A thermodynamic model for electrical current induced damage

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Abstract

Electromigration-induced damage, which is in principal an irreversible mass diffusion under high current density, has been a concern for VLSI design for a long time. Miniaturization of electronic device sizes down to nano-scale will make electromigration a concern for all conducting components. This paper uses thermodynamics, statistical mechanics and mass transport (diffusion) principals to propose a model for electromigration process and a damage evolution model to quantify the degradation in microelectronics (and micro electromechanical system) solder joints subjected to high current densities. Entropy production in the system is used as a damage metric. The irreversible thermodynamic damage model utilized in this work has previously been successfully applied to thermo-mechanical fatigue of microelectronic solder joints. In this paper we extend this model to electromigration-induced degradation.

Electromigration process is modeled by the atomic vacancy flux (mass diffusion) process. The proposed unified model is compared with several existing analytical and empirical models. A comparison of the damage evolution model proposed in here agrees well with empirical models proposed in the literature.
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Keywords: Electromigration; Damage mechanics; Solder joints; Void growth; Nanomechanics; Diffusion; Nanoelectronics

1. Introduction

1.1. Physics of electromigration process

When a solid conductor is subjected to an electrical potential difference, the current enters from the anode side and travels to cathode side, and the electrons travel from the cathode to the anode side. As a result the degradation of the conductor occurs mainly in two forms, in the anode side the atoms will accumulate and finally form hillocks and the vacancy condensation in the cathode side will form voids. Both hillocks and voids will cause the degradation of the material and eventual failure. The damage evolution due to electromigration can be modeled as an irreversible mass transport process. The purpose of this paper

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is to model the electromigration induced material degradation process in terms of continuum damage mechanics framework using thermodynamics, statistical mechanics and atomic vacancy flux.

Electromigration is a mass diffusion-controlled phenomenon. When a conductor solid is subject to a high current density, the so-called electron-wind transfers part of the momentum to the atoms (or ions) of solid to make the atoms (or ions) move in the direction of the current. The physical mechanism of electromigration has been extensively investigated for pure metal confined thin films [film attached to a thick non-conducting substrate, primarily VLSI lines. Black (1969) established the relationship between the mean time to failure and current density for confined thin films. The experiments by Blech (1976) revealed that the stress gradient could act as a counter force to electromigration under high current density. In addition, for thin films, he proposed a length scale called 'Blech's critical length' below which mass diffusion due to electrical driving force will be totally counter balanced by stress gradient driving force.

From the engineering perspective, the electromigration studies conducted so far have been mostly empirical studies aimed at developing a relationship between the current density and the time to failure (rupture of a thin film) (Black, 1969; Shatzkes and Lloyd, 1986; Korhonen et al., 1993). Several researchers reported their observations of electromigration in solder joints (Zeng and Tu, 2002; Lee et al., 2001; Tang and Shi, 2001; Brandenburg and Yeh, 1998; Liu et al., 1999, 2000; Hu and Harper, 1998; Ye et al., 2002, 2003a,b,c,d,e). These studies are basically experimental observations in Pb/Sn solder alloys with no attempt to model the damage evolution process from computational damage mechanics perspective.

In order to solve an arbitrary boundary value problem with irregular boundaries or initial value problem with arbitrary conditions and composite material properties involving electromigation, there is a need for a mechanics based current density-strain constitutive relation and a continuum damage mechanics based damage evolution model. Then this model can be implemented in a finite element method (or any other computational mechanics procedure). At the present time, such a damage mechanics model does not exist in the reported literature for microelectronics solder joints (Ye et al., 2003b). Relatively little work has been done on continuum damage mechanics of electromigration in solids in general. The state of the art knowledge base in thin film electromigration work is very helpful in providing an insight into the problem, yet there are major differences between a confined pure metal thin film and low melting point solder alloys, such as the state of stress, diffusion mechanism, interaction of phases in an alloy (Ye et al., 2003a,b,c,d). Moreover, the state of stress in a solder joint is three-dimensional versus the two-dimensional case in most VLSI thin films.

The classical definition of electromigration refers to the structural damage caused by ion transport in metal as a result of high current density. Electromigration is usually insignificant at low current density levels. Qualification of what is "high current density" is studied extensively by Ye et al. (2003c) hence it is outside the scope of this paper. Electromigration is a mass transport in a diffusion-controlled process under certain driving forces. The driving force here is more complicated than what is involved in a pure diffusion process, in which the concentration gradient of the moving species is the only component. The electrical driving forces for electromigration consist of the electron-wind force and the direct-field force. The electron-wind force refers to the effect of momentum exchange between the moving electrons and the ionic atoms when an electrical charge—a direct-field force—is applied to a conductor. When current density, which is proportional to the electron flux density, is high enough, this momentum exchange effect becomes significant, resulting in a noticeable mass transport referred to as electromigration. Low melting point alloys when used at elevated homologous temperature ($> 0.5 T_{melt}$) are prone to have considerable atomic diffusivity. Solder joints in microelectronics (and in micro electromechanical systems) are prime examples of this category, where melting point of eutectic Pb37/Sn63 solder alloy is 183C. The nature of electromigration in solder alloys (especially lead free solder alloys) is currently investigated and is expected to be different from that in metal interconnect lines, i.e. Cu and Al (Ye et al., 2003d). This is primarily due to the differences in the materials properties and the microstructures of a typical solder alloy and pure metal VLSI interconnect lines. The fact that there are more than one diffusive species in solder alloy makes the problem

more complex. Based on the first and second laws of thermodynamics, continuum damage mechanics is a good approach to address the electro-mechanical reliability issue of solder joints under electrical stressing since electromigration is an irreversible damage process. Despite the extreme complexity of micromechanics involved, the continuum damage mechanics can serve as a bridge between the microscopic damage process due to electromigration and macroscopic structural response.

