incubation of tiny void is the early stage of Electromigration in which the stable critical nucleus (tiny void) is formed. The creation of a nucleus implies the formation of an interface at the boundaries of a new phase (the tiny void, or the vacancy cluster in this study) in the metal material. Vacancy supersaturation due to the high temperature, current density and stress is the driving force to form the nucleus. During
the incubation, some of the energy is consumed to form a new interface, based on the surface energy of nucleus. Before a stable critical nucleus is formed, there is a distribution of sub-tiny voids (known as an unstable nucleus or "embryo") in the metastable matrix [104]. The incubation process of nucleus generally occurs with much more difficulty in the interior of a uniform substance. However, in practical interconnect process technology, there are always incubation sites in the metal thin film due to the inhomogeneity of microstructure/texture, such as different grain orientation, defects, dislocations and the interfaces of the different materials. At such preferential sites, the effective surface energy is lower, thus facilitating incubation. Vacancies and sub-tiny voids are not stable objects in a material. They interact easily with dislocations, grain boundaries and other defects in the material, and they may be created or annihilated in the material. The life time of a vacancy is very short and it is in the range of mini-second[105]. During such a short lifetime, a single vacancy is not able to diffuse from its initial locations to the final void growth location without annihilation. Despite the short lifetime of vacancies, they have high possibility to aggregate and form a tiny void at any of the above-mentioned possible incubation sites as illustrated in Fig. 38(b). If a hypothetical nucleus is too small, the energy that would be released by forming its volume is not enough to create its surface and the embryo will shrink to reduce the surface energy at the new interface, it will render an unsuccessful nucleation. When the void radius is about 10nm, it can hardly be broken up but to remain as a relatively stable object during the void nucleation process[106]. These tiny voids are more stable than the vacancies themselves, and this process is called tiny void incubation. Compared with the incubation time, the process of the
void nucleation due to the movement and coalescence of the tiny voids occupy most part of the MTF of an interconnect and it is the primary damage mechanism in EM failure [107].

The tiny void can be treated as a new inhomogeneity inside the material, and it attracts more vacancies nearby to sink into it while it moves through the material under the influence of various driving forces. This movement is preferred for vacancies since the system energy will be reduced. The tiny void moves by means of the diffusion of its surrounding atoms around its inner surface, as indicated by the small solid arrows in Fig 38(b).

As the size of the tiny void grows, the diffusivity of the tiny void reduces since it needs to re-arrange more atoms around its surface to move forward. As a result, it will be caught up by other tiny voids which have smaller sizes with higher mobility as shown in Fig 38(c) and (d). In this way, the tiny voids join together and the resultant void grows in size while moving through the material, and the voids can become visible under microscope. This behavior of movement and coalescence of visible voids is observed during the in-situ interconnect EM test reported in the literature[49, 71].

Because of the low energy status of the triple points of grain boundaries and the end of the cathode, the movement of the tiny void is pinned at these locations while continue to grow in size. When its size grows larger, it becomes a source of atomic flux...
divergence that causes the void to growth bigger in a much faster rate as simulated by Li et. al.[48], and causes the interconnect to fail ultimately.

The process of the void nucleation due to the movement and coalescence of the tiny voids occupy most part of the MTF of an interconnect since the duration of void growth is comparatively short for narrow interconnects[62] and it is the primary damage mechanism in EM failure[107]. Therefore, in the present study, our focus is on the theoretical derivation of the void nucleation time as described above. The movement and the coalescence of tiny voids can be simulated using Monte Carlo simulation together with FEA. The formula to predict the MTF can be derived based on the EM driving forces and the diffusivity of the tiny void. The details analysis and derivation will be elaborated in the following sections.

5.2.2. Derivation of the void nucleation time

During the tiny void incubation, the tiny void is formed at different inhomogeneity sites. The time for this process is negligible when we consider the MTF for the void nucleation. This is because the lifetime of a vacancy is in the range of mini seconds[105] and the vacancy needs to aggregate with each other within its lifetime.

Once the tiny voids are formed, they start to move under various EM driving forces as more stable objects than a single vacancy. Owing to their small size, the change in the electrical properties of the metal line will not be significant until they coalesce into a large void at weak spot in the interconnect. Therefore, the prediction of the time of
void nucleation is essentially the formation and the movement of the tiny voids during its process of aggregation.

The time for void nucleation and movement is inverse proportionally to the net drift velocity of the tiny void, $v$, given as

$$TTF = \frac{\Delta d}{v}$$

(5.1)

where $\Delta d$ is the average distance to be traveled by all the tiny voids from their original locations to the final tiny void aggregation location. But $v = M_{\text{void}} \cdot F_{EM}$, where $F_{EM}$ represents the various EM driving forces, and $M_{\text{void}}$ is the mobility of the tiny voids which is given as $M_{\text{void}} = D_{\text{void}} / k_B T$, following the Nernst-Einstein relationship[25], and we have

$$TTF = \frac{\Delta d}{v} = \frac{\Delta d}{M_{\text{void}} \cdot F_{EM}} = \frac{k_B T}{D_{\text{void}}} \cdot \frac{\Delta d}{F_{EM}} = \frac{k_B T}{D_{\text{void}}} \cdot \frac{\Delta d}{F_{EM} \cdot D_{\text{void}}} = \frac{k_B T \cdot \Delta d^2}{D_{\text{void}} \cdot \Delta E_{EM}}$$

(5.2)

Here $\Delta E_{EM}$ is the average work done by EM driving forces during the void nucleation and movement process. The derivation of $D_{\text{void}}$ will be given in the following section.

