Modeling Electromigration for Microelectronics Design*

Xiao ZHU**, Hiren KOTADIA***, Sha XU****, Hua LU**,
Samjid MANNAN***, Chris BAILEY** and Yancheong CHAN****

** School of Computing and Mathematical Sciences, University of Greenwich,
30 Park Row, London SE10 9LS, UK

E-mail: X.ZHU@gre.ac.uk

*** Physics Department, School of Natural & Mathematical Sciences, King's College London,
Strand, London WC2R 2LS, UK

**** Department of Electronic Engineering, City University of Hong Kong,
83 Tat Chee Avenue, Kowloon Tong, Hong Kong, China

Abstract

Computer simulation of electromigration (EM) in microelectronics devices has been reviewed and a multi-physics numerical simulation method has been proposed and developed so that the electric current, temperature, stress can be solved simultaneously and the vacancy concentration can be predicted in a seamless framework. The design considerations for resisting EM is also discussed in this work and a shunt structure for solder joint pad is proposed and its potential for the reduction of EM risk is demonstrated.

Key words: Electromigration, Simulation, Shunt, Solder Joint

1. Introduction

Electromigration (EM) is a mass migration phenomenon that occurs in conductors under the influence of strong electric current, temperature, temperature gradient, and mechanical stress Ref. (1). The main process is a diffusion of ions that is driven by their collision with charge carriers, i.e. electrons in metals. In recent years, high density packaging (HDP) in electronics manufacturing has been increasingly adopted to meet the needs for device miniaturization and performance in electronic products. As a result, maximum electric current density in electronic devices has increased tremendously and is expected to increase even further. Because of this trend, EM is now a major challenge for electronics designers and manufacturers. In this paper, computer simulation methods for EM have been reviewed, and a new multi-physics EM simulation method that combines electric, thermal, atomic diffusion and stress analysis has been described. The new integrated method can be used to predict vacancy evolution in conductors so that EM-aware electronics designs can be carried out.

EM was first reported by M. Gerardin in 1861 Ref. (2), and was confirmed to be correlated with the type of majority charge carriers by W. Seith and H. Wever in the 1950s Ref. (3). In 1967, J.R. Black first proposed an EM model Eq. (1) to predict the mean time to failure (MTTF) of electric conductors:

$$MTTF = \frac{A}{j_e^n} \exp\left(\frac{E_a}{kT}\right) \quad (1)$$

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where A is a material and geometry constant, J_n is the current density, E_a is the activation energy, T is the absolute temperature, and k is Boltzmann's constant Refs. (4) and (5). The Black model is an empirical model and the reported values of n varies and $n = 2$ has been quoted in most EM analysis.

As EM occurs, hydrostatic stress builds up. In 1975, I. A. Blech found EM this stress may stop EM if the conductor's length is shorter than a critical value. He proposed a model to describe the relationship between this critical length, the current density, and the stress Eq. (2) Refs. (6) and (7).

$$\Delta x = \frac{\Delta \sigma \Omega}{Z^* e E} \quad (2)$$

where σ is the hydrostatic stress, Ω is the atomic volume, Δx is the critical length of the conductor, Z^* is the effective charge, e is the elementary charge, E is the electric field, Eq. (2) can also be written as Eq. (3).

$$(\Delta x \cdot J_e) = \frac{\Delta \sigma \Omega}{Z^* e \rho} \quad (3)$$

where $(\Delta x \cdot J_e)$ is the so called critical product which can be used to characterize the EM resistance capability of conducting metals. For example, the critical product of copper is about 2000 to 10000 A/cm Refs. (6) - (9).

Since the development of the above models, more detailed theoretical and experimental analysis work of EM has been carried out by many researchers. In 1988, A.P. Schwarzenberger et al. Ref. (10) used a one-dimensional model to simulate the stress evolution in their experiments. Chang et al. Ref. (11) simulated the change of the voltage distribution in the solder joint to predict the site of void formation caused by EM. Xia and et al. Ref. (12) analyzed the evolution of voids due to strain and diffusion effect using the finite element method (FEM). In 1986, Shatzkes and Lloyd Ref. (13) proposed a one dimensional diffusion-convection EM model and since then computer modeling has gradually become more focused on EM under the influence of multiple physical processes. Lee et al. Ref. (14) modeled both the heat flow and the current density in a solder bump to explore the relation between the combined effects of these two factors on the atomic flux. Hieu and Salm Ref. (15) analyzed the current crowding effect in a solder joint and predicted the failure location and the lifetime of the solder joint. Singh et al. Ref. (16) simulated the nucleation and growth of voids in a realistic interconnecting test structure. Some researchers have used numerical methods to evaluate in details the influence of temperature, stress, and geometry on EM. For example, Liu et al. used the commercial FEM software package ANSYS and a separate diffusion-convection equation solver to calculate the divergence of atomic vacancy caused by electric, thermal, and stress effects to predict intensity of EM Ref. (17), and similarly, Cacho and his colleagues used Comsol in their work to solve the divergence of atomic vacancy and concluded that the intensity of mechanical effect, or the so called stress migration (SM), is as strong as the EM Ref. (18).