1.2. Driving forces of electromigration process

1.2.1. The electric field driving forces
In an electrical field there are two driving mechanisms; one is attributed to the electron-wind force, which refers to the effect of the momentum exchange between the moving electrons and the ionic atoms. On the other hand, the atoms move in the opposite direction of the applied electric field when they are ionized, the latter mechanism is considered the direct-field force. The net effect of these two forces is the so-called electrical field driving force of the electromigration.

1.2.2. Stress gradient
Mechanical stress gradient influences the electromigration process. There is an interaction between the stress gradient and the electromigration driving forces. Stress gradient can counteract or enhance the electromigration process, depending upon the interaction of the stress fields due to boundary conditions and stress fields due to atomic vacancy gradient.

1.2.3. Thermal gradient
The heat generated under high electrical current density is highly localized. Hence, there is a thermal gradient in the medium, which leads to thermo-migration. Thermomigration cannot be ignored especially when the thermal gradient is large, in which case the thermomigration can be the dominant migration process (Ye et al., 2003a).

1.2.4. The atomic vacancy concentration gradient
It has been estimated that, the mass flux due to vacancy concentration gradient is small compared to those induced by electrical field forces, stress gradient and thermal gradient.

2. Modeling electromigration process

Electromigration is an electron flow assisted diffusion process. The process can be assumed to be controlled by a vacancy diffusion mechanism, in which the diffusion takes place by vacancies switching lattice sites with adjacent atoms. In isothermal condition, the process is driven by electrical current caused mass diffusion, stress gradient induced diffusion, and diffusion due atomic vacancy concentration. In the presence of electrical current, due to electrical resistance, there is always heat production that leads to thermomigration, which interacts, with other diffusive forces. Under the presence of these four forces the atomic vacancy flux equation can be given by combining Hungtington (1972) and Kircheim (1992) flux definitions adding the influence of temperature gradient and vacancy concentration yields,

$$\frac{\partial C_v}{\partial t} = -\vec{\nabla} \cdot \vec{q} + G \tag{1}$$

$$\vec{q} = -D_v \left[\vec{\nabla} C_v + \frac{C_v Z^* e}{kT} (-\rho \vec{j}) - \frac{C_v}{kT} (-f\Omega) \vec{\nabla}\sigma + \frac{C_v Q^*}{kT} \frac{\vec{\nabla} T}{T} \right] \tag{2}$$

combined these two equations yield

$$\frac{\partial C_v}{\partial t} = D_v \left[\nabla^2 C_v - \frac{Z^* e\rho}{kT} \vec{\nabla} \cdot (C_v \vec{j}) + \frac{f\Omega}{kT} \vec{\nabla} \cdot (C_v \vec{\nabla}\sigma) + \frac{Q^*}{kT^2} \vec{\nabla}(C_v \nabla T) \right] + G \tag{3}$$

where C_v, vacancy concentration; D_v, vacancy diffusivity; $\vec{q}$, vacancy flux vector; Z^*, vacancy effective charge number; e, electron charge; ρ, metal resistivity; $\vec{j}$, current density vector; f, vacancy relaxation ratio, the ratio of the volume of an atom and the volume of a vacancy; Ω, atomic volume; Q^* heat of transport, the isothermal heat transmitted by moving the atom in the process of jumping a lattice site less the intrinsic enthalpy; k, Boltzman's constant; T, absolute temperature; $\sigma = \text{trace}(\sigma_{ij})/3$, hydrostatic or spherical part of the stress tensor (Sarychev and Zhinikov, 1999); G, vacancy generation rate,

$$G = -\frac{C_v - C_{ve}}{\tau_s} \tag{4a}$$

C_{ev}, thermodynamic equilibrium vacancy concentration

$$C_{ve} = C_{v0} e^{\frac{(-f)\Omega\sigma}{kT}} \tag{4b}$$

C_{v0}, equilibrium vacancy concentration in the absence of stress, τ_s, characteristic vacancy generation/annihilation time.

If we define $C \equiv C_v/C_{v0}$ as the normalized concentration, then the vacancy diffusion equation could be re-written as

$$\frac{\partial C_v}{\partial t} = D_v \left[\nabla^2 C - \frac{Z^* e\rho}{kT} \vec{\nabla} \cdot (C\vec{j}) + \frac{f\Omega}{kT} \vec{\nabla} \cdot (C\vec{\nabla}\sigma) + \frac{Q^*}{kT^2} \vec{\nabla}(C\vec{\nabla}T) \right] + \frac{G}{C_{v0}} \tag{5}$$

where initially, $C = 1$ (or $C_v = C_{v0}$).

