

A unified model of mean-time-to-failure for electromigration, thermomigration, and stress-migration based on entropy production

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Abstract: We have revisited Black's equation of mean-time-to-failure (MTTF) for electromigration from the viewpoint that in irreversible processes, entropy production is the controlling behavior. We justify that the power factor on current density is $n = 2$, as given in the original Black's equation. Furthermore, on the basis of entropy production, we provide a unified model of MTTF for thermomigration and stress-migration. We note that up to now, no MTTF for thermomigration and stress-migration are given.

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I. Introduction

As we enter the big data era, 5G communication technology and artificial intelligence (AI) applications are ubiquitous due to the use of mobile internets and devices. The continuing demand in mobile devices for smaller size, more functionality, lower power consumption, and reduced cost is challenging, because Moore's law of miniaturization in Si technology is ending. Actually, a paradigm change, from 2-dimensional integrated circuits (2D IC) to 3D IC, has occurred in microelectronics industry for more than ten years. Yet, the transition to 3D IC has not been successful due to high cost and low reliability. [1 - 3] Currently, the use of 5G technology in AI applications has provided the impetus to promote 2.5D IC, instead of 3D IC, into mass production. Reliability has become a critical issue.

Owing to the strong attraction of the huge market in 5G + AI applications, some microelectronic companies tend to push out their 2.5D IC device in mass production without a detailed study of reliability. Compare to 2D IC devices, the adding of a Si interposer in 2.5D IC devices requires one more redistribution layer (RDL) and one more level of solder joints due to use of vertical interconnects. It has been shown that if the new RDL was not designed properly, it becomes the weak-link in the system and fails quickly. [4, 5] On the other hand, if we strengthen the RDL, relatively speaking, we just move the weak-link in the interconnect system from RDL to other interconnect units such as micro-bumps.

In the past, when we study electromigration in Al or Cu lines, we may care about stress-migration because of back-stress, [6] but not thermomigration. This is because Soret effect occurs in alloys. Thus, we have to wait until the wide applications of flip chip C-4 (control-collapse-chip-connection) solder joint, which is an alloy, and also when its reliability became an issue, the study of thermomigration

began. [7] Across a C-4 solder joint of 100 μm in diameter, if there is a temperature difference of 10 $^{\circ}\text{C}$, the temperature gradient is 1000 $^{\circ}\text{C}/\text{cm}$, which enables thermomigration to occur.

In the dense 2.5D IC packaging, not only Joule heating is serious, but also heat dissipation is poor. To enhance heat dissipation, we need to have a high temperature gradient. Unfortunately, the gradient can lead to thermomigration. This is especially true in small structures; for a micro-bump of 10 μm in diameter, if there is a temperature difference of only 1 $^{\circ}\text{C}$ across it, the temperature gradient is 1000 $^{\circ}\text{C}/\text{cm}$. Furthermore, the use of Si interposer enhances the lateral heat transfer along the interposer, and it has caused an unexpected thermomigration failure. [8]

To analyze thermomigration failures, however, we found that there is no analysis of mean-time-to-failure (MTTF) for thermomigration, nor for stress-migration too. In electromigration, Black's equation of MTTF is well established. [9] The goal of this paper is to find a common theme of failure analysis, so that we can have a unified model of MTTF for all three of them. To do so, we have based on entropy production in irreversible processes as the common theme. What is very interesting is that the exponential parameter of $n = 2$ on current density in Black's equation can be justified, which has been a controversial issue for a long time! [10-16]

Actually, the exponent $n = 2$ was obtained in the paper of Shatkez and Lloyd [11] which was an important step in the analysis of electromigration-induced failures. Yet, their model was based on the unrealistic assumption of vacancy electromigration without vacancy sinks and sources. Authors of Ref. [11] solved the equation of vacancy redistribution under electromigration in semi-infinite line with blocking boundary (zero flux) without vacancy sinks in the line and at the boundary. Failure criterion in this paper was taken as reaching some critical value of vacancy concentration at the blocking boundary. This approach was later significantly changed

and improved (by simultaneous account of vacancy sinks and stresses) in the papers by Kirchheim, etal [12] and by Korhonen, etal [13].