5.2.2.1. Derivation of diffusivity of the tiny void

As the movement of a tiny void is the collective result of the continuous displacement of atoms around the void, the diffusivity of the tiny voids can be obtained from the diffusivity of the atoms as follows.
In Fig.39, the small arrow shows the moving direction of one of the atoms on the tiny void surface, while the bulky arrow shows the moving direction of the tiny void as the result of the displacement of the atom. For a given temperature and EM driving forces, the ratio of their velocity is equal to the ratio of their diffusivity. The diffusivity of the tiny void can be derived by the relationship of the displacement of the atom and the tiny void as follows.

\[
\frac{D_{\text{void}}}{D_{\text{atom}}} = \frac{v_{\text{void}}}{v_{\text{atom}}} = \frac{\frac{d_{\text{void}}}{t_{\text{atom}}}}{d_{\text{atom}}} = \frac{d_{\text{void}}}{d_{\text{atom}}} \quad (5.3)
\]

where \(D\), \(v\), and \(d\) are the diffusivity, velocity and distance travelled by either the tiny void or the atom, indicated by the corresponding subscript of void and atom.
respectively. If we take the size of the tiny void and a single atom into the consideration, the moving distance of tiny void due to the movement of a single atom from one end of the tiny void to the other can be estimated as the ratio of the volume of the atom and the tiny void, and multiple by moving distance of the single atom. The detail of derivation is shown in the Appendix.

\[ d_{\text{void}} = \frac{V_{\text{atom}}}{V_{\text{void}}} \cdot d_{\text{atom}} \]  \hspace{1cm} (5.4)

where \( V_{\text{atom}} \) and \( V_{\text{void}} \) are the volumes of atom and void respectively.

However, this is just the scenario of the displacement of one atom. In the real situation, the tiny void is moving through the displacement of several atoms simultaneously and continuously, and the number of atoms that can move simultaneously is estimated by the size of the tiny void and the number of vacancies around its surface as the atoms are moved via occupying the vacancy. Therefore, we have

\[ \frac{D_{\text{void}}}{D_{\text{atom}}} = d_{\text{void}} \cdot d_{\text{atom}} \cdot N_{\text{vacancy}} = \frac{V_{\text{atom}}}{V_{\text{void}}} \cdot d_{\text{atom}} \cdot N_{\text{vacancy}} = \frac{V_{\text{atom}}}{V_{\text{void}}} \cdot S_{\text{void}} \cdot c_{\text{vacancy}} \] \hspace{1cm} (5.5)

where \( N_{\text{vacancy}} \) (\( N_{\text{vacancy}} = S_{\text{void}} \cdot c_{\text{vacancy}} \)) is the number of vacancies available on the surface of the tiny void, \( c_{\text{vacancy}} \) is the vacancy concentration and \( S_{\text{void}} \) is the surface area of the tiny void. The vacancy concentration depends on both the temperature[25, 108] and the stress[14, 25]. Mathematically, the two factors can be expressed respectively as

\[ c_{\text{vacancy}} = c_0 \exp\left(-\frac{E_{a\text{vacancy}}}{k_B T}\right) \] \hspace{1cm} (5.6)
\[ c_{\text{vacancy}} = c_0 \exp\left(\frac{\Omega\sigma_H}{k_B T}\right) \quad (5.7) \]

where \( c_0 \) is the equilibrium vacancy concentration, \( E_{a,vacancy} \) is the thermal activation energy of vacancy formation which has an approximate value of 0.6 eV for Al [107].

Substitute Eqn. 5.6, 5.7 into Eqn. 5.5, we have

\[ D_{\text{void}} = D_{\text{atom}} \cdot \frac{V_{\text{atom}}}{V_{\text{void}}} \cdot S_{\text{void}} \cdot c_0 \cdot \exp\left(\frac{\Omega\sigma_H - E_{a,vacancy}}{k_B T}\right) \quad (5.8) \]

To estimate the average diffusivity of all the tiny voids during the void nucleation, an estimated average \( r_{\text{void}} \) is used as we assume the spherical shape of void. In our study, \( r_{\text{void}} \) is around 10nm as we mentioned earlier[106], and we also observe in our simulation that most of the tiny voids move independently inside the metal and aggregate into a slightly bigger void at the metal-barrier layer interface only when they are very close to the final nucleation location. Hence, average \( r_{\text{void}} \) of 10 nm is used in this work.

The diffusivity of Al atom is depended on temperature and stress[25], and it can be mathematically expressed as[25]

\[ D_{\text{atom}} = D_0 \exp\left(-\frac{E_{a,\text{diff}}}{k_B T}\right) \quad (5.9) \]

And

\[ D_{\text{atom}} = D_{\text{atom}} \cdot \exp\left(\frac{\sigma_H}{B}\right) \quad (5.10) \]
Where $D_0$ is the pre-factor of the diffusivity of Al atom, $E_{a,\text{diff}}$ is the activation energy of diffusion, $B$ is the appropriately defined modulus for the metal-dielectric composite[23, 25].

5.2.2.2. Overall Median Time to Failure (MTF) formula

Substituting Eqn. 5.8 – 5.10 into 5.2, and using the average $V_{\text{void}}$ and $\Delta d$, i.e. the MTF as given by

$$M_{\text{TF}} = \frac{k_b T \cdot \Delta d^2}{D_0 \exp \left( -\frac{E_{a,\text{diff}}}{k_b T} + \frac{\sigma_H}{B} \right) \cdot \frac{V_{\text{atom}}}{V_{\text{void}}} \cdot \frac{c_0}{S_{\text{void}}} \cdot \exp \left( \frac{\Omega \sigma_H - E_{a,\text{vacancy}}}{k_b T} \right) \cdot \Delta E_{\text{EM}}} \quad (5.11)$$

With this equation, the MTF can be estimated theoretically and the effect of the influencing physical parameters can be studied quantitatively. Compared with the Black’s equation given in Eqn. 5.12, the detailed physics of the EM is revealed in our MTF formula.

$$M_{\text{TF}} = A(J^\alpha) \exp \left( \frac{E_{a,\text{effective}}}{k_b T} \right) \quad (5.12)$$

From Eqn. 5.11 and 5.12, we can see that the effective activation energy of the failure $E_{a,\text{effective}}$ from the Black’s equation actually consists of three components, namely the activation energy of the atom diffusivity $E_{a,\text{diff}}$, the activation energy of vacancy formation $E_{a,\text{vacancy}}$ and the effect of the hydrostatic stress. We can obtain the value of $E_{a,\text{vacancy}}$ and $\Omega \sigma_H$ from the literature and simulation respectively. However, we need the experimental data fitting to find the exact the value of $E_{a,\text{diff}}$ due to its
dependence on dominant diffusion path which in turn dependent on temperature and other process related factors[102].

\( (J^{-n}) \) in the Black’s equation represents the sole effect of electron wind force due to the high current density, while \( \Delta E_{EM} \) in our MTF formula accounts for not only the electron wind force, but also other various EM driving forces.