The vacancy can be considered as a substitutional species at the lattice site with a smaller relaxed volume than the volume of an atom. When a vacancy switches lattice site with an atom or a vacancy is generated/annihilated at a grain boundary local volumetric strain occurs. Proposed by Sarychev and Zhinikov (1999), the vacancy causes volumetric strain in the metal, because the volume of the vacancy is different than the volume of the atom. This volumetric strain is composed of two parts, ε_{ij}^m, the volumetric strain due to vacancy flux divergence, and ε_{ij}^g, the volumetric strain due to vacancy generation. Since diffusion is a time dependent process, these volumetric strains are naturally expressed in the form of strain rates,

$$\dot{\varepsilon}_{ij}^m = \frac{1}{3} f\Omega \vec{\nabla} \cdot \vec{q} \delta_{ij} \tag{6}$$

$$\dot{\varepsilon}_{ij}^g = \frac{1}{3}(1-f)\Omega G \delta_{ij} \tag{7}$$

where δ_{ij} is the Kronecker's delta.

Thus, the combined volumetric strain rate due to current stressing is

$$\dot{\varepsilon}_{ij}^{elec} = \dot{\varepsilon}_{ij}^m + \dot{\varepsilon}_{ij}^g = \frac{\Omega}{3}[f\vec{\nabla} \cdot \vec{q} + (1-f)G]\delta_{ij} \tag{8}$$

The total volumetric strain rate due to current stressing is then:

$$\dot{\varepsilon}^{elec} = \Omega[f\vec{\nabla} \cdot \vec{q} + (1-f)G] \tag{9}$$

By analogy to thermal strain (which is the volumetric strain caused by temperature variation), the volumetric strain caused by the current stressing is superimposed onto the strains tensor with strains due to other loadings, thus total strain can be given by

$$\varepsilon_{ij}^{total} = \varepsilon_{ij}^{mech} + \varepsilon_{ij}^{therm} + \varepsilon_{ij}^{elec} \tag{10}$$

where $\varepsilon_{ij}^{\text{total}}$ is the total strain tensor, $\varepsilon_{ij}^{\text{mech}}$ is the strain due to mechanical loading, $\varepsilon_{ij}^{\text{therm}}$ is the strain due to thermal load, and $\varepsilon_{ij}^{\text{elec}}$ is the volumetric strain due to electromigration.

2.1. Thermodynamics of damage evolution due to electromigration

Damage, in the context of continuum damage mechanics is defined as the progressive deterioration of materials before final failure. Damage mechanics establishes fundamental principles for prediction of fatigue life of solid structures. In this paper damage nucleation at atomic scale is defined as vacancy generation at a lattice site and it is modeled by formulation given above where vacancy generation and vacancy flux is defined. We cannot model a solder joint (usually 50 μm or less in height for next generation microelectronics) atom by atom in a finite element analysis due to computational limitations. Therefore, atomic scale behavior must be connected with macroscale behavior. The biggest challenge in continuous damage mechanics has always been to find a metric to quantify evolution of degradation at macroscopic scale, which represents initiation of damage at multiple lattice sites at atomic scale. Fortunately, thermodynamics provide us such a tool, Valanis (1997), Basaran and Yan (1998), Basaran and Tang (2003), Basaran and Tang (2002, 2001), Tang and Basaran (2001) and Basaran and Nie (in press) have shown that entropy can be used as damage metric for thermo-mechanical load induced degradation. In this paper this concept is extended to electromigration-induced damage. Traditionally, statistical Weibull function or a damage potential surface is used for modeling the evolution of the damage at the macroscale, even when the void nucleation at the micro level is modeled by dislocation mechanics (Stolkarts et al., 1999). Both Weibull function and damage potential surface require parameters that is difficult to attach any physical characteristic of the material, hence they may be considered as curve fitting approaches, as far as macro level damage evolution modeling is concerned. On the other hand entropy is an intrinsic system state variable and every system (when not in phase transition) must follow the laws of thermodynamics.

Boltzmann (1898), using statistical mechanics gave a precise meaning to disorder and established the connection between disorder and entropy by the following relation:

$$s = k \ln W \tag{11}$$

where s is the entropy of the system, k is the Boltzmann's constant and W is the disorder parameter, which is the probability that the system will exist in the state it is relative to all the possible states it could be in.

The entropy of a unit volume then can be given as

$$s = N_0 k \ln W \tag{12}$$

From the above equation, we can write:

$$W = \mathrm{e}^{s/N_0 k} \tag{13}$$

If we select an initial reference state of the solid body with disorder W_0; then the change in disorder at any arbitrary time with respect to the initial reference state is given by

$$\Delta W = W - W_0 = -(\mathrm{e}^{s_0/N_0 k} - \mathrm{e}^{s/N_0 k}) \tag{14}$$

Let us define a variable D as the ratio of the change in disorder parameter to the original reference state disorder parameter defined as follows:

$$D = D_{\text{cr}} \left(\frac{\Delta W}{W_0} \right) = D_{\text{cr}} \left(1 - \mathrm{e}^{\left(\frac{s_0}{N_0 k} - \frac{s}{N_0 k} \right)} \right) \tag{15}$$

D_{cr} is the critical damage parameter used to define the failure point. It can also be used in a function form to correlate entropy production with specific mechanical property degradation. But in this work it is only used as critical damage parameter.

