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NEW THERMODYNAMIC APPROACHES TO FAILURE ANALYSIS IN MICROELECTRONIC MATERIALS

Failure of the microelectronic device may be treated in the frame of non-equilibrium thermodynamics applied to open systems under the condition of incompatibility of steady states for different processes. The criterion of failure can be related to some threshold amount of the structural entropy produced and accumulated in the system by the external forces. This hypothesis provides a simple interpretation of the empirical Black equation for the mean time to failure in the case of electromigration, and helps to predict similar equations for the cases of thermo- and stress migration. The failure itself can be treated as a phase/structure transformation in the open system and described by kinetics similar to Kolmogorov-Avrami kinetics of the first-order phase transformations.

Keywords: entropy production, vacancies, voids, failure, open system, flux, diffusion.

1. Introduction.

Failure of any concrete microelectronic device is a stochastic event and, as a rule, cannot be predicted deterministically, but the mean time to failure and even distribution of times to failure can be predicted with good accuracy. Actually, this is the main task of reliability theory [1-4]. This paper will be about some fundamental, even philosophical aspects of reliability. The key issues and questions of our thermodynamic approach to failure are:

1. Interconnect or solder joint is an open system under the heterogeneous external (boundary) conditions producing the thermal and structural entropy
2. Failure is a result of incompatibility of steady-state for different non-equilibrium processes.
3. Failure is a result of the accumulation of some threshold structural entropy
4. Failure is a kind of phase transition, including nucleation, growth, and ripening, but all this in open heterogeneous systems.
5. All living creatures are mortal. All microelectronic devices are also, most probably, mortal. Is it possible to make an immortal interconnect?

Let us remind shortly some fundamentals of thermodynamics of the closed and open systems. Our definitions of closed and open systems are similar to but not coinciding with traditional descriptions. This is summarized in Table 1.

If a system is isolated and in a non-equilibrium state, it may have various evolution paths to equilibrium (Fig. 1). What is the criteria of choice among these paths - is not known for sure, but many people believe that the most probable evolution path corresponds to the maximal entropy production rate among all possible paths. The final state of an isolated system (if one forgets about fluctuations) corresponds to maximum entropy and it is a second law of thermodynamics.

If a system is surrounded by (and in good thermal contact with) a thermal bath with uniform fixed temperature and fixed volume, it may have also various evolution paths to equilibrium. What is the criteria of choice among these paths - is also not known for sure, but many people believe that the most probable evolution path corresponds to the maximal rate $(-\frac{dF}{dt})$ of the Helmholtz free energy F=U-TS decrease among all possible paths. The final state of the system in thermal bath and with constant volume corresponds to minimum Helmholtz free energy. It is a well-proved consequence of the second law of thermodynamics.

If, instead of volume, the pressure is fixed (which is typical for condensed phases), the final state is characterized by the minimum of Gibbs free energy G=U-TS+pV, and many people believe that the choice of evolution path corresponds to the maximum release rate of Gibbs free energy, $(-\frac{dG}{dt})$.
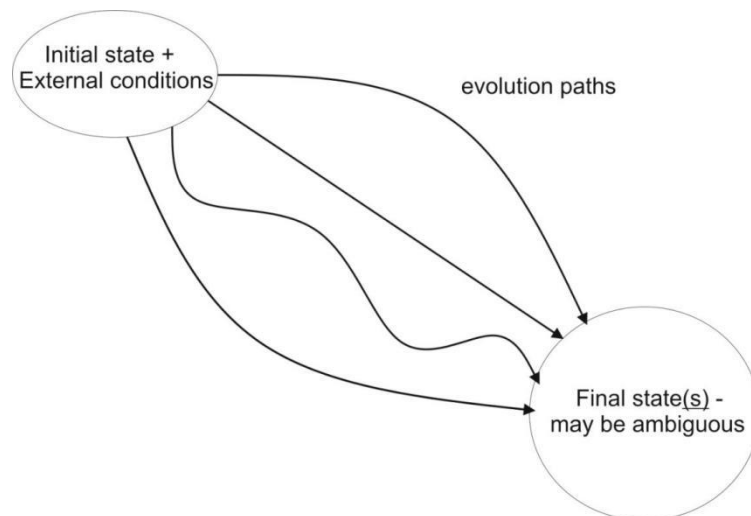