In this work, a new multi-physics computer modeling method is described. This method is based on a tightly coupled solution of all governing equations that describe EM and it offers an integrated numerical solution that can be used to analyze the whole EM process from vacancy diffusion to void formation and void evolution. In the following this method is described. Also in this paper cases of improving microelectronics design are discussed to demonstrate the concept of EM-aware design using Finite Element method.

2. Numerical Simulation Methodology

As mentioned above, EM is caused by the diffusion of ions/atoms in metal conductors. In EM related microelectronics reliable analysis, vacancy concentration C_v , rather than atomic concentration C_a is preferred because it leads directly to void formation in conductors. Therefore, based on Fick's laws of diffusion, the governing diffusion equation for vacancy concentration evolution can be written as:

$$\frac{\partial C_v}{\partial t} + \nabla \cdot \mathbf{J}_v = r \quad (4)$$

where $\mathbf{J}_v$ is the total vacancy flux vector, r is the source/sink term. The vacancy flux vector is shown in Eq. (5) Refs. (1), (17) and (20).

$$\mathbf{J}_v = -D_v \nabla C_v + \frac{|Z^*|e}{kT} D_v C_v \mathbf{E} + \frac{Q^*}{kT^2} D_v C_v \nabla T - \frac{f\Omega}{kT} D_v C_v \nabla \sigma \quad (5)$$

Where

$$D_v = D_0 \exp\left(-\frac{E_a}{kT}\right) \quad (6)$$

and, D_v is the diffusivity of vacancy, Q^* is the heat of transport associated with vacancy transport, f is the vacancy relaxation factor, Ω is the vacancy volume, and D_0 is the pre-exponential factor. In Eq. (5), the terms on the right hand side represent contributions to the total vacancy flux from self-diffusion, electric current, temperature gradient and hydrostatic stress gradient force. The Eq. (4) can also be written as the following convection-diffusion equation:

$$\frac{\partial C_v}{\partial t} + \nabla \cdot (C_v \mathbf{u}) = \nabla \cdot (D_v \nabla C_v) + r \quad (7)$$

where

$$\mathbf{u} = \frac{|Z^*|eD_v}{k} \left(\frac{\mathbf{J}_e}{T}\right) + \frac{Q^*D_v}{kT^2} \left(\frac{\nabla T}{T^2}\right) - \frac{f\Omega D_v}{k} \left(\frac{\nabla \sigma}{T}\right) \quad (8)$$

where $\mathbf{u}$ is called the drift velocity. Eqs. (7) and (8) show that if the distributions of stress, temperature and current density are known, the vacancy distribution equation (Eq. (7)) can be solved numerically as a diffusion-convection problem.

In this work, a multi-physics modeling method has been proposed to solve Eqs. (7) and (8) and to further solve voids formation and propagation in conductors. This method uses unstructured Finite Volume (FV) for diffusion, electric current, and heat transfer and Finite Element Method (FEM) for stress analysis. The electric, thermal, stress and the diffusion transient solvers are coupled sequentially as outlined in Fig. 1. This allows EM to be modeled seamlessly from electric current prediction to void formation. The model has been implemented using the commercial multi-physics software package PHYSICA Ref. (19) which has all the FV and FEM solvers. So far as we know, this fully coupled solution is a new development in EM simulation.

The development of the method is on-going. A 1D EM problem that had been solved by R.L. de Orio and his colleagues analytically Ref. (20) was used as a test case for the method. The simulated vacancy distribution and evolution results agreed very well with the analytical solution Refs. (20) and (21). There is no general analytical solution for Eq. (4). Preliminary work on a 3D Blech structure showed that the simulated atomic flux divergence is consistent with experimental results Ref. (22).

The voids formation and growth capability of the model is being developed. It will be implemented using 'element death' method, i.e. when a pre-assumed vacancy concentration value is reached the element is taken out of the numerical model for current density simulation. This method can be demonstrated using current density based void formation criteria and a simplified solder joint model as follows.

Figure 1 the flow chart of model

The solder joint model is shown in Fig 2. It's a 3D slice model, i.e. in the out of plane direction there is only one layer of elements. The material properties are listed in table 1. A current load of 2 A is applied. For the void formation, it is assumed that voids form when current density exceeds 40000 A/cm^2 .