Expanding the exponent term in this equation to Taylor's series, and ignoring the higher order terms, yields the following simplification:

$$D = D_{cr} \left[1 - e^{\frac{-\Delta s}{N_0 k}} \right] \tag{16}$$

Using principles of continuum damage mechanics Eq. (16) can be implemented in stress–strain relations by Lemaitre and Chaboche (1998)

$$d\sigma = (1 - D)C \, d\varepsilon \tag{17}$$

where $d\sigma$ is the incremental effective stress tensor, C is the tangential material constitutive tensor, and $d\varepsilon$ is the incremental total strain tensor.

According to the hypothesis in Eq. (16) when change in entropy Δs is equal to zero the material is at original state hence D is equal to zero. In this state there is no additional disorder with respect to the original state. When Δs is equal to infinity material must fail according to the second law of thermodynamics and D will be equal to D_{cr}. In reality material fails (or considered to be failed) long before entropy change becomes infinity. In most engineering applications failure point is defined at a stage long before actual collapse of the structure occurs. There is always a factor safety. In traditional damage mechanics D value ranges between zero (at initial state) and one (at final collapse state). Actually failure definition can vary from application to application, owing to the fact that the factor of safety value is different in each engineering application. In Eq. (16) D_{cr} allows defining failure point with respect to the problem at hand.

At this point it should emphasized again that we are not suggesting to use Eq. (16) to use as a criterion for vacancy generation rate or as void nucleation criterion at atomic scale, that is done by the formulation given in the previous section (see Eq. (3)). Eq. (16) only provides an evolution criterion for degradation of the system with respect to the intrinsic state variable entropy, which is defined at macro level. In the finite element formulation entropy is computed at each Gauss point, and the virtual work equation is written for the entire system not for a discreet lattice point, entropy is a variable that bridges micro behavior (atomic flux) with macro response (effective stress). Traditionally Weibul function is used by the dislocation mechanics community e.g. Stolkarts et al. (1999) and damage potential surface is used by the researchers who belong to phenomenological modeling school of thought, e.g. Lemaitre and Chaboche (1998). Based on our laboratory experience (Basaran and Tang, 2001) both Weibull function and damage potential surface are unattractive for engineering use due to extensive testing needed to find the necessary constants. The proposed model does not require a potential surface, there are no curve fitting material parameters involved just the entropy production rate.

At this point we need to answer the fundamental question, which is, does all entropy change contribute to damage? If we inspect the traditional entropy production equation, we can see that entropy change happens in two categories, one is caused by the entropy flowing into the system and the other one is due to the internal entropy production. We may argue that only the internal entropy production leads to degradation of the system, which we call as damage. The relation between entropy production rate and entropy can be given by

$$\Delta s = \int_{t_0}^{t} \gamma \, dt \tag{18}$$

3. Entropy production for an irreversible process

In this section the entropy production rate function will be derived in a way appropriate for implementation in Eq. (18). In this section for the sake of completeness, and clarity, some obvious thermo-

dynamics relations are stated. Including this textbook information in the paper may seem unnecessary, yet we feel it is essential for smooth flow of the paper.

According to the second law of thermodynamics for any macroscopic system the entropy, S, of the system is a state function.

The variation of the entropy, dS, may be written as the sum of two terms

$$dS = dS_e + dS_i \tag{19}$$

where dS_e is the entropy supplied to the system and dS_i is the entropy produced inside the system. The second law of thermodynamics states that dS_i must be equal to zero for reversible and positive for irreversible processes.

$$dS_i \geqslant 0 \tag{20}$$

Classical thermodynamics deals with the reversible process for which the internal entropy production is zero. In the thermodynamics of irreversible processes, the objective is to relate the internal entropy production to the various irreversible phenomena within a solid continuum. For this purpose, we need to establish the local form of entropy, as

$$S = \int_V \rho s \, dV \tag{21}$$

$$\frac{dS_e}{dt} = -\int_\Omega \mathbf{J}_{s,\text{tot}} \cdot d\Omega \tag{22}$$

$$\frac{dS_i}{dt} = \int_V \gamma \, dV \tag{23}$$

where s is the entropy per unit mass, $\mathbf{J}_{s,\text{tot}}$ is the total entropy flow per unit area and unit time, and γ the entropy source strength or entropy production per unit volume per unit time.

Using the local form of entropy, we can get the local form of the variation of entropy as follows:

$$\frac{\partial \rho s}{\partial t} = -\text{div}\mathbf{J}_{s,\text{tot}} + \gamma \tag{24}$$

$$\gamma \geqslant 0 \tag{25}$$

With the help of the material time derivative of the volume integral, which is given by

$$\frac{d}{dt} = \frac{\partial}{\partial t} + v \cdot \text{grad} \tag{26}$$

Eq. (24) can be rewritten in a slightly different form as

$$\rho \frac{ds}{dt} = -\text{div}\mathbf{J}_s + \gamma \tag{27}$$

where the entropy flux, J_s is the difference between the total entropy flux and a convective term:

$$\mathbf{J}_s = \mathbf{J}_{s,\text{tot}} - \rho s \mathbf{v} \tag{28}$$

In obtaining (25) and (27), we have assumed that the definition given by Eqs. (19) and (20) also hold for infinitesimally small parts of the system. This assumption is in agreement with the Boltzmann (1898) relation where the entropy state is related to the disorder parameter via Boltzmann constant using statistical mechanics (Malvern, 1969; Boltzmann, 1898).