Fig. 1. Illustration of multiple evolution paths.
Рис. 1. Ілюстрація неоднозначності шляхів еволюції

Table 1
Таблиця 1

Evolution paths and final state of the closed and open systems
Шляхи еволюції та кінцевий стан закритих і відкритих систем

Initial state + External conditions		Choice of evolution path and level of understanding	Final state and level of understanding
Closed system	Isolated	Maybe, $\frac{dS}{dt} = max$, but it is not proved	S->max -second law of thermodynamics

	In homogeneous thermal bath, T=const, V=const	Maybe ($-\frac{dF}{dt} = max$) or maybe transformation velocity =max or…?	F=U-TS-> min checked and proved
	In the homogeneous thermal bath, T=const, p=const	Maybe($-\frac{dG}{dt} = max$) or maybe transformation velocity =max or…?	G=U-TS+pV-> min checked and proved
Open system	Under gradient of electric potential with constant conductivity	Not very well studied but taking a small time interval	Steady-state, characterized by a minimum of entropy production, $\frac{dS_{total}}{dt} = min$
	Under gradient of temperature with constant heat conductivity	Temperature redistribution according to heat diffusion parabolic equation	Steady-state, characterized by a minimum of entropy production, $\frac{dS_{total}}{dt} = min$
	Under gradient of electric potential inducing the electron wind effect	Electron wind effect induces electro-migration, and corresponding redistribution of atoms, vacancies. Also, electro-migration induces stresses and corresponding stress migration. Also, current induces nonuniform Joule heating and corresponding temperature gradients which induce the thermomigration.	Failure - formally, also "steady-state" effect but with effective conductivity tending to zero, $j_{el} = 0$

2. Evolution of open systems
2.1. Open system - one parameter - one steady-state process is approached
Now we come to an open system. We will treat as an open system any system, which finds itself in the heterogeneous or/and time-dependent external (boundary) conditions which means global gradients of temperature or electric potential, chemical potential, or any flux over the system. In this sense, maybe it would be better to call such a system "driven" as Georges Martin from Nuclear Centre Saclay in France used to call it. Yet, we will keep the more general term "open system".

For us, the system is open if its boundary conditions are incompatible with reaching the equilibrium. If we keep the different electric potentials in different points of the conducting

system, the equilibrium is not possible because the current will always pass between boundaries with different potentials, unless the effective conductivity will decrease to zero due to a large void or crack (and it means failure) (Fig. 2). **Instead of equilibrium, the system may reach the steady state**: non-zero fluxes but zero time derivatives. Simple mathematics shows that, if conductivity is constant, then the steady state corresponds to the globally minimal entropy production among all possible distributions of electric potential and current, compatible with boundary conditions for potential.
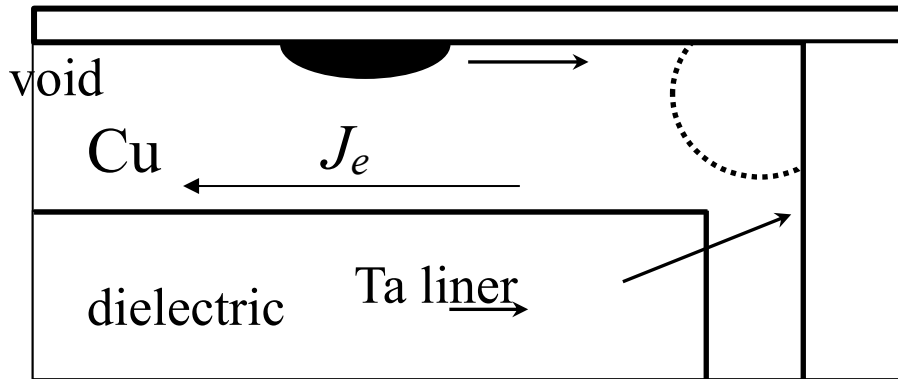