II. A unified model of MTTF for electromigration, thermigration, and stress-migration

II.A Revisit Black's equation of MTTF for electromigration

On studying electromigration, we can vary time, temperature, and the applied current density. Black's equation of MTTF for electromigration has been given as,

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

where the time (MTTF) is related to temperature and current density by three parameters; the pre-factor A, the current density power factor $n = 2$, and the activation energy E_a . The factor E_a is the activation energy of atomic diffusion in electromigration.

Conventionally, let J be the atomic flux driven by electromigration, we have

$$J = C \frac{D}{kT} Z^* e \rho j \quad (2)$$

where C is concentration; $D = D_0 \exp(-E_a/kT)$ is atomic diffusivity and for electromigration in Cu interconnects at the device operation temperature near 100 °C, it is surface diffusion, and D_0 is pre-factor; E_a is activation energy; kT is thermal energy; and the driving force is $Z^* e \rho j$, where Z^* is effective charge number; e is charge; ρ is resistivity; and j is applied current density. [17]

Eq. (2) is a simplification because the atomic flux contains, in addition to the gradient of electric potential, also the gradients of stress and concentration. A

general model for mechanical stress evolution during electromigration has been considered by Nix, et al. [15]

To understand the physics better, we try to distinguish processes, in which electromigration, thermomigration, or stress-migration may play the major role. Of course, sometimes such distinguishing becomes impossible. For example, in Nabarro-Herring explanation of Blech experiment for critical products of current density and length, the total atomic (and vacancy) flux (consisting from electromigration and stress migration parts) becomes zero, meaning also zero entropy production (except Joule heating compensated by heat out-flux). However, we only try to discuss our subject in the simplest cases below.

Now, let V^* be the critical volume of the void formation at the cathode end, which has led to opening failure, we have $V^* = \Omega J A t$, where Ω is atomic volume, A is the cross-section of the diffusion, and t (or MTTF) is time to failure, so

$$t = V^*/\Omega A J. \quad (3)$$

The above equation shows that MTTF is proportional to $1/j$, thus $n = 1$.

To revisit Black's equation, we consider entropy production in irreversible processes. [18, 19] The link between entropy production and microstructure change under mechanical damage has been given. [20] According to Onsager, the entropy production rate is given as,

$$\frac{TdS}{Vdt} = JX \quad (4)$$

where T is temperature, dS/dt is rate of entropy production, V is volume of the test

sample, and J and X are the conjugated flux and driving force, respectively.

In general, the entropy production is a sum of all products of driving forces and corresponding fluxes. In this paper we try to consider different terms one by one, under appropriate external conditions. There are atomic flux, heat flux, and charge flux in irreversible processes. In electromigration, which is a cross-effect between charge flux and atomic flux, J has been given by Eq. (2), and $X = Z^*eE = Z^*ej$, where $E = -d\phi/dx = \rho j$ is electric field.

Now, we consider entropy production during electromigration. We treat MTTF as a time to accumulate some threshold entropy, $S_{\text{threshold}}$. At that, we take into account the entropy produced by electron flow (Joule heating) is evacuated by the heat out-flux. Thus, we may assume that the accumulation of entropy proceeds via electromigration of atoms. We exclude entropy production by Joule heating, from the entropy balance. A detailed analysis of entropy production will be given in Section III on Discussions. So far, let us exclude also thermomigration and stress-migration. The total entropy production until failure is

$$J_e X_e t^{\text{failure}} = TS_{\text{threshold}}/V \quad (5)$$

$$\text{MTTF} \approx t^{\text{failure}} = \frac{TS_{\text{threshold}}}{VJ_e X_e} = A' \frac{1}{j^2} \frac{1}{D} = Aj^{-2} \exp\left(\frac{E_a}{kT}\right) \quad (6)$$

which is Black's equation and it means that $n = 2$ is justified. We use Wilbull's distribution to obtain the MTTF where 50% failure occurs.