4. Entropy balance equations

Based on above definitions, the change in the mechanical properties (such as degradation) of the system can be related to the rate of change of the entropy. This will enable us to obtain more explicit expressions for the entropy flux and internal entropy production rate.

With the assumption of a caloric equation of state, Helmoltz free energy Ψ in differential form can be written as

$$\mathrm{d}\Psi = \mathrm{d}u - T\,\mathrm{d}s - s\,\mathrm{d}T \tag{29}$$

where u is internal energy, T is temperature. (Here we use upper case Ψ to distinguish from the potential ϕ.)

Rearranging leads to

$$T\,\mathrm{d}s = \mathrm{d}u - \mathrm{d}\Psi - s\,\mathrm{d}T \tag{30}$$

in order to get the expression for free energy, we need to specify a function with a scalar value concave with respect to temperature T and convex with respect to other variables. Here we use:

$$\Psi = \Psi(\varepsilon, \varepsilon^e, \varepsilon^p, T, V_k) \tag{31}$$

where V_k can be any internal variable determined by the specific application at hand and physical processes.

In small strain theory, the strain can be written in the form of their additive decomposition

$$\varepsilon - \varepsilon^p = \varepsilon^e \tag{32}$$

so that:

$$\Psi = \Psi((\varepsilon - \varepsilon^p), T, V_k) = \Psi(\varepsilon^e, T, V_k) \tag{33}$$

time derivative of the free energy is given by

$$\frac{\mathrm{d}\Psi}{\mathrm{d}t} = \frac{\partial\Psi}{\partial\varepsilon^e} : \frac{\mathrm{d}\varepsilon^e}{\mathrm{d}t} + \frac{\partial\Psi}{\partial T} : \frac{\mathrm{d}T}{\mathrm{d}t} + \frac{\partial\Psi}{\partial V_k} : \frac{\mathrm{d}V_k}{\mathrm{d}t} \tag{34}$$

From Eq. (30), we obtain:

$$T\frac{\mathrm{d}s}{\mathrm{d}t} = \frac{\mathrm{d}u}{\mathrm{d}t} - \frac{\mathrm{d}\Psi}{\mathrm{d}t} - s\frac{\mathrm{d}T}{\mathrm{d}t} \tag{35}$$

Using the first principle of thermodynamics the conservation of energy equation can be given by Groot (1962)

$$\rho\frac{\mathrm{d}u}{\mathrm{d}t} = -\mathrm{div}\mathbf{J}_q + \sigma : \mathrm{Grad}(\mathbf{v}) + \sum_k \mathbf{J}_k \cdot \mathbf{F}_k \tag{36}$$

u is the total internal energy, $\mathbf{J}_q$ is the heat flux, σ is the stress tensor, v is the rate of deformation, $\mathbf{J}_k$ is the diffusional flux of component k and F_k is the body force acting on the mass of component k.

Using the conservation of energy equation in the form given by Eq. (36) and Eqs. (27) and (28), we can write the rate of change of entropy density as follows:

$$\rho\frac{\mathrm{d}s}{\mathrm{d}t} = \frac{1}{T}\left(-\mathrm{div}\mathbf{J}_q + \sigma : \mathrm{Grad}(\mathbf{v}) + \sum_k \mathbf{J}_k \cdot \mathbf{F}_k - \rho\left(\frac{\partial\Psi}{\partial\varepsilon^e} : \frac{\mathrm{d}\varepsilon^e}{\mathrm{d}t} + \frac{\partial\Psi}{\partial T} : \frac{\mathrm{d}T}{\mathrm{d}t} + \frac{\partial\Psi}{\partial V_k} : \frac{\mathrm{d}V_k}{\mathrm{d}t} - s\frac{\mathrm{d}T}{\mathrm{d}t}\right)\right) \tag{37}$$

where

$$\sigma : \mathrm{Grad}(\mathbf{v}) = \sigma : (\mathbf{D} + \mathbf{W}) \tag{38}$$

and $\mathbf{D}$ (symmetric) and $\mathbf{W}$ (skew symmetric) are the rate of deformation tensor and spin tensor, respectively.

Due to the symmetry of σ

$$\sigma : (D + W) = \sigma : D \tag{39}$$

For small deformation, we can make the following assumption

$$\sigma : \mathbf{D} = \sigma : \frac{d\varepsilon}{dt} = \sigma : \left(\frac{d\varepsilon^e}{dt} + \frac{d\varepsilon^p}{dt} \right) \tag{40}$$

Rearrange Eq. (37) and comparing with (27) we can get $\mathbf{J_s} = \frac{1}{T}\mathbf{J}_q$ and the following entropy production rate term

$$\gamma = -\frac{1}{T^2}\mathbf{J}_q \cdot \mathrm{Grad}(T) + \frac{1}{T}\sum_k \mathbf{J}_k \cdot \mathbf{F}_k + \frac{1}{T}\sigma : \frac{d\varepsilon^p}{dt} + \frac{1}{T}\left(\sigma : \frac{d\varepsilon^e}{dt} - \rho\frac{\partial\Psi}{\partial\varepsilon^e} : \frac{d\varepsilon^e}{dt} \right)$$
$$+ \frac{\rho}{T}\left(s + \frac{\partial\Psi}{\partial T} \right)\frac{dT}{t} - \frac{\rho}{T}\frac{\partial\Psi}{\partial V_k} : \frac{dV_k}{dt} \tag{41}$$

In solids with internal friction all deformations cause positive entropy production rate $\gamma \geqslant 0$. (Which is also referred as the Classius–Duhem inequality, Malvern, 1969.)