Fig. 2. Failure mechanism - migration of void under electron wind along the interface metal/dielectric towards via

Рис. 2. Механізм відмови - міграція пори до перехідного з'єднання під дією електронного вітру вздовж інтерфейсу метал/діелектрик

2.2. Entropy production minimization for steady-state current
The density of entropy production by current, multiplied by temperature, is just a product of current and minus gradient of electric potential and is equal to Joule heating density. When approaching the steady state, entropy production tends to a minimum. Indeed, entropy production density times temperature is a sum of products of flux densities and the driving forces generating these fluxes. In our case, the flux density is the current density, and force is a minus gradient of electric potential. Flux and force are related by conductivity λ. In a steady state, the integral of this product over all volume of conductor should tend to minimum. Mathematically, call such integrals the functionals of potential and current didtribution.

$$T\frac{dS}{dt} = \iiint \overrightarrow{J_{el}}(-\overrightarrow{\nabla}\varphi)dV = \iiint \lambda(\overrightarrow{\nabla}\varphi)^2 dV = \min \qquad (1)$$

Putting variation of this functional (under fixed constant conductivity λ) and equalizing it to zero at the arbitrary variation of electric potential immediately leads us (by the standard procedure of variational analysis) to the Laplace equation for electric potential:

$$\text{div(grad } \varphi) = 0 \qquad (2)$$

This distribution of potential and current may exist unchanged forever if the conductivity will be constant. BUT! Conductivity, in the long term, is not constant because it depends on morphology (including changing cross-section of interconnect due to voids and cracks), morphology changes due to migration of atoms, and especially due to migration, accumulation, and generation of vacancies.

3. Structural entropy production during diffusion, vacancy generation, and annihilation.
Now we will concentrate on the entropy production as a **reason**, or at least, as a **marker** of failure.
Failure is, typically, a result of an accumulation of some threshold level of structural defects in one place. On the other hand, the evolution of an open system is described by the entropy production in local relaxation processes. This entropy production, in general, contains thermal

and structural parts. The thermal part of entropy production (in our case, Joule heating) usually just dissipates in the ambient and is not accumulated, but the structural part may accumulate in the form of extra defects. Thus, failure may be treated as the result of reaching the threshold of the structural part of entropy production. Let us consider some obvious examples of the structural part of entropy production.

3.1. Diffusional redistribution of tracer atoms in chemically homogeneous pure material or chemically homogeneous alloy.

If the concentration gradient $\text{grad}(C^*)$ of the tracer concentration and corresponding driving force - the minus gradient of chemical potential, $-\frac{k_b T}{C^*} \cdot \text{grad}(C^*)$, then the entropy production density (times temperature) will be the product of flux density $-D \cdot \text{grad}(C^*)$ and the driving force and of course, will be positive. Yet, redistribution of tracer atoms (isotopes of the main matrix components) does not change any energy or enthalpy - thus, this entropy production does not produce any heat - it changes only configurational entropy (increasing it). So, the self-diffusion of isotopes produces only structural entropy.

3.2. Structural entropy production by vacancy diffusion.

In the solid material with vacancies but with vacancy sinks and sources only at the external boundaries, the following conservation law is valid inside the material:

$$\frac{\partial C_v}{\partial t} = -div(\Omega \overrightarrow{J_v}) . \tag{3}$$

($\overrightarrow{J_v}$ is a local vacancy flux density, Ω is the mean volume per site which we approximately take as equal to vacancy volume).