Figure 2 the structure of a typical solder joint

Material	Density (kg/m ³)	Electrical Resistivity ($\Omega \cdot m$)	Thermal Conductivity (W/m ² *K)	Specific Heat (J/kg*K)
Al	2710	2.61×10^{-8}	240	902
95.5Sn4.0Ag0.5Cu	7390	13.3×10^{-8}	57	219
Cu	8900	1.58×10^{-8}	393	385
Material	CTE (/k)	Elastic Modulus (GPa)	Poisson's Ratio	Effective Charge Number (Z*)
Al	23×10^{-6}	69	0.33	-33
95.5Sn4.0Ag0.5Cu	23×10^{-6}	26.2	0.35	-20
Cu	17.1×10^{-6}	127.7	0.31	-20

Table 1 Materials properties

Fig. 3 shows the current density distribution in part of the solder joint where the maximum current density in solder alloy is located at a corner. Fig. 4 shows the voids and current density at the end of the first step in the simulation. After the first iteration, current density is recalculated and used for void formation in the next iteration step. Figs. 5 and 6 show the shape of voids and current density at the 6 and 18 iterations respectively. This example takes into account the current density only. In the final model where vacancy distribution is used as void formation criteria, void shape may be different because of self-diffusion and other effects (as described in Eq. 4) are taken into account.

Figure 3. the cross section view of the current distribution of a typical solder joint. The unit is A/m².

Figure 4 (a) the voids as the area (red area), and (b) the current density distribution (A/m^2) at the second iteration.

Figure 5 (a) the voids at iteration 6 and (b) the current density distribution.

Figure 6 (a) the voids at iteration 18, and (b) the current density distribution (A/m^2).

3. EM-Aware Design

EM-Aware designs are designs that have taken into account the possible effects of EM and efforts have been made to reduce or prevent EM damage. In this section, we demonstrate and discuss a few examples of EM-aware designs that can be achieved using computer simulation. A current shunt structure to reduce current crowding in and around solder bumps has been analyzed in detail.

3.1 Design Factors

In order to carry out EM-Aware design, it's important to understand the factors that affect EM process. First of all, EM is caused by electric current and therefore current density is very important in EM process. To reduce EM risk, the first thing to do is to avoid excessive current crowding. This can be done through careful design of conductor lay out as demonstrated later in this paper.

The second important factor in EM is the temperature. From Eq. (1), we can see the MTF is exponentially dependent on the temperature. Because the temperature in conductors is determined by the ambient temperature as well as the heat that's generated by electricity (Joule heat), it's closely linked to the current density issue.

The third factor is material selection. Even at the same current density and temperature, different conductors have different levels of tolerance to electric current. For a long time, since Al has low resistivity, excellent adhesion to dielectrics can be easily deposited and can be dry etched, Al-based metallization has been widely used in IC packaging. However, O. Kraft and et al. Refs. (23) - (25) found that Al-Cu alloys can significantly improve the EM resistance because of AlCu alloy's higher activation energy. Similarly, Lee, Hu, and Tu Ref. (26) found that adding Sn can also significantly increase activation energy and reduce EM drift velocity Ref (26).

	Blech Product (A cm⁻¹)	Effective Charge Number, Z*	Activation Energy E_a (eV) (373K - 473K)
Al	244	18	0.6
98Al2Cu	833	5	0.79

Table 2 EM resistance comparison between pure Al and AlCu. The higher Blech product value of AlCu alloy means it has higher EM resistance than pure Al.

This work is focused on the design that minimizes the current crowding and thus minimizes the EM risk caused by excessive current density and temperature increase caused by Joule heat. This design optimization process can be achieved by using numerical analysis method to predict current density for conductors of a range of geometric shapes.

3.2 Current Crowding

To illustrate the effect of geometry on current density distribution, electric current density in cornered copper conductors are modeled. Assuming copper bent structures with material properties in the Table 1 and a loaded 2A current to same contacting area (200μm x 200μm) of bent structures, we get the current density distribution as Fig. 7 and maximum current density reduce from 1.79×10^4 A/cm² (90° angle) to 9.86×10^3 A/cm² (45° angle), and 6.95×10^3 A/cm² (round corner).

Figure 7 the current density (A/m²) distribution of bent structure with different angle.
(a) 90° (b) 135° (c) round corner

The purpose of this work is not an accurate prediction of the variables in the simulation and therefore relative coarse meshes have been used to obtain qualitative results. Fig. 8 shows how the predicted maximum current density in a bent conductor. The material properties of copper in Table 1 are used and it can be seen that the difference in maximum current density is about 7% between the values of the coarsest and the finest meshes.

Figure 8 the current density (A/m) distribution of round bent at different mesh density.
From (a) to (d) the mesh edge length is halved consecutively at each step change.

Tungsten vias are widely used in semiconductor manufacturing. Due to its limited ampacity of each via, an array of tungsten vias are usually used. As shown in Fig. 9, by redistributing the vias, maximum current density can be reduced significantly.