Using the following relations,

$$\sigma = \rho(\partial\Psi/\partial\varepsilon^e) \tag{42}$$

$$s = -\frac{\partial\Psi}{\partial T} \tag{43}$$

we can simplify Eq. (41) as follows:

$$\gamma = -\frac{1}{T^2}\mathbf{J}_q \cdot \mathrm{Grad}(T) + \frac{1}{T}\sum_k \mathbf{J}_k \cdot \mathbf{F}_k + \frac{1}{T}\sigma : \dot{\varepsilon}^p - \frac{\rho}{T}\frac{\partial\Psi}{\partial V_k} : \frac{dV_k}{dt} \tag{44}$$

or if the heat flux term $\mathbf{J}_q$ is replaced by

$$\mathbf{J}_q = \frac{1}{T^2}C|\mathrm{Grad}(T)|^2 \tag{45}$$

where is C is the thermal conductivity tensor, the entropy production rate can be given by

$$\gamma = -\frac{1}{T^2}C|\mathrm{Grad}(T)|^2 + \frac{1}{T}\sum_k \mathbf{J}_k \cdot \mathbf{F}_k + \frac{1}{T}\sigma : \dot{\varepsilon}^p - \frac{\rho}{T}\frac{\partial\Psi}{\partial V_k} : \frac{dV_k}{dt} \tag{46}$$

We identify $\mathbf{J}_k$ in Eq. (46) as $\vec{q}$ in Eq. (2) and the effective driving force terms F_k as

$$F_k = \left[Z^*ej\rho + (-f\Omega)\vec{\nabla}\sigma - \frac{Q}{T}\vec{\nabla}T - \frac{kT}{C}\vec{\nabla}C \right] \tag{47}$$

From Eq. (46), we can see that the irreversible dissipation includes two parts, the first term is called heat dissipation caused by conduction inside the system, while the second, third and fourth terms account for other irreversible processes in the system, we will call it intrinsic dissipation.

According to second law of thermodynamics all systems must fail when entropy is at maximum and the production rate is at minimum. Based on this law, entropy production rate given in the form shown in Eq. (46) allows accounting for electromigration-induced entropy production in the system. Because electromigration is an irreversible process and leads to failure of the system, we assume that it must fall within the laws of thermodynamics. Entropy production rate given in Eq. (46) could be written in many different forms, but this form of this equation is the most appropriate for our purpose.

With the help of Eqs. (46) and (47), we can write Eq. (16) as

$$\Delta s = \int_{t_0}^{t} \left(\frac{1}{T^2} C |\text{Grad}(T)|^2 + \frac{C_v D_{\text{effective}}}{kT^2} \left(Z_l^* e\rho j - f\Omega\nabla\sigma + \frac{Q\vec{\nabla}T}{T} + \frac{kT}{C}\vec{\nabla}C \right)^2 + \frac{1}{T}\sigma : \varepsilon^p - \frac{\rho}{T}\frac{\partial\Psi}{\partial V_k} : \frac{dV_k}{dt} \right) dt \tag{48}$$

If we only consider the damage caused by electrical driving forces and disregard other factors such as stress gradient, temperature gradient, atomic vacancy concentration the damage evolution formula can be given by

$$D = D_{\text{cr}} \left[1 - e^{\frac{\int_{t_0}^{t} -\frac{C_v D_{\text{effective}}}{kT^2}(Z^* e\rho j)^2 \, dt}{N_0 k}} \right] \tag{49}$$

If we assume that the solder joint has failed when the degradation reaches some critical value (e.g. it is 5% drop in electrical resistance of a solder joint in the US microelectronics industry), defined as D_{cr}, the time required to reach the failure can be obtained from Eq. (49) as

$$t = \frac{N_0 T^2 k^2}{C_v D_{\text{effective}} (Z^* e\kappa j)^2} \ln\frac{1}{(1 - D_{\text{cr}})} \tag{50}$$

From Eq. (49), we observe that the dependence on temperature is to the power of two. One may wonder why the time to failure is larger when the temperature is larger. The fact is that the diffusivity is going to change with temperature too. The relationship between the temperature and the diffusivity is represented by Arrnhenius function,

$$D_{\text{effective}} = D_0 e^{-\frac{Q}{kT}} \tag{51}$$

Inserting Eq. (51) into Eq. (49), we can get:

$$t = \frac{N_0 T^2 k^2}{N_l D_0 (Z_l^* e\kappa j)^2} \left(\ln\frac{1}{(1 - D_{\text{cr}})} \right) e^{\frac{Q}{kT}} \tag{52}$$

The last term (exponent) dominates the temperature effect so the time to failure decreases with temperature as expected.