On the other hand, if we consider Joule heating in electrical conduction, it is

$$\frac{TdS}{Vdt} = j\left[-\frac{d\phi}{dx}\right] = jE = j^2\rho \quad (7)$$

where $j^2\rho$ is “joule heating” per unit volume per unit time. Its unit is energy/cm³-sec.

In Eq. (4), we note that entropy production cannot be in a steady state. While the applied current can be steady or the rate of charges being transported is constant, the entropy production increases, so the temperature without heat dissipation will rise. To reach a steady state, the system needs an outgoing heat flux of $J_Q = j^2\rho$, which simultaneously will be accompanied by the outgoing entropy fluxes of J_Q/T .

Usually, the power of joule heating is written as

$$P = I^2R = j^2\rho V \quad (8)$$

where I is applied current and $I/A = j$, and A is the cross-sectional area of the sample, R is resistance of the sample and $R = \rho A/l$, and l is the length of the sample, so the volume of sample $V = Al$. Thus, I^2R is Joule heating per unit time (power = energy/time) of the entire sample, and $j^2\rho$ is Joule heating per unit volume per unit time of the sample. What is shown in the above is that j^2 is intrinsic in entropy production in electrical conduction as well as in electromigration.

To make a comparison of entropy production between electrical conduction and electromigration, we consider an Al interconnect. If we take $j = 10^6$ A/cm² and $\rho = 10^{-6}$ Ω-cm for Al, the Joule heating in electrical conduction is,

$$\frac{TdS}{Vdt} = jE = \rho j^2 = 10^6 \frac{\text{joule}}{\text{cm}^3 \text{ sec}}$$

For electromigration in Al interconnect, we have

$$\frac{TdS}{Vdt} = JX = \left(C \frac{D}{kT} F\right) F = C \frac{D}{kT} (Z^* e \rho j)^2 \quad (9)$$

We take $C = 10^{23} / \text{cm}^3$, $T = 400 \text{ K}$, $D = 10^{-16} \text{ cm}^2/\text{sec}$, $Z^* e = 10^{-18} \text{ coulomb}$, $\rho = 10^{-6} \Omega\text{-cm}$, and $j = 10^6 \text{ A/cm}^2$. Substituting these data into Eq. (9), we obtain

$$\frac{TdS}{Vdt} = \frac{10^{-29} \text{ joule}^2}{(0.033 \text{ eV}) \text{ cm}^3 \text{ sec}} = 2 \times 10^{-9} \frac{\text{joule}}{\text{cm}^3 \text{ sec}}$$

where $kT = 0.033 \text{ eV}$ at $T = 400 \text{ K}$, and $1 \text{ joule} = 6.24 \times 10^{18} \text{ eV}$. Clearly, the Joule heating due to electrical conduction is much larger.

II.B MTTF for thermomigration

Similar to the above, the major entropy production in thermomigration is due to heat propagation under a temperature gradient, [21]

$$\frac{TdS}{Vdt} = \left(-\kappa \frac{dT}{dx}\right) \left(-\frac{1}{T} \frac{dT}{dx}\right) \quad (10)$$

If we take heat conduction in solder as $\kappa \approx 50 \text{ J/msK}$, $dT/dt = 1000 \text{ K/cm}$, and $T = 400 \text{ K}$, we obtain $TdS/Vdt = 1.2 \times 10^9 \text{ J/m}^3\text{sec}$.