The process and geometry related arbitrary parameter \( A \) in the Black’s equation actually consists of many physical factors[101] where are not presented explicitly due to the absence of theoretical treatment. From our MTF formula in Eqn 5.11, the key physical factors contained in the parameter \( A \) are revealed and can be analyzed quantitatively. One can see that the parameter \( A \) is actually temperature dependent as is indeed shown by Shatzkes and Lloyd[17].

### 5.2.3. Finite element model and Monte Carlo simulation of void nucleation

Multi-physics FEA software ANSYS is used to create a 3-dimensional finite element model of a via-line structure. Only half of the structure is modeled due to the mirror symmetrical nature of the structure as shown in Fig. 35. For experimental comparison, Al interconnect is employed in the simulation, and the metal line thickness is 0.45 \( \mu \)m with the via diameter of 0.288 \( \mu \)m. The stress free temperature in the model is set at 410 °C which is the final annealing temperature of the wafers. In order to obtain more accurate results in the critical region which is along the via-line interface, a submodel
with a much higher mesh density is created. Its position is highlighted in the coarse finite element model shown in Fig. 35.

Void nucleation is a process of movement of tiny voids, vacancies and atoms in order to minimize the system energy. Following the FEA of the physical environment of the test structure, Monte Carlo method is employed to simulate the process of the void nucleation. The detailed implementation of the Monte Carlo methodology can be found in Chapter 4 and our previous work[48]. The simulation result and experimental observation will be discussed in the subsequent sections.

Figure 35: Coarse finite element model of the test structure and its submodel
5.2.4. Result and discussion

In this section, both the simulation and experimental result will be presented and the MTF estimation formula is verified based on the experimental data. The experimental EM failure data was obtained by performing an accelerated package level EM tests on an aluminum Via-line structure where the via-filling material is Tungsten (W), the barrier metal is TiN/Ti composition and the TARC layer is Ti. Fig. 36(a) shows the initial randomized locations of the tiny voids in the finite element submodel. The test condition is 200°C and 3.5MA/cm². The simulation continues until a 1% change in the resistance of the metal interconnection.

1% resistance change criterion is chosen because the size of the nucleated void up to 1% resistance change does not alter the distribution of various EM driving forces in the model as verified by our simulation work, and we consider this period of the EM

![Figure. 36: The Monte Carlo simulation of the void nucleation](image-url)
process as the phase of void nucleation. Experimentally, we also observed that the resistance change rapidly after the 1% change. This rapid change in resistance is due to the dramatic increase of the EM driving forces as a result of large atomic flux divergence around the nucleated void[48].

The final simulation result in shown in Fig. 36(b) which shows that the void nucleation site is under the W plug and slightly close to the edge of the metal line. From the locations of the initial tiny voids and their final nucleation location, the average $\Delta d$ in our MTF formula can be estimated by taking the difference between their median values.

Fig.37 is the experimental observation of the EM testing sample after 1% resistance change is recorded. As indicated in the figure, a small void nucleation site is indeed observed under the W plug and close to the outer edge of the via-line interface as predicted by the simulation.
With our MTF formula derived in the previous section and the information we have obtained from the simulation, $E_{a,diff}$ under the EM test condition can be determined by fitting the experimental MTF into our MTF formula. In our MTF formula, we assume the spherical shape of atoms and void, and the following input values were used:

$$ r_{atom} = 0.182\text{nm} \quad [106], \quad r_{void} = 10\text{nm} \quad [106], \quad S_{void} = 4\pi r_{void}^2 = 1.26 \times 10^3 \text{nm}^2, $$

$$ D_0 = 9.5 \times 10^{-8} \text{m}^2/\text{s} \quad [109], \quad E_{a,vacancy} = 0.6\text{eV} \quad [107], \quad \Omega = 1.66 \times 10^{-29} \text{m}^3 \quad [109], $$

$$ B = 50\text{GPa} \quad [109], \quad c_0 = 9.85 \times 10^{22} \text{/cm}^3 \quad [107]. $$

$r_{atom}$ and $r_{void}$ are the radii of atom and void respectively.

The value of $\Delta d$, $\Delta E_{EM}$ and $\sigma_H$ is estimated from the EM simulation where the material properties of the test structure used in the simulation is adopted from our previous study[48]. Under the testing condition of 200°C and 3.5MA/cm², we found that $E_{a,diff} \sim 0.52\text{eV}$.

With this value of $E_{a,diff}$, the MTF of the interconnect under other test temperatures can be estimated using our MTF formula and the simulation. Another two accelerated EM tests with the same current density but different test temperatures were performed. The results of the predicted MTF, MTF from experiments, the overall effective activation energy of void nucleation are summarized in Table 8.
Table 8: Testing and simulation result at different temperature ($E_{a,vacancy} = 0.6$ [107])

<table>
<thead>
<tr>
<th>Testing Condition</th>
<th>Estimated MTF</th>
<th>Experiment MTF</th>
<th>$E_{a,\text{diff}}$</th>
<th>$\Omega \sigma_H$ (Stress)</th>
<th>$E_{a,\text{effective}}$ (Simulation)</th>
<th>$E_{a,\text{effective}}$ (Black Eqn)</th>
</tr>
</thead>
<tbody>
<tr>
<td>150°C &amp; 3.5MA/cm²</td>
<td>2.51E+05</td>
<td>2.82E+05</td>
<td>0.52ev</td>
<td>0.021ev</td>
<td>1.09ev</td>
<td></td>
</tr>
<tr>
<td>200°C &amp; 3.5MA/cm²</td>
<td>1.35E+04</td>
<td>1.32E+04</td>
<td>0.52ev</td>
<td>0.029ev</td>
<td>1.09ev</td>
<td>1.02ev</td>
</tr>
<tr>
<td>250°C &amp; 3.5MA/cm²</td>
<td>1.31E+03</td>
<td>1.16E+03</td>
<td>0.52ev</td>
<td>0.036ev</td>
<td>1.1ev</td>
<td></td>
</tr>
</tbody>
</table>

As shown in Table 8, the estimated MTF has a good agreement with the MTF from the EM experiments over the temperature range of 150-250°C. Also the effective activation energy predicted by MTF formula and the Black equation are quite close. It is believed that the small discrepancy in the effective activation energy of the void nucleation is due to the approximate physical consideration in the Black’s equation, e.g. the temperature independence of the factor A in the Black’s equation.