4.1. Comparison with other models in the literature

Eq. (52) indicates that damage evolution in electromigration is related to the square of the current density, which was first proposed by Black's test. The Black's (1969) formulation is in the form of

$$t = \frac{wh}{Aj^2} \exp\frac{Q}{kT} \tag{53}$$

where t is mean time to failure, w is the conductor width and h is the film thickness, Q is the activation energy, k is Boltzman constant and T is temperature, and the constant A is related to several factors such as,

(1) the volume resistivity of the metal,
(2) the electron-free time between collisions or the electron free path and average velocity,
(3) the effective ionic scattering cross-section for electrons,
(4) the frequency factor for self diffusion (e.g. aluminum in aluminum).

Shatzkes and Lloyd (1986) starting with following atomic flux assumption equation

$$J = D\left(\frac{Z^*e\kappa j}{kT}C_v - \frac{\partial C_v}{\partial x}\right) \tag{54}$$

For a blocking boundary condition with the assumption of the time to failure is the time to achieve a specific vacancy concentration, they proposed the following time to failure equation:

$$t_f = \frac{2C_f k^2 T^2}{D_0(Z^*e\rho j)^2}e^{\frac{\Delta H}{kT}} \tag{55}$$

For thin films, Korhonen et al. (1993) considered the stress gradient as counter force to electrical field forces, starting with the following atomic flux equation

$$J = \frac{C_v D}{kT}(\nabla(\sigma\Omega) + Z^*(\rho j)) \tag{56}$$

They defined failure as the time to reach a critical hydrostatic stress value, "yield stress" for initiation of a void, for a blocking boundary condition, they proposed the following time to failure equation,

$$t_f = \frac{\pi\Omega kT}{4DB(\rho jZ^*e)^2} \tag{57}$$

where B is applicable modulus, which depends on the elastic properties and the aspect ratio of the cross-section, other variables have the usual meaning as before.

It should be pointed out that these time to failure equations, may be able to predict the time to failure for thin films on thick substrate, yet these empirical equations cannot be used for solution of a boundary value or initial value problem using finite element (or similar) method. Comparing (52) with (55), dependence of the mean time to failure on temperature and current density is the same, the difference is that (55) has a N_f term which is the critical vacancy concentration and while (52) has a critical damage term. In classical continuum damage mechanics the damage variable is defined by Lemaitre and Chaboche (1998)

$$D = \frac{\delta S_d}{S} \tag{58}$$

where δS_d is the void area on the principle surface and S is the original total surface area. If we treat the voids (accumulated atomic vacancies) as damaged area, we can see that the critical damage is related to critical vacancy concentration (assuming that the void nucleation is caused by critical vacancy concentration, Gleixner and Nix, 1996) as it appeared in Eq. (54).

Comparing Eq. (57) with Eq. (52), we can observe that the main difference is that the mean time to failure dependence on temperature is to the first power in Eq. (57). Korhonen et al. (1993) assumed that in confined metal line the lattice site vacancy concentration is related to stress change by the following relation

$$\frac{dC_v}{C_c} = \frac{-d\sigma}{B} \tag{59}$$

According to this relation Korhonen et al. (1993) as the stress reaches the critical value ("yield stress" (as they call it)), the atomic concentration also reaches a critical value and which can then be directly related to the critical damage value (assuming that a critical vacancy concentration value need to be reached for void nucleation). It can be interpreted that critical damage value in the proposed model corresponds to critical vacancy concentration in Shatzkes and Lloyd (1986) model and critical stress in Korhonen et al. (1993) model.

5. Conclusions

Based on thermodynamics, statistical mechanics, continuum damage mechanics and atomic diffusion principals a damage evolution model has been proposed for electromigration-induced damage. The model agrees with Black's empirical model, which was obtained by experimental data where it is shown that the mean time to failure is related to the inverse power of two of the current density. The model also yields time to failure result similar to other mean time to failure models proposed in the literature. In this paper entropy production due to electromigration has been proposed as a damage metric. This concept previously has been shown to be very successful for thermo-mechanical fatigue life predictions. This damage model combined with the strain-electrical current density material constitutive model for solder alloys (developed by Ye et al. (2003e)) can be used for finite element analysis of any electromigration boundary/initial value problem which cannot be done with the empirical mean time to failure models available in the literature. The proposed model can explain the fact that the mean time to failure is related to the inverse power of two of the current density established by Black's test, without any physical assumption imposition. The proposed damage evolution model includes the effect of the electrical field forces, stress gradient effect, vacancy concentration and the thermal gradient. It can be implemented in finite element procedure for solution of boundary and initial value problems involving electrical current to compare with the observed behavior.