On thermomigration, we have,

$$\frac{TdS}{Vdt} = \left(C \frac{D}{kT} X_h\right) X_h = C \frac{D}{kT} \left(3k \frac{dT}{dx}\right)^2 \quad (11)$$

where we have roughly taken the conjugated driving force $X_h = 3k (dT/dx)$, where k is Boltzmann's constant, and $3kT$ is local thermal energy per atom, and by taking dT/dx

= 1000 K/cm, we obtain $TdS/Vdt = 3 \times 10^{-6} \text{ J/m}^3\text{sec}$. which is much smaller than that due to heat conduction. To calculate the MTTF of thermomigration, we take the atomic flux in themomigration to be,

$$J_h = C \frac{D}{kT} \frac{Q^*}{T} \left(-\frac{\partial T}{\partial x}\right) \quad (12)$$

where Q^* is defined as heat of transport in thermomigration and Q^* has the same dimension as μ , so it is the heat energy per atom. The conjugated driving force is,

$$X_h = \frac{Q^*}{T} \left(-\frac{dT}{dx}\right) \quad (13)$$

Thus, we have $J_h X_h t^{\text{failure}} = TS_{\text{threshold}}/V$

$$MTTF \approx t^{\text{failure}} = \frac{TS_{\text{threshold}}}{VJ_h X_h} = B \left(-\frac{dT}{dx}\right)^{-2} \exp\left(\frac{E_a}{kT}\right) \quad (14)$$

where B is a constant.

II.C MTTF for stress-migration

Conceptually, there is a fundamental difference between stress-migration and electromigration or thermomigration. The latter are cross-effects on the basis of irreversible processes. This is because the atomic flow in electromigration or thermomigration is accompanied by electron flow or heat flow, respectively. Yet, there is no “stress flow” accompanying the atomic flow in stress-migration, especially if we assume elastic stress. Stress-migration is a primary flow of atoms, driven by stress potential gradient, which is a chemical potential gradient. Often,

stress-migration is called a steady state diffusional creep. [22, 23]

Stress potential is defined as $\sigma \Omega$, where σ is stress and Ω is atomic volume.

Thus, the driving force of stress-migration is given as,

$$X_s = \frac{d\sigma\Omega}{dx} \quad (15)$$

and the atomic flux in stress-migration is given as,

$$J_s = CMF = C \frac{D}{kT} \left(\frac{d\sigma\Omega}{dx} \right) = \frac{D}{kT} \left(\frac{d\sigma}{dx} \right) \quad (16)$$

We have $J_s X_s t^{\text{failure}} = TS_{\text{threshold}}/V$

$$MTTF \approx t^{\text{failure}} = \frac{TS_{\text{threshold}}}{VJ_s X_s} = G \left(\frac{d\sigma}{dx} \right)^{-2} \exp\left(\frac{E_a}{kT}\right) \quad (17)$$

Where G is a constant.

III. Discussions

III.A A comparison of driving forces among electromigration, thermomigration, and stress-migration

Here, we make a comparison among the driving forces of electromigration, thermomigration, and stress-migration in solder. Specially, the growth of Sn whisker under a compressive stress is used to evaluate stress-migration because synchrotron radiation measurement has been done.

We first consider electromigration. It occurs in Sn-based solder joints when the applied current density is above 10^4 A/cm² or 10^8 A/m² at temperatures above

100 °C. The driving force is $X_e = Z^*eE = Z^*ej$. For calculation, we take $Z^* = 10$, $e = 1.6 \times 10^{-19}$ comb, $\rho = 10 \times 10^{-8} \Omega\text{m}$, and $j = 1 \times 10^8 \text{ A/m}^2$, we obtain $F = 1.6 \times 10^{-17} \text{ N}$. The work done by an atomic jump distance driven by this force will be

$$\Delta w = X_e \times a = (1.6 \times 10^{-17} \text{ N})(3 \times 10^{-10} \text{ m}) = 4.8 \times 10^{-27} \text{ Nm} = 4.8 \times 10^{-27} \text{ J}$$

Next, we consider thermomigration in solder joint under a temperature gradient of 1000 °C/cm near 100 °C. Across an atom of diameter of $3 \times 10^{-8} \text{ cm}$, the ΔT due to the temperature gradient of 1000 °C/cm is about $3 \times 10^{-5} \text{ K}$. The change of thermal energy across an atom is

$$3k\Delta T = 3 \times 1.38 \times 10^{-23} \text{ (J/K)} \times 3 \times 10^{-5} \text{ K} = 1.3 \times 10^{-27} \text{ J}$$

which is of the same order of magnitude as the work done under electromigration given in the above.