Additional two accelerated EM testing were also performed at 6MA/cm² and 2MA/cm² while keeping the temperature at 150°C so as to study the current density dependence of our estimated MTF. The value of $E_{a,\text{diff}}$ is taken to be 0.52eV as obtained from the previous experiments. Fig. 40 shows that the experimental MTF presents a linear relationship with $1/J^2$, where $J$ is the current density. The value of 2 in the current exponent indicates that the EM process considered (with 1% resistance change) is indeed void nucleation as reported in the literature[16, 17, 23].
Comparing the experimental MTF and the estimated MTF in Table 9, the discrepancy is found at both high and low current density conditions. This is believed to be due to the dependence of the overall effective activation energy on current density, which was reported in the literature[110-112]. A fitting parameter, $E_j$, is added to $E_{a,diff}$ to account for such a dependence. The value of $E_j$ is obtained by fitting the estimated MTF to experimental MTF, and the results are shown in Table 9. From Table 9, one can see that the activation energy decreases with increasing current density, which is consistent with the trend reported in the literature[112, 113]. This fitting parameter should be included in the extrapolation if the prediction is over different current density.
Table 9: Testing and simulation result at different current density

<table>
<thead>
<tr>
<th>Testing Condition</th>
<th>Estimated MTF</th>
<th>Adjusted Estimated MTF</th>
<th>Adjusted MTF</th>
<th>( E_{a,\text{diff}} + E_l ) (adjusted)</th>
</tr>
</thead>
<tbody>
<tr>
<td>150°C &amp; 2MA/cm²</td>
<td>3.83E+05</td>
<td>6.58E+05</td>
<td>6.53E+05</td>
<td>0.54ev</td>
</tr>
<tr>
<td>150°C &amp; 3.5MA/cm²</td>
<td>2.51E+05</td>
<td>2.51E+05</td>
<td>2.82E+05</td>
<td>0.52ev</td>
</tr>
<tr>
<td>150°C &amp; 6MA/cm²</td>
<td>4.56E+04</td>
<td>1.63E+04</td>
<td>1.27E+04</td>
<td>0.48ev</td>
</tr>
</tbody>
</table>

5.2.5. Summary

In the present study, a concept of three physical stages during EM is proposed. The three physical stages are the tiny void incubation, void nucleation and void growth. Combining the Finite element submodelling and Monte Carlo method, an alternative EM model for void nucleation is developed. Using the developed simulation methodology, the process of void nucleation during EM is simulated. We presented the derivation of physics-based MTF formula for void nucleation, and the physical formulation of MTF reveals the key physical factors that are hidden in the Black’s equation. With the aid of the simulation, the effect of the key physical parameters on MTF can be studied and analyzed quantitatively. Various accelerated EM testing are performed and the experimental observation shows a good agreement with our simulation prediction.
5.3 Application of Black’s equation to today interconnect – A revisit

The Black’s equation is a simple empirical EM model, which is widely accepted in the industry as the most common method to extrapolate the median time to failure (MTF) from the accelerated testing condition to the normal operating condition. Although the empirical model of the Black’s equation is simple in implementation, its validity has been a great controversy in the literature. In this section, we revisit the Black’s equation for its success in the industry and the validity of its inherent assumptions. Due to neglecting of additional stress factors in ULSI interconnects, we found that the application of the Black’s equation in today ULSI interconnects fails as evident experimentally. The alternative MTF model proposed in previous section is compared with Black equation in this section.

5.3.1 Black’s equation for interconnection – A revisit

5.3.1.1 The origin of Black’s equation and its controversy

The most popular EM model in the industry today is introduced by J. R. Black from Motorola in 1967[101]. Through his various experiments, an empirical EM model is proposed as follows

\[
MTF = A \cdot (j)^{-2} \cdot \exp \left( \frac{E_a}{k_B T} \right) \quad (5.13)
\]

where \( A \) is a constant depending on the geometry property of the interconnect structure, \( j \) is the current density, \( E_a \) is the activation energy, \( k_B \) is the Boltzman’s
constant and $T$ is the film temperature. Subsequent research and experiment suggest that EM testing data does not always follow the relationship strictly and the current density exponential is not necessary equal to 2[114], and the Black’s equation is rewritten as follows

$$MTF = A \cdot (j)^{-n} \cdot \exp \left( \frac{E_a}{k_n T} \right)$$

(5.14)

Due to its reasonable good fitting of EM experimental data and the simplicity of implementation, the Black’s equation is widely accepted in the industry as the most common method to extrapolate the MTF from the accelerated testing condition to the normal operating condition. The application of the Black’s is not only limited to various Al-based interconnect system[115], but also to Cu-based interconnect system[88], highly accelerated Wafer Level EM testing[116] and Solder Bump EM testing with good success[117].

Since the proposal of the Black’s equation in 1960s, the interconnect technology has advanced dramatically. New thin film stack, new materials and the ever shrinking interconnect dimension has introduced new EM physics[47, 48]. The validity of application of the Black’s equation in these new situations becomes questionable. For example, due to the simplicity of the Black’s equation, it fails to consider new stress factors which can seriously affect the accuracy of its lifetime prediction in the nano-interconnects[5, 16]. Moreover, it has been a great controversy on the choice of the critical values, such as current density exponent and the activation energy in its basic formula, which brings it a large potential error [25, 102, 103, 111].
The inaccuracy and the contradiction of the Black’s equation have received researchers’ attention and several predictive EM models have been proposed in the literature to modify the Black’s equation in order to have a better fitting to the experimental results [17, 18, 31, 118]. However, all of them are only addressing one of several issues of the Black’s equation, such as current density, pre-exponential constant or the effect of hydrostatic stress, and modify the equation accordingly. Moreover, the modification and improvement of the Black’s equation still have their root on the Black’s equation. It is hard to believe such adjustment in the expression of a purely empirical equation can be used to predict even changing interconnect technology. In the following sections, we will review the inherent implications of the Black’s equation and discuss their validity.

5.3.1.2 The inherent assumptions of the Black’s equation and their validity

The Black’s equation is actually a combination model that combine the Arrhenius model and the inverse power rule model[62, 119]. From the Black’s equation, the inherent implications made in the equation can be summarized as follows.