Configurational entropy of vacancy distribution within the material is

$$S_v = -k_b \iiint (C_v ln C_v + (1 - C_v)ln(1 - C_v))\frac{dV}{\Omega} . \tag{4}$$

The chemical potential of vacancies is equal to zero for the case of vacancies in equilibrium and is determined by vacancy super- or undersaturation:

$$\mu_v = k_b T ln\frac{C_v}{C_v^{eq}} , \tag{5}$$

so that

$$ln C_v = \frac{\mu_v}{k_b T} + ln C_v^{eq} . \tag{6}$$

Here C_v^{eq} is an equilibrium vacancy concentration. After some elementary algebra, one gets from Eqs. (3-6) and taking into account that $C_v << 1$:

$$\frac{dS_v}{dt} = \frac{-k_b}{\Omega} \iiint \frac{\partial C_v}{\partial t}(ln C_v - ln(1 - C_v))dV =$$
$$= \frac{-k_b}{\Omega} \iiint (-div(\Omega \overrightarrow{J_v}))(\frac{\mu_v}{k_b T} + ln C_v^{eq})dV \tag{7}$$

The equilibrium vacancy concentration is determined by the vacancy formation enthalpy H_{1v}:

$$C_v^{eq} = exp(-\frac{H_{1v}}{k_b T}) \tag{8}$$

At that, $H_{1v} = TS_{1v}$, here S_{1v} is an entropy increase due to adding one vacancy to the system. Our result is:

$$T\frac{dS_v}{dt} = \oiint(\mu_v - H_{1v})\overrightarrow{J_v}d\vec{\Sigma} + \iiint \overrightarrow{J_v}(-\vec{\nabla}\mu_v)dV \tag{9}$$

Here, the first term is an entropy production due to vacancy diffusion, and it is purely structural, not related to any heat generation or absorption:

$$\overrightarrow{J_v}(-\vec{\nabla}\mu_v) = \frac{D_v}{k_b T C_v}(\vec{\nabla}C_v)(\vec{\nabla}C_v) \tag{10}$$

3.3. Structural entropy production by vacancies with an account of vacancy sinks/sources in relaxation approximation.

Now we consider the more realistic case of entropy production by vacancies in the real crystal with vacancy sinks and sources. Here we consider the simplest relaxation approximation when these sinks/sources are "smashed" over all crystal continuously and characterized by the single parameter – relaxation time. Mathematically it is a second term in the right-hand side of the kinetic equation (11) for vacancy concentration.

$$\frac{\partial C_v}{\partial t} = -div(\Omega \overrightarrow{J_v}) - \frac{C_v - C_v^{eq}}{\tau_v} \tag{11}$$

The first term is a minus divergence of vacancy flux, and the second describes going extra vacancies to sinks if the vacancy concentration is higher than the equilibrium value, and the generation of lacking vacancies by sources if the vacancy concentration is lower than the equilibrium one. Here τ_v - vacancy relaxation time determined by the mean free path for vacancy migration from sinks to sources and by vacancy diffusivity.

If supersaturation or undersaturation by vacancies is relatively small, the difference of actual and equilibrium vacancy concentration is easily transformed into the chemical potential of non-equilibrium vacancies.

$$C_v - C_v^{eq} = C_v^{eq}(\frac{C_v}{C_v^{eq}} - 1) \approx C_v^{eq} \exp(\frac{C_v}{C_v^{eq}}) = C_v^{eq}\frac{\mu_v}{k_b T} \tag{12}$$

In such terms, the relaxation rate is proportional to the difference of actual vacancy chemical potential and equilibrium vacancy potential (which is, of course, zero).

$$\frac{\partial C_v}{\partial t} \cong -div(\Omega \overrightarrow{J_v}) - \frac{C_v^{eq}}{k_b T}\frac{\mu_v}{\tau_v} \tag{13}$$