Finally, we consider stress-migration by calculating the driving force of Sn whisker growth. The driving force $X_s = -d\sigma\Omega/dx$, where σ is normal stress and Ω is atomic volume. The stress distribution around the root of a Sn whisker has been measured by x-ray diffraction using synchrotron radiation, as shown in [Table I in Ref. \[23\]](#). We estimate the stress gradient between the origin ($x = 0, y = 0$) and the lower left corner point at ($x = -0.5400, y = 0.8475$), where $\Delta x \approx 10 \mu\text{m}$ and $\Delta\sigma \approx 4 \text{ MPa}$, and we take the atomic volume of Sn atom to be $27 \times 10^{-24} \text{ cm}^3$. The force is given below,

$$\begin{aligned} X_s &= -\frac{\Delta\sigma\Omega}{\Delta x} = \frac{4 \times 10^6 \text{ (N/m}^2\text{)} \times 27 \times 10^{-24} \text{ (cm}^3\text{)}}{10^{-3} \text{ (cm)}} = \frac{4 \times 10^7 \text{ (dyne/cm}^2\text{)} \times 27 \times 10^{-24} \text{ (cm}^3\text{)}}{10^{-3} \text{ cm}} \\ &= \frac{108 \times 10^{-17} \text{ erg}}{10^{-3} \text{ cm}} \approx 10^{-12} \text{ erg/cm} \end{aligned}$$

The work done by this force over a distance of atomic diameter of 0.3 nm is 3×10^{-27} joule, which is of the same order of magnitude of those calculated in the above for electromigration and thermomigration. It is worth mentioning that in Ref. [23], while the stress distribution was measured, but no calculation of the driving force was given at that time because of no comparison!

The above calculations show that the conjugated forces of electromigration, thermomigration, and stress-migration in Sn or Sn-rich solder are nearly the same. This provides the justification of the following analysis of MTTF of three of them by equating their driving forces.

$$Z^* e \rho j = 3k \frac{dT}{dx} = - \frac{d\sigma\Omega}{dx}$$

Thus, we have

$$j = \frac{3k}{Z^* e \rho} \frac{dT}{dx} = \frac{-1}{Z^* e \rho} \frac{d\sigma\Omega}{dx}$$

Then, by substituting j^2 into the original Black' equation, we obtain MTTF for thermomigration and stress-migration below. For thermomigration, we obtain

$$MTTF_h = A \left(\frac{3k}{Z^* e \rho} \frac{dT}{dx} \right)^{-2} \exp\left(\frac{E_a}{kT}\right) \quad (18)$$

And for stress-migration, we obtain,

$$MTTF_s = A \left(\frac{1}{Z^* e \rho} \frac{d\sigma\Omega}{dx} \right)^{-2} \exp\left(\frac{E_a}{kT}\right) \quad (19)$$

III.B Link between entropy production and microstructure failure

It is important to provide a receipt for predicting the threshold entropy corresponding to failure. In general, it is a very complicated problem because failure have various mechanisms (modes). In this paper we limit ourselves with the case of voiding formation at the cathode end in electromigration, as a mechanism of failure.