1) There are only two stress factors during EM, temperature and current density

2) The pre-exponential term is a temperature independent constant

3) There is no interaction between temperature and current density/other stress factor

4) The overall effective activation energy is independent on current density/other stress factor
Considering the implication (1), it has been reported that in the modern ULSI interconnect system, the electron wind force is not the sole driving force during EM[48, 61], and hydrostatic stress has been identified as an increasing significant factor during EM as interconnect linewidth reduces toward sub-micron scale and below as reported by many[14, 25, 100]. For the implication (2), both our recent study[120] and report from others[17, 22, 24, 121] have shown the temperature dependence of the pre-exponential term. For the implication (3), since hydrostatic stress is induced from the thermal mismatch of the metal interconnect and its surrounding, the magnitude of the hydrostatic stress depends on the interconnect temperature and its uniformity which in turn depends on the current density because of the Joule heating effect. Hence, obviously there is an interaction between current density and temperature as well as the other stress factor, and this is not accounted for in the Black’s equation. The evidence of the temperature interaction with hydrostatic stress during EM testing is reported in several experimental result[47, 100, 122] and theoretical studies[26, 100].

The final implication is the independence of the activation energy with the stresses. However, this is not true even in the era of Al interconnect as reported by Partridge and Litterfield[112], and Fig. 41 reproduced their experimental result for clarity. Furthermore, Eyring[123-125] pointed out that the free energy of activation is a sensitive function of intensive stress factors in general.
The work by McPherson[110] showed that the activation energy becomes stress-dependent when two necessary requirements are satisfied, namely the applied stress must be of the same order of magnitude as the strength of the material, and the stress acceleration parameter must be a function of temperature. The encapsulation constrains and confinement due to the surrounding materials in a practical interconnects lead to high mechanical stress, estimated to be of the order 600MPa \textasciitilde 1.3GPa[126, 127]. Thus the applied stress is indeed of the same order of magnitude as the strength of the metal in term of void nucleation and its effect has been studied in various reports in the literature[23, 24, 109]. Also, the hydrostatic stress is a function of temperature as mentioned earlier. Hence, the activation energy should be stress dependent.

Also, the use of the Arrhenius model for extrapolation is found to be inconsistence with the physical concept of the Arrhenius theory as pointed out by Kececioglu and
Sun in Chapter 12 in their book[128] and hence direct use of the Arrhenius model for extrapolation can be inaccurate.

With the invalidity of the inherent assumptions in the Black’s equation, the lifetime data extrapolation based on the Black’s equation is expected to be inaccurate in assessing the reliability performance of today interconnection which will be shown in the subsequent section. As an alternative to Black’s equation, we adopt the physics-based MTF formula proposed in previous section to analyze the data from EM accelerated lifetime testing. The equation of the MTF formula is as follows

\[
MTF = \frac{k_B T \cdot \Delta d^2}{D_0 \exp \left( -\frac{E_{a,\text{diff}}}{k_B T} + \frac{\sigma_H}{B_m} \right) \cdot V_{\text{atom}} \cdot S_{\text{void}} \cdot c_0 \exp \left( \frac{V_{\text{atom}} \cdot \sigma_H - E_{a,\text{vacancy}}}{k_B T} \right) \cdot \Delta E_{\text{EM}}}
\]

(5.15)

where \(D_0\) is the pre-factor of the diffusivity of Al atom, \(E_{a,\text{diff}}\) is the activation energy of diffusion, \(T\) is the stress temperature, \(\sigma_H\) is the hydrostatic stress, \(V_{\text{atom}}\) is the atomic volume, \(V_{\text{void}}\) and \(S_{\text{void}}\) is the volume and surface area of the tiny void[120] considered in the modeling, \(B_m\) is the appropriately defined modulus for the metal-dielectric composite[23, 25], \(c_0\) is the equilibrium vacancy concentration, \(E_{a,\text{vacancy}}\) is the thermal activation energy of vacancy formation which has an approximate value of 0.6 eV for Al [107], \(\Delta E_{\text{EM}}\) is the total work done by EM driving forces during the void nucleation and \(\Delta d\) is the average traveling distance of all the tiny voids in the EM testing structure.
5.3.2 Experimentation

5.3.2.1 Accelerated EM testing

In this study, the accuracy of the Black’s equation under different test temperatures is investigated. We predict the EM lifetime at various stress conditions from a reference stress condition using both the Black’s equation and the recent MTF model in Eqn. 5.15 while keeping the stress current unchanged so that the accuracy of the prediction by both models can be analyzed and compared at different test temperatures.

The experimental EM failure data are obtained by performing an accelerated package level EM tests on an aluminum Via-line structure where the via-filling material is Tungsten (W), the barrier metal is TiN/Ti composition and the TARC layer is Ti. The width of the Al line and the via diameter are 0.288um. The final anneal temperature of the wafer is at 410°C. The test temperatures are 250°C, 200°C and 150°C at the same stress current density of 3.5MA/cm². The test continues until a 1% change in the resistance of the metal interconnection is observed. The time to failure data are analyzed and extrapolated to low stress condition (100°C & 3.5MA/cm²) based on the Black’s equation and the physics-based MTF formula. Al interconnects are used in this work due to the availability of the samples, and the same principle can be applied to other metal interconnection such as Cu.

5.3.2.2 Lifetime extrapolation

The acceleration factor based on the Black’s equation can be calculated as below
\[ A_j = \frac{MTF_{predict}}{MTF_{ref}} = \frac{A \cdot (j_{predict})^{-n} \cdot \exp \left( \frac{E_a}{kT_{predict}} \right)}{A \cdot (j_{ref})^{-n} \cdot \exp \left( \frac{E_a}{kT_{ref}} \right)} = \left( \frac{j_{predict}}{j_{ref}} \right)^{-n} \exp \left[ - \frac{E_a}{k} \left( \frac{1}{T_{predict}} - \frac{1}{T_{ref}} \right) \right] \]  

(5.16)

where the \( MTF, j \) and \( T \) are the median time to failure, current density and temperature of either the reference stress condition or the predicting stress condition, indicated by the corresponding subscript of \( ref \) and \( predict \) respectively. As the current density is kept unchanged in this study, the acceleration factor can be reduced to

\[ A_j = \frac{MTF_{predict}}{MTF_{ref}} = \exp \left[ - \frac{E_a}{k} \left( \frac{1}{T_{predict}} - \frac{1}{T_{ref}} \right) \right] \]  

(5.17)

Taking the logarithm on the both sides of Eqn. 5.17, one can see the linear relationship of \( \ln(MTF) \) and \( 1/kT \), and \( E_a \) can be extracted by fitting the experimental result from three stress conditions with different temperatures. Fig. 42 shows the linear regression fitting of experimental result from 150\(^o\)C, 200\(^o\)C and 250\(^o\)C, and \( E_a \) is found to be 1.02 eV

![Figure 42: Extraction of activation energy of the Black's equation](image)

\( Ea = 1.02\text{eV} \)
Taking the MTF at 200°C as reference, the value of MTF at 250°C, 150°C and 100°C is estimated based on Eqn. 5.17.