Again we write down andtransform the expressions for vacancy configurational entropy and the rate of its change:

$$S_v = -k_b \iiint (C_v ln C_v + (1 - C_v)ln(1 - C_v))\frac{dV}{\Omega} \tag{14}$$

$$\frac{dS_v}{dt} = \frac{-k_b}{\Omega} \iiint \frac{\partial C_v}{\partial t}(ln C_v - ln(1 - C_v))dV =$$

$$= \frac{-k_b}{\Omega} \iiint (-div(\Omega \overrightarrow{J_v}) - \frac{C_v^{eq}}{k_b T}\frac{\mu_v}{\tau_v})(\frac{\mu_v}{k_b T} + ln C_v^{eq})dV =$$

$$= \iiint \frac{\mu_v - H_{1v}}{T} div(\overrightarrow{J_v})dV + \frac{1}{T\Omega} \iiint \frac{C_v^{eq}}{k_b T}\frac{(\mu_v)^2}{\tau_v}dV + \frac{k_b C_v^{eq} ln C_v^{eq}}{\Omega k_b T \tau_v} \iiint \mu_v\, dV \tag{15}$$

$$\iiint (\mu_v - H_{1v})div(\overrightarrow{J_v})dV = \iiint div(\overrightarrow{(\mu_v - H_{1v})J_v})dV - \iiint \overrightarrow{J_v}\vec{\nabla}\mu_v dV \tag{16}$$

Here,

$\iiint \overrightarrow{J_v}(-\vec{\nabla}\mu_v)$ - entropy production by vacancy migration

$\oiint(\mu_v - H_{1v})\overrightarrow{J_v}d\vec{\Sigma} = \frac{dS^{ext}}{dt}$ — out-flux of entropy (if any)

Due to the out-flux of vacancies to the external boundaries which act as a vacancy sink, one gets:

$$\iiint \frac{C_v^{eq}}{k_b T}\frac{\mu_v}{\tau_v}dV \cong \iiint \frac{C_v - C_v^{eq}}{\tau_v}dV = \frac{\iiint C_v dV - C_v^{eq}\iiint dV}{\tau_v} = \frac{\Omega N_v - \Omega N_v^{eq}}{\tau_v} = \Omega\frac{\Delta N_v}{\tau_v} \tag{17}$$

On the other hand,

$$\frac{dV^{tot}}{dt} = \Omega\frac{dN_v^{tot}}{dt} \tag{18}$$

(total shrinking rate $= \frac{dV^{tot}}{dt} < 0$)

Finally, our result is:

$$T\frac{dS_v}{dt} = \oiint(\mu_v - H_{1v})\overrightarrow{J_v}d\vec{\Sigma} + H_{1v}(-\frac{N_v - N_v^{eq}}{\tau_v}) +$$

$$+ \iiint \overrightarrow{J_v}(-\vec{\nabla}\mu_v)dV + \iiint \frac{C_v^{eq}}{k_b T}\frac{(\mu_v)^2}{\tau_v}\frac{dV}{\Omega} \tag{19}$$

Here, the first term is an entropy change due to the out-flux of vacancies.

The second term is a global entropy change due to the creation or annihilation of vacancies at the sinks/sources.

The third term is entropy production due to vacancy diffusion.

The fourth term is an entropy production due to the relaxation of non-equilibrium vacancy concentration.

4. Structural entropy production as a reason for failure

4.1. What is the fraction of structural entropy in the total entropy production by diffusion, electromigration, thermomigration, and stress migration?

If the driving force of vacancy flux is purely configurational, the produced entropy is purely structural. What is the form (thermal or configurational or both) of the produced entropy, if the driving force is an electron wind in electromigration or temperature gradient thermomigration or stress gradient in stress migration, is not very clear so far.

Let us consider electromigration. The elementary act of electromigration – atomic jump (and opposite vacancy jump) under electron wind force, of course, proceeds with heat generation during electron scattering on the jumping atom and its deformed vicinity. Yet, at least a significant part of this heat generation is actually a Joule heating already taken into account in entropy production by electron current under a gradient of electric potential.