Figure 9 current crowding can be reduced by rearranging tungsten via array.

3.3 Solder Interconnect

Solder alloy has lower resistance to EM than Al or Cu due to its low melting point and therefore lattice diffusion is dominant over grain diffusion and surface diffusion. Higher atom mobility is expected when lattice diffusion is strong Ref. (1). In designing a solder interconnect, solder joint cross section must be large enough so that EM does not cause significant damage. In the situation where solder joint dimensions are restricted, there is the risk that current crowding cause local current density to rise above the threshold for EM to be significant even if the average current density is below the threshold. This is caused by the uneven distribution of current density in solder joint.

In Figs. 2 and 3, current crowding can be seen to occur at solder joint corners. By reducing current density at these current crowding locations, the reliability of solder joints can be improved. Under pure electric loading, the lifetime of solder joint is inversely proportion to the square of current density based on the Black's model Eq. (1).

One of the solutions to resolve the current crowding problem is to divide the current path so that the current enters a solder joint at more than one location. To achieve this, "current shunt" can be used. The current shunt design works by dividing current in a few steps. The more steps are built in, the more evenly distributed the current will be in solder joints. In Fig. 10, an ad hoc solder joint structure is used to demonstrate the current shunt concept and in Fig. 11 current density distributions are shown in solder joints that make use of this technique.

To demonstrate how this design works, we define n as the number of steps the current is divided and $1/2^n$ is the temporal name of the different shunt structures with n steps. In order to make comparison of different shunt structures, the total contact area between the structures and the solder bump is the same for $1/2$, $1/4$, and $1/8$ shunt structure. The thickness of the Al/Cu conductors is kept constant and therefore the width of contacting area at each level, W_n , can be calculated using Eq. (11) from W_{Al} which is the cross section area of the thickest conductor in the $1/2$, $1/4$ and $1/8$ structures. The solder bump in this study has a diameter of 500 μm .

$$W_n = \frac{W_{Al}}{2^n} \quad (11)$$

Figure 10 (a) Basic structure without current division, (b) 1/2 shunt structure, (c) 1/4 shunt structure and (d) 1/8 shunt structure.

Figure 11 top view of the current density distribution in solder joints.

The properties of copper and aluminum are listed in Table 1 and a current of 1.8 A is applied to the solder joints. The current density distributions the solder interconnects are shown in Fig. 11. The maximum current density of the solder bumps is $8.27 \times 10^2 \text{ A/cm}^2$, $3.54 \times 10^2 \text{ A/cm}^2$, $3.5 \times 10^2 \text{ A/cm}^2$, and $3.2 \times 10^2 \text{ A/cm}^2$ respectively. This means that the maximum current density can be reduced by 57.3% if the 1/8 structure is adopted in the design, and this may prolong the solder joint lifetime time by about 5 times according to the Black's model. The reduction in the maximum current density is the results of more even current density distribution as shown in Fig. 12. These results show that the current shunt

design has great potential in reducing current crowding and enhancing solder joint EM resistance.

Figure 12 the top view of the current density (A/m) distributions in solder bump

3.4 Atomic Divergence

In the previous section, current density is used as a measure of EM strength. For more detailed analysis, atomic/vacancy flux divergence can be calculated. The atomic divergence is a measure of mass transport in material and it's directly linked to void formation. Assuming the activation energy $E_a = 0.8$ eV; pre-exponential factor $D_0 = 0.016$ m²/s; heat of transport $Q^* = 0.0094$ eV; heat transfer coefficient 20 W/mK with ambient temperature 293K, vacancy volume $\Omega = 2.48 \times 10^{-29}$ m³/atom. All terms in Eqs. (4) and (5) can be obtained and get atomic divergence from them calculated. In Fig.13, for example, the divergence of the atomic flux caused by electric force, i.e. the second term in Eq. 5, is shown. According to Ref. (16), this is the most important EM. The results in Fig. 13 clearly show the significant impact of current density reduction on the reduction of atomic flux divergence.

Figure 13 Atomic divergence (atoms/m³s) distribution caused by current flow in solder bump at $t = 1000$ s

4. Conclusion

An integrated multi-physics modeling framework that couples diffusion, electric current distribution, heat transfer and mechanical stress as well as void formation and evolution has been developed. The framework is based on the finite volume/finite element software package PHYSICA. Compared to other works in this area, this approach offers a seamless method that can be used to predict failures caused by EM. The framework is still under development. One dimensional result agrees very well with analytical result and a 3D slice model has been used to demonstrate the method capability of capturing the growth of voids caused by EM.

To highlight the importance of virtual design in the designing microelectronics products, a current shunt structure is analyzed to show how current crowding can be reduced by changing the design of conductors leading to solder bumps. The results show that the shunt structure can reduce maximum current density by over 20%.

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