With the physics-based MTF formula in Eqn 5.15 and the information we have obtained from the simulation, \( E_{a,diff} \) under the EM test condition can be determined by fitting the experimental MTF into our MTF formula. Here we assume the spherical shape of atoms and voids, and the following input values are used:

- \( r_{atom} = 0.182 \text{nm} \) \[106\], \( r_{void} = 10 \text{nm} \) \[106\], \( S_{void} = 4\pi r_{void}^2 = 1.26 \times 10^3 \text{nm}^2 \),
- \( D_0 = 9.5 \times 10^{-8} \text{m}^2/\text{s} \) \[109\], \( E_{a,vacancy} = 0.6 \text{eV} \) \[107\], \( \Omega = 1.66 \times 10^{-29} \text{m}^3 \) \[109\],
- \( B = 50 \text{GPa} \) \[109\], \( c_0 = 9.85 \times 10^{22}/\text{cm}^3 \) \[107\]. \( r_{atom} \) and \( r_{void} \) are the radii of atom and void respectively. The value of \( \Delta d \), \( \Delta E_{EM} \) and \( \sigma_H \) is estimated from the simulation and the material properties of the test structure used in the simulation is adopted from our previous study[48]. Under the testing condition of 200°C and 3.5MA/cm², we found that \( E_{a,diff} \sim 0.52 \text{eV} \). With this value of \( E_{a,diff} \), the MTF of the interconnect under other test temperatures at 250°C, 150°C and 100°C can be estimated using the MTF formula of Eqn 5.15.

To evaluate the accuracy of the two models, an unbiased extrapolation method is needed as a reference. This unbiased method is based purely on statistics so that the physical assumptions used in any physical model can be avoided. As the probability plot of the time to failure data at the three test temperatures are parallel as shown in Fig. 43, we have the true linear acceleration[119] in our results, and hence statistics
based model for the computation of acceleration factor can be employed. This method can be found in most of the textbooks on reliability statistics[119, 129].

![Lognormal CDF plot for testing data at 250C, 200C and 150C](image)

**Figure 43: Lognormal CDF plot for testing data at 250C, 200C and 150C**

Plotting the ln(MTF) vs. stress level (i.e. temperature), our results indeed appear as straight line in the plot as shown in Fig. 44. The prediction results due to the Black’s equation and the recent MTF formula are also shown in Fig.44 for comparison, and Table 10 summaries the comparison results.
Figure 44: The result of experiments and predictions

From Table 10, we find that although both the Black’s equation and MTF model have a reasonable accuracy in the MTF prediction at 150°C, 200°C and 250°C, the prediction error at 100°C using the Black’s equation is significant.

Table 10: The result of predictions by MTF model and the Black’s equation

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Current Density (MA/cm²)</th>
<th>MTF Model</th>
<th>Black Equation</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Predicted</td>
<td>Experiment</td>
<td>Error</td>
</tr>
<tr>
<td>250C 3.5MA/cm²</td>
<td></td>
<td>1.31E+03</td>
<td>1.16E+03</td>
<td>12.93%</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.23E+03</td>
<td>1.16E+03</td>
<td>6.16%</td>
</tr>
<tr>
<td>150C 3.5MA/cm²</td>
<td></td>
<td>2.51E+05</td>
<td>2.42E+05</td>
<td>3.72%</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2.52E+05</td>
<td>2.42E+05</td>
<td>3.72%</td>
</tr>
<tr>
<td>100C 3.5MA/cm²</td>
<td></td>
<td>5.79E+06</td>
<td>4.41E+06</td>
<td>31.21%</td>
</tr>
<tr>
<td></td>
<td></td>
<td>9.32E+06</td>
<td>4.41E+06</td>
<td>111.24%</td>
</tr>
</tbody>
</table>
As $E_{a,diff}$ is a constant with the value around 0.52eV determined from our test data, the prediction result from the physics-based MTF model does not depend on any particular reference temperature. It gives comparable results at all testing conditions. However, the prediction result from the Black’s equation depends on the activation energy, the MTF at reference stress condition and the acceleration factor between the reference stress condition and the predicting stress condition. Table 11 shows the error of extrapolation result at 100°C using the Black’s equation with different stress condition as the reference point.

<table>
<thead>
<tr>
<th>Reference</th>
<th>Estimated MTF at 100°C</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>150C 3.5MA/cm²</td>
<td>7.77E+06</td>
<td>76.19%</td>
</tr>
<tr>
<td>200C 3.5MA/cm²</td>
<td>9.31E+06</td>
<td>111.09%</td>
</tr>
<tr>
<td>250C 3.5MA/cm²</td>
<td>9.52E+06</td>
<td>115.71%</td>
</tr>
</tbody>
</table>

The overestimation of the Black’s equation is due to the neglection of the effect of thermo-mechanical stress in the interconnect system. At high testing temperature, the stress in the metal line is moderate as the testing temperature is closer to the stress free temperature, which was set at the final annealing temperature of the wafer. However, at low testing temperature, the stress in the metal line is significant and becomes another stress factor during EM testing. The extrapolation from high stress condition thus underestimates the acceleration effect due to the thermo-mechanical stress and overestimates the EM lifetime at the low stress condition.
5.3.3 Summary

In this study, the inherent implications in the Black’s equation are revisited and their validity is discussed. As the development of interconnect system into the submicron and below, the validity of the inherent assumptions of the Black’s equation is challenged, and inevitable error in the extrapolation of the test data is resulted. Such inaccuracy is shown experimentally, and the EM lifetime at low testing temperature is overestimated. As the purpose of accelerated life test is to predict the reliability performance at normal operating condition, over-estimation of the life time can render serious consequences. On the other hand, the recently proposed MTF formula shows considerable accurate result on all the predicting stress conditions regardless of the choice of the reference stress condition.