Let us assume that the structural entropy production by electromigration is a constant fraction f of total entropy production by the electromigration, $(0 < f < 1)$

$$T \frac{dS_{struct}}{dt} = f \cdot J \cdot X = f \cdot \left(\frac{C \cdot D}{k_b T} \cdot Z_e \rho j_{el}\right) \cdot Z_e \rho j_{el} \tag{20}$$

Now we will try to apply this assumption for the explanation and prediction of parameters in the Black equation for MTTF.

Our task is to understand the Black equation for MTTF and to provide receipts for the prediction of its parameters n, Ea, A.

$$MTTF = A(j^{-n}) \exp\left(\frac{E_a}{k_b T}\right) \tag{21}$$

4.2. Treating MTTF as a time to accumulate the threshold structural entropy

Now, we consider entropy production during electromigration. We treat MTTF as a time to accumulate some threshold entropy, S 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. So far, let us exclude also thermomigration and stress-migration. The total entropy production until failure is

$$J \cdot X \cdot MTTF = \frac{TS_{threshold}}{V} \tag{22}$$

$$\frac{f \cdot C \cdot D}{k_b T} \cdot (Z_e \rho j_{el})^2 \cdot MTTF = \frac{TS_{threshold}}{V} \tag{23}$$

$$t^{failure} = \frac{TS_{threshold}}{V J_e X_e} = A' \frac{1}{j^2} \frac{1}{D} = A j^{-2} \exp\left(\frac{E_a}{k_b T}\right) \tag{24}$$

4.3 Threshold structural entropy

It is important to suggest some receipt for predicting the threshold entropy corresponding to failure. In general, it is a very complicated problem since failure has various mechanisms (modes). In this paper, we limit ourselves to the case of voiding (pore formation) at the cathode end, as an immediate mechanism of failure.

To nucleate and grow the viable void, the cathode end should accumulate the nonequilibrium vacancies. If the supersaturation by vacancies is not large, then the accumulation of N_v extra

vacancies increases entropy by $\frac{N_v E_v}{T}$. Indeed, the equilibrium of the vacancy subsystem means zero derivative of Gibbs free energy:

$$\frac{d}{dN_v}(N_v H_v - TS(N_v)) = 0 = H_v - T\frac{dS}{dN_v} \Rightarrow \frac{dS}{dN_v} = \frac{H_v}{T} \tag{25}$$

It immediately gives that the increase of entropy by adding one extra vacancy to the system is just a vacancy formation enthalpy divided by temperature.

4.4. Vacancies as the "quants" of entropy and carriers of entropy

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

$$\Delta S \approx \Delta N_v^{\text{extra}}\frac{E_v}{T} \tag{26}$$

Sooner or later these extra vacancies will unite into the void or crack stopping the current. To stop the current completely, the void should have cross-section A of the interconnect and at least $\delta \approx 0{,}2$ nm of thickness:
Then the threshold entropy may be VERY ROUGHLY approximated as

$$S^{threshold} \approx \frac{A \cdot \delta}{\Omega}\frac{E_v}{T} \tag{27}$$

4.5. Competition of K (Kirkendall) - and F (Frenkel) - vacancy sinks

Relaxation of the vacancy subsystem can proceed in two ways:
1) The first way is voiding as a result of vacancy relaxation at the so-called F-sinks (Frenkel sinks - the terminology of Ya. E. Geguzin), which means just joining vacancies into voids.
2) The second way is vacancy relaxation without voiding, at the so-called K-sinks, (Kirkendall sinks, according to the same terminology of Ya. E. Geguzin, localized at dislocation kinks or the surface of crystal grains).