Acknowledgements

References

Basaran, C., Nie, S. An irreversible thermodynamic theory for damage mechanics of solids. Int. J. Damage Mech., in press.
Basaran, C., Tang, H., 2002. Implementation of a thermodynamic framework for damage mechanics of solder interconnects in microelectronic packaging. Int. J. Damage Mech. 11 (1), 87–108.
Basaran, C., Tang, H., 2003. A damage mechanics based fatigue life prediction model for solder joints. Trans. ASME, J. Electron. Packaging 125 (March), 120–125.
Basaran, C., Tang, H. Experimental damage mechanics of microelectronics solder joints. J. Damage Mech., in press.
Basaran, C., Yan, C.-Y., 1998. A thermodynamic frame work for damage mechanics of solder joints. Trans. ASME, J. Electron. Packaging 120, 379.
Basaran, C., Tang, C.-Y., 2001. Computer simulations of solder joint reliability tests. Adv. Packaging 1, 17–22.
Black, J.R., 1969. Electromigration failure modes in aluminum metallization for semiconductor devices. Proc. IEEE 57 (9).
Blech, I.A., 1976. Electromigration in thin aluminum films on the titanium nitride. J. Appl. Phys. 47 (4).
Boltzmann, I., 1898. Lectures on Gas Theory. University of California Press, Berkley, CA (Translation by S. Bush, 1964).
Brandenburg, S., Yeh, S., 1998. Electromigration studies of flip chip bump solder joints. In: Surface Mount International Conference Proceedings, 8-23-1998.
Gleixner, R.J., Nix, W.D., 1996. An analysis of void nucleation in passivated interconnect lines due to vacancy condensation and interface contamination. MRS Symp. Proc., p. 428.
Groot, D., 1962. Non Equilibrium Thermodynamics. North-Holland Publishing Company.
Hu, C.-K., Harper, J.M.E., 1998. Copper interconnections and reliability. Mater. Chem. Phys. V 52 (1), 5–16.
Hungtington, H.B., 1972. Electro- and thermomigration in metals. Diffusion Papers Presented at a Seminar of the American Society of Metals, pp. 155–184.
Kircheim, R., 1992. Stress and electromigration in al-lines of integrated-circuits. Acta Metall. Mater. 40 (2), 309–323.
Korhonen, M.A., Borgesen, P., Tu, K.N., Li, C.Y., 1993. Stress evolution due to electromigration in confined metal line. J. Appl. Phys. 73, 3790.
Lee, T.Y., Tu, K.N., Kuo, S.M., Frear, D.R., 2001. Electromigration of eutectic SnPb solder interconnects for flip chip technology. J. Appl. Phys. 89 (6), 3189–3194.

Lemaitre, J., Chaboche, J.-L., 1998. Mechanics of Solid Materials. Cambridge University Press.

Liu, C.Y., Chen, C., Liao, C.N., Tu, K.N., 1999. Microstructure-electromigration correlation in a thin stripe of eutectic SnPb solder stressed between Cu electrodes. Appl. Phys. Lett. 75 (1), 58–60.

Liu, C.Y., Chen, C., Tu, K.N., 2000. Electromigration in Sn–Pb solder strips as a function of alloy composition. J. Appl. Phys. 88 (10), 5703–5709.

Malvern, L., 1969. Introduction to the Mechanics of a Continuous Medium. Prentice Hall.

Sarychev, M.E., Zhinikov, Yu., 1999. General model for mechanical stress evolution during electromigration. J. Appl. Phys. 86 (6), 3068–3075.

Shatzkes, M., Lloyd, J.R., 1986. A model for conductor failure considering diffusion concurrently with electromigration resulting in a current exponent of 2. J. Appl. Phys. 59, 3890.

Stolkarts, V., Keer, L.M., Fine, M.E., 1999. Damage evolution governed by microecrack nucleation with application to the fatigue of 63Sn37Pb solder alloy. J. Mech. Phys. Solids 47 (12), 2451–2468.

Tang, H., Basaran, C., 2001. Influence of microstructure coarsening on thermomechanical fatigue behavior of Pb/Sn eutectic solder joints. Int. J. Damage Mech. 10, 1–14.

Tang, Z., Shi, F.G., 2001. Stochastic simulation of electromigration failure of flip chip solder bumps. Microelectron. J. 32 (1), 53–60.

Valanis, K.C., 1997. Some thoughts on thermodynamics of internal variables. Arch. Mech. 49 (2), 443–445.

Ye, H., Lin, M., Basaran, C., 2002. Failure modes and FEM analysis of power electronic packaging. J. Finite Elem. Anal. Des. 38 (7), 601–612.

Ye, H., Basaran, C., Hopkins, D., 2003a. Thermomigration in Pb–Sn solder joints under Joule heating during electric current stressing. Appl. Phys. Lett. 82 (8).

Ye, H., Basaran, C., Hopkins, D., 2003b. Damage mechanics of microelectronics solder joints under high current densities. Int. J. Solids Struct. 40 (15), 4021–4032.

Ye, H., Basaran, C., Hopkins, D., 2003c. Measurement of high electrical current density effects in solder joints. J. Microelectron. Reliability, in press.

Ye, H., Basaran, C., Hopkins, D., 2003d. Mechanical degradation of solder joints under current stressing. Int. J. Solids Struct., in press.

Ye, H., Basaran, C., Hopkins, D., 2003e. Numerical simulation of stress evolution during electromigration in IC interconnet lines. IEEE Trans. Components Packaging Technol., in press.

Zeng, K., Tu, K.N., 2002. Six cases of reliability study of Pb-free solder joints in electronic packaging technology. Mater. Sci. Eng. 38 (2), 55–105.