5.4 Conclusion

In this chapter, we focus on the prediction of EM MTF. It consists of two parts, one part is the theoretical and experimental study of the EM physics and its acceleration, the other part is to review the Black’s equation and its comparison with our MTF formula. In our study, an alternative concept of EM physics is proposed. It consists of three physical stages, namely the tiny void incubation, void nucleation and void growth. The degradation process of EM during each physical stage is described in detail and formularized in our study. It enhances not only our understanding of the physics of EM, but also the predictive simulation of EM. With the MTF formula, we
are able to perform the physics-based EM simulation for a particular testing structure and predict its MTF accurately in different testing condition by extrapolation. From both our experiments and reported data in the literature, we also find the inaccurate prediction results from the Black’s equation. We review the validity of inherent implications of the Black equation and find that its inaccuracy is due to the neglection of additional stress factors in the advanced interconnect system. In contract, those additional stress factors are taken into consideration in our proposed MTF formula. Our formula has a much better prediction result as evident experimentally.
Chapter 6: Conclusion and Future work

6.1 Conclusion

Demand for higher speed ULSI with more complex functionality is driving the continuous change in the interconnects’ structures and materials as well as the interconnects processing technology. On the other hand, their reliability requirements are expected to be higher with the increasing complexity of ULSI. Therefore, reliability evaluation and improvement of new interconnects require a more thorough understanding of the physics of EM, and experimental investigation can be too costly and too slow to cope with the changing interconnect systems. Physics-based modeling of the EM becomes necessary to complement the experimental investigation.

Our study starts with a comprehensive review on the EM models in the interconnections and their evolution over the last three decades. Along the evolution of the physics-based EM simulation in the last three decades, some aspects of the EM physics are dropped for simplification, and some are added to accommodate our new understanding of the EM physics as well as for the new development of the interconnect technology. With the continuous change in the metallization system and materials, the aspects of physics that have been dropped may become important again. New physics might also occur with these changes in metallization system. Therefore, a review on the development of physics-based modeling for EM will be a useful reference for researchers who are working on the EM modeling.
In our study of the physics of EM, the multi-physics FEA software is used. The application of multi-physics FEA on the interconnect system of ULSI is rather limited in both industry and academic field. However, decades of advances in computational science have brought us smarter algorithms and faster, more powerful hardware that puts multi-physics FEA tools within reach for all engineers and scientists. It opens up new opportunities for modeling and simulating real-world applications as well as a world of technological investigation in the interconnect system of the integrated circuit (IC).

In Chapter 3, our study demonstrates the real-world application of FEA with theory of EM physics and advance statistical analysis method in the development of highly accelerated EM testing in a wafer fab, which is one of the potential utilizations of multi-physics FEA. We also shows how the linkage between MatLab and ANSYS can leverage the FEA on reliability analysis of EM in advance interconnect system.

In Chapter 4, a holistic EM simulation methodology that combines Monte Carlo algorithm and FEA is presented to study the dynamic physical process of EM. The inhomogeneity of the interconnect microstructure and the resulting different atomic diffusivities along the various diffusion paths are considered in the model. The presence of the various driving forces of EM is also included in the analysis. Our model demonstrates the vacancy trapping, void nucleation and void growth during EM, and the results are found to agree well with the experimental observations reported in literatures. In this Chapter, we also demonstrate how the Monte Carlo simulation can
be performed on a more realistic EM testing structure with complicated geometry with the by using the advance FEA technical, submodeling. It is shown that the submodeling technique can extend the application of Monte Carlo simulation of EM to the testing structure with more general geometry without compromising its accuracy in prediction of void nucleation location.

An alternative concept of EM physics is proposed in Chapter 5. It consists of three physical stages of EM, namely the tiny void incubation, void nucleation and void growth. Physics-based MTF formula for void nucleation is derived and present in the study, and the physical formulation of MTF reveals the key physical factors that are hidden in the Black’s equation. With the aid of the simulation, the effect of the key physical parameters on MTF can be studied and analyzed quantitatively. Various accelerated EM testing are performed and the experimental observation shows a good agreement with our simulation prediction. The validity of Black’s equation is further explored in the second part of this chapter. The inherent implications in the Black’s equation are revisited. It is found that the validity of the inherent implications of the Black’s equation is challenged and inevitable error in the extrapolation of the test data is resulted as the development of interconnect system into the submicron and below. On the other hand, the proposed MTF formula shows considerable accurate result on all the predicting stress conditions regardless of the choice of the reference stress condition.
6.2 Suggestion for future work

Looking at the evolution of the EM models over the past three decades, and with the advancement in interconnect process technology as well as the change in interconnect system in term of both the materials and structures, we can comment on the following future progress needed for the EM modeling.

6.2.1 Advanced 3-Dimensional EM simulation

6.2.1.1 3-Dimensional EM simulation at circuit level

Most of the early proposed 1-D and 2-D models studied the EM within the interconnect material itself, and the effect of the surrounding materials on the interconnect EM is not taken into consideration. As the interconnect line width goes into 150 nm and below, and with the use of the low-k dielectric, the impact of the surrounding materials on the interconnect EM becomes significant[48]. Although the EM model in our study has take the surrounding material into the consideration, the simulation is performed locally on one portion of the interconnect system. The current density and the temperature due to the heat generated by transistors and joule heating are not equally distributed in the whole interconnect system. Depending on their locations in the chip, a particular interconnect structure can have significantly different reliability performance even with the same surrounding material and structure. In other words, the future EM simulation can no longer be limited to the interconnect material and particular structure. It should be able to assess the integrated EM
reliability performance in the entire interconnect network in the chip, including the
consideration of design layout of the entire chip in 3-Dimensions.