This classification appeared due to an investigation of interdiffusion. Since 1947, thanks to Ernst Kirkendall, we know that the inequality between the diffusivities of components in binary diffusion couple leads to compensating vacancy flux from the slow component side to the fast component side, and divergency of this vacancy flux leads simultaneously to two effects – Kirkendall shift and Frenkel or Kirkendall voiding. The Kirkendall shift is a movement of inert markers, embedded in the crystal lattice, shifted due to dislocation climb generated by vacancy annihilation at one side of diffusion couple and vacancy generation at another side. Frenkel or Kirkendall voiding is just uniting extra vacancies into voids.

The difference between K-sinks and F-sinks of vacancies in the case of interdiffusion generating the vacancy flux from the side of slow component B to the side of fast component A. Vacancies coming to the A-side have two possibilities – (1) to annihilate at the dislocation generating its climb and causing the lattice shift? And (2) to join the void and increase it, instead of causing lattice shift. In the case of electromigration, the vacancies migrate from anode to cathode due to electron wind onto the atoms. If there are no preexisting voids, then they can be created only at the K-sources at the anode end, but they have two possibilities at the cathode end. Therefore, the total amount of "emptiness" in the interconnect increases (Fig. 3).
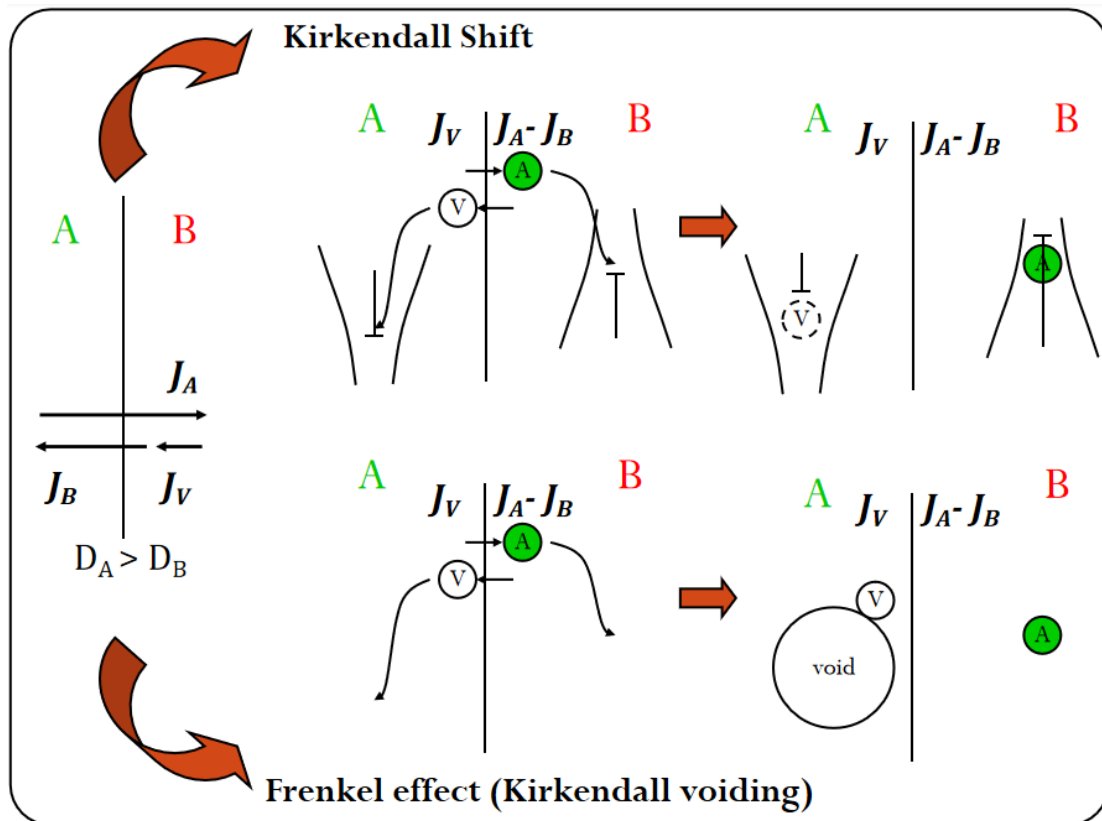
Fig. 3. Mechanisms of Kirkendall and Frenkel effects (Drawing for description of competition between the Kirkendall shift and Kirkendall voiding was made by Dr. T. Zaporozhets)
Рис. 3. Механізми ефектів Кіркендалла та Френкеля (Малюнок для опису конкуренції між зсувом Кіркендалла та утворенням пор виконано доктором Т. Запорожець)