To nucleate and grow the void, the cathode end should have accumulated a sufficient amount of non-equilibrium vacancies. If the super-saturation by vacancies is not large, the accumulation of extra vacancies of N_v increases entropy by $N_v \cdot E_v / T$, where E_v is the formation energy of a vacancy. Then, equilibrium of vacancy subsystem means zero derivative of Gibbs free energy:

$$\frac{d}{dN_v} (N_v H_v - TS(N_v)) = 0 = H_v - T \frac{dS}{dN_v} \Rightarrow \frac{dS}{dN_v} = \frac{H_v}{T} \quad (20)$$

Thus, the adding of one vacancy to the almost equilibrium system means the adding of additional entropy equal to enthalpy of vacancy formation divided by temperature. In usual conditions of small pressures (typically less than gyga-pascal) the vacancy formation enthalpy is close to vacancy formation energy, so that

$$\Delta S \approx \Delta N_v^{extra} \frac{E_v}{T} \quad (21)$$

Sooner or later these extra vacancies will unite into the void or crack stopping the current and leading to failure. To stop the current completely, the void should have

cross-section A of the interconnect and at the least the thickness of $\delta \approx 0.2 \text{ nm}$. Then the threshold entropy may be very roughly approximated as

$$S^{threshold} \approx \frac{A \cdot \delta E_V}{\Omega T} \quad (22)$$

The rate of entropy production is

$$\begin{aligned} T \frac{dS}{V dt} &= \frac{CD}{kT} (Ze\rho j)^2 \approx \\ &\approx \frac{10^{29} \left(\frac{1}{m^3}\right) 10^{-20} \left(\frac{m^2}{s}\right)}{0.4 \cdot 1.38 \cdot 10^{-20} \text{ (Joule)}} \left(10^{-18} \text{ (coulomb)} \cdot 10^{-8} \text{ (\Omega m} \cdot \text{m)} \cdot 10^{10} \left(\frac{A}{m^2}\right)\right)^2 \approx 1.8 \cdot 10^{-3} \frac{\text{Joule}}{m^3 s} \end{aligned}$$

Then we may evaluate the MTTF from Eq. (6),

$$\left(\frac{CD}{kT} (Ze\rho j)^2\right) \cdot A \cdot l \cdot MTTF \approx TS^{threshold} = T \frac{A \cdot \delta E_V}{\Omega T} = \frac{A \cdot \delta E_V}{\Omega} ,$$

$$MTTF = \frac{\delta E_V}{\Omega \left[\frac{CD}{kT} (Ze\rho j)^2\right]} \approx \frac{2 \times 10^{-10} \times 1.6 \times 10^{-19}}{10^{-29} \times 10^{-5} \times 1.8 \times 10^{-3}} = 1.9 \times 10^8 \text{ sec} \approx 6 \text{ years}$$

Here $A \cdot l$ is the volume of the line, and l is the length of the line, which we take it to be about $10 \mu\text{m}$. No doubt, the accumulation of N_v extra vacancies will increase entropy by $N_v \cdot E_v / T$, but the gathering of these vacancies into void or going out from the crystal will decrease entropy by the same magnitude.

Thus, the accumulation of non-equilibrium vacancies indeed is related to entropy production, but their transformation into a void means a drop of entropy after increase.

According to Gleixner et al [24] voids may nucleate not due to the accumulation of vacancies but due to mechanical stress. But it makes prediction not of failure but of void nucleation at the interfaces. For failure, the nuclei of the void should develop and grow and/or migrate, and for this, void needs supply of vacancies. Moreover, as shown in [25-27] failure can be the result of the electromigration of previously formed interface nano-voids along the interface metal/dielectric and their accumulation at the cathode end. It proves that the transport of empty space is at least one of the main reasons of failure.

IV. Summary

Black's equation of mean-time-to-failure (MTTF) for electromigration has been revisited from the viewpoint based on entropy production in irreversible processes. We have justified that the power factor on current density is $n = 2$, which has been a controversial issue for a long time. Furthermore, on the basis of entropy production, we provide a unified model of MTTF for thermomigration and stress-migration.

In general, input of all sources of entropy production should be taken into account simultaneously – each of such inputs can lead to earlier arriving of the entropy threshold, and decreasing of MTTF. Decreasing of MTTF due to thermal gradients was experimentally found in [28]. We use the accumulated entropy as a parameter of failing of the device, in turn as the link between MTTF and threshold entropy.

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