6.2.1.2 Electron windless modeling

One of the modeling concepts adopted in our simulation and the MTF derivation is
that the root cause of void nucleation and movement is the redistribution of the
vacancies and atoms, which is the result of uneven distribution of energy due to the
external source, such as current density, temperature gradients, stress gradients and
surface energy. Our study presents the methodology to simulate the physical process
of EM based on the energy distribution. C.T. Sah has presented a windless, neutral
atomic diffusion and trapping void model in his two publications [130, 131]. Although
our simulation methodology is different from the windless void model with only
atomic diffusion and releasing/trapping as proposed by C.T. Sah, we are actually
consistent in terms of basis physics as the change in the distribution of energy
(electrical, thermal, strain and surface) essentially relates to the strength of the metallic
bonding of atom with its surrounding atoms, which directly affects the
releasing/trapping rate and the diffusion of the atom in the metal conductor. In our
study, although the concept of electron wind force is still adopted for the calculation
of the energy distribution, our further work is to calculate the energy change due to the
electron flow without involving the concept of electron wind force. In fact, it is shown
that in presence of excessive electron during EM, the bonding energy of an atom to its
surrounding is weakened [132], thus increase the possibility of atoms dislodging from
their neighbor, and such an increase in the possibility is found to be anisotropic [132].
Because of the inhomogenous distribution of the excessive electron in an interconnect, the direction to a state with lower energy is favored for the moving atoms. To correlate and formulate the quantitative relationship of energy due to aforementioned external energy sources with the windless model of Sah requires the knowledge of many body physics, and most importantly, how to realize it in a simulation methodology that can be easily accepted by industry are indeed a great challenge in the future.

6.2.1.3 Tiny void incubation in advanced nanointerconnections

With the development of nano-interconnect technology, not only the nucleation of void is critical to Electromigration reliability of an interconnect system, but also the incubation of the tiny void. The model proposed in this dissertation is to address the primary reliability degradation issue in today’s interconnections. The future nanointerconnection will be even more vulnerable to the void nucleation, and furthermore, the void nucleation during the Electromigration is an irreversible process which causes the inevitable reliability degradation of interconnections. Hence, the study of the mechanism of tiny void incubation in a heterogeneous metal material and the development of the method to prevent or retard the formation of a stable nucleus before the nucleation process (and hence the irreversible reliability degradation) even start will be valuable for the reliability of future interconnections. To further assess the reliability degradation due to Electromigration and the improvement method for the future nano-interconnections, the modification to current model is needed so that the incubation of the tiny void in the future nano-interconnection is also considered.
6.2.2 The MTF prediction formula for the application in industry

The Black’s equation is purely empirical, and it has been known for years that the current exponent and activation energy found in experiments varies widely from experiments to experiments. The application of the Black’s equation on advance technology has been questioned by many researchers in the literature. However, most of the evidence of the failure of the Black’s equation is from various reported experiments. The justification of the failure of the Black’s equation should be based on both the basic physical derivation and numerous experiments. Moreover, the modification and improvement of the Black’s equation still have their root on the Black’s equation. It is hard to believe such adjustment in the expression of a purely empirical equation can be used to predict even changing interconnect technology. That is also the reason why there are many modifications of the Black’s equation but none of them is generally accepted by the industry.

The Black’s equation is well accepted in the industry due to its simple application and its success in the early technologies. In our study, we derived an alternative MTF formula to assess the EM reliability performance. Although we have found the evidence of its advantage over the black’s equation, there is still a lot of work to do to propose a practical MTF prediction formula for industry. The MTF formula is able to predict the MTF accurately with the help of physics-based EM simulation, the complexity of the formula and simulation make its application in industry very difficult. The formula can be simplified by dropping the insignificant terms or replacing the complex mathematic expressions with general constants. However, such
modification needs to be carefully justified based on the EM physics and the alternative equation has to be verified by numerous experiments and advance statistical analysis. The development of the methodologies to determine the values of the various parameters in the alternative formula accurately will be great challenge in the future work. Furthermore, the formula needs to be reviewed and adjusted constantly with the development of interconnect technology as the new technology may introduce new physical aspects in EM or make the insignificant parameters in the formula become critical in the new technology.

6.2.3 The development of simulation tools

The development of the computer hardware and the computational software has released researchers from enormous numerical calculation limitations. This development enables us to simulate the process of EM with higher accuracy, more complicated geometrical structure and in much greater details. Some of the computer intensive methodologies, such as Monte Carlo method, could become a common tool with the ever increasing computational power.

The intercommunication or interface between different software also allows us to take the advantages of the strength of each software, thus providing more than one analysis tools to serve the purpose of our simulation. Hence, one should also be familiar with the advancement of the simulation tools available and re-examine the various assumptions made during the EM simulation as a result of the computing power.
limitations, and to build a more comprehensive EM model so that design-in reliability for interconnect system can become a reality.
Appendix

Determination of Void Displacement due to its element movement

This is to derive the movement of a mass center of a given volume due to the movement of one of its small element. As shown in the figure below, the volume consists of numbers of small units.

Assuming all the elements has the same volume of $V_{elem}$, and the x-coordinate of the $i^{th}$ element is $x_i$, the x-coordinate of the mass center of the volume, $\bar{x}$ can be calculated as

$$V_{elem} \cdot \sum_{i=1}^{N} x_i = V_{volume} \cdot \bar{x} \quad (A1)$$

$$\bar{x} = \frac{\sum_{i=1}^{N} x_i}{N} \quad (A2)$$

Figure A-1: The movement of one element in a volume
where $N$ is the number of units in the volume ($N = \frac{V_{\text{volume}}}{V_{\text{elem}}}$)

When an element $a$ is moved from $x_a$ to $x'_a$, the new mass centre of the volume, $\bar{x}'$, can be calculated as

\[ V_{\text{elem}} \left( \sum_{i=1}^{N} x_i - x_a + x'_a \right) = V_{\text{volume}} \cdot \bar{x}' \quad (A3) \]

\[ \bar{x}' = \frac{\left( \sum_{i=1}^{N} x_i - x_a + x'_a \right)}{N} \quad (A4) \]

and

\[ \bar{x}' - \bar{x} = \frac{\left( \sum_{i=1}^{N} x_i - x_a + x'_a \right)}{N} - \frac{\sum_{i=1}^{N} x_i}{N} = \frac{x'_a - x_a}{N} = \frac{V_{\text{elem}}}{V_{\text{volume}}} \cdot (x'_a - x_a) \quad (A5) \]

Similarly to the y- and z-coordinates. Thus, the moving distance of the mass center of the volume due to the movement of an element of $d_{\text{elem}}$ is given by

\[ d_{\text{volume}} = \frac{V_{\text{elem}}}{V_{\text{volume}}} \cdot d_{\text{elem}} \quad (A6) \]
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