Vacancies lead to failure if they go to F-sinks, and they annihilate without causing damage if they go to K-sinks. Thus, one should help K-sinks in their competition with F-sinks.

For this, we may try to increase the dislocation density. Yet, it will increase the resistivity, which is not good. Professor Chih Chen et al. discovered about 10 years ago that nanotwinned copper may be a good candidate. Nanotwinned copper can absorb vacancies without forming voids and has a resistivity almost the same as "ideal" copper without defects.

4.6. MTTF for thermomigration. Prediction of MTTF for thermomigration-caused failure
Similar to electromigration, the major entropy production in thermomigration is due to heat propagation under a temperature gradient:

$$\frac{TdS}{Vdt} = (-\kappa \frac{dT}{dx})(-\frac{1}{T}\frac{dT}{dx}) \tag{28}$$

In thermomigration of atoms, we have, very roughly

$$\frac{TdS}{Vdt} = (C \frac{D}{k_bT} X_h)X_h = C \frac{D}{k_bT}(3k_b\frac{dT}{dx})^2 \tag{29}$$

$$f \cdot J_h X_h t^{failure} = \frac{TS_{threshold}}{V} \tag{30}$$

$$MTTF \approx t^{failure} = \frac{TS_{threshold}}{VJ_hX_h} = B(-\frac{dT}{dx})^{-2}\exp\left(\frac{E_a}{k_bT}\right) \tag{31}$$

$$J_h = C \frac{D}{k_bT}\frac{Q^*}{T}(-\frac{\partial T}{\partial x}) \tag{32}$$

$$X_h = \frac{Q^*}{T}(-\frac{\partial T}{\partial x}) \tag{33}$$

So, we predict that the MTTF for thermomigration is inversely proportional to the squared temperature gradient.

4.7. MTTF for stress-migration

We can practically repeat the same time of derivation of MTTF for the case of stress migration. In this case, the driving force is the gradient of the stress tensor, $\text{grad}(\sigma\Omega)$.

$$X_s = \frac{d\sigma\Omega}{dx} \tag{34}$$

$$J_s = CMF = C\frac{D}{k_bT}\left(\frac{d\sigma\Omega}{dx}\right) = \frac{D}{k_bT}\frac{d\sigma}{dx} \tag{35}$$

$$f \cdot J_s X_s \text{t}^{\text{failure}} = \frac{\text{TS}_{\text{threshold}}}{\text{V}} \tag{36}$$

$$\text{MTTF} \approx \text{t}^{\text{failure}} = \frac{\text{TS}_{\text{threshold}}}{\text{V}J_s X_s} = G\left(-\frac{d\sigma}{dx}\right)^{-2}\exp\left(\frac{E_a}{k_bT}\right) \tag{37}$$

So, we predict that the MTTF for stress migration is inversely proportional to the squared stress gradient.

5. Failure as a phase/structure transformation in open system

One of the basic equations in the general kinetic theory of the first-order phase transformations is the Kolmogorov-Avrami equation for the time dependence of the transformed fraction of the parent phase

$$Y = 1 - \exp[-K \cdot t^n] \tag{38}$$

where K includes nucleation frequency and growth velocity of the new phase precipitates. The kinetics of K-A evolution is a typical S-curve (Fig. 4a), which gives, in a double-logarithmic scale, the linear dependence (Fig. 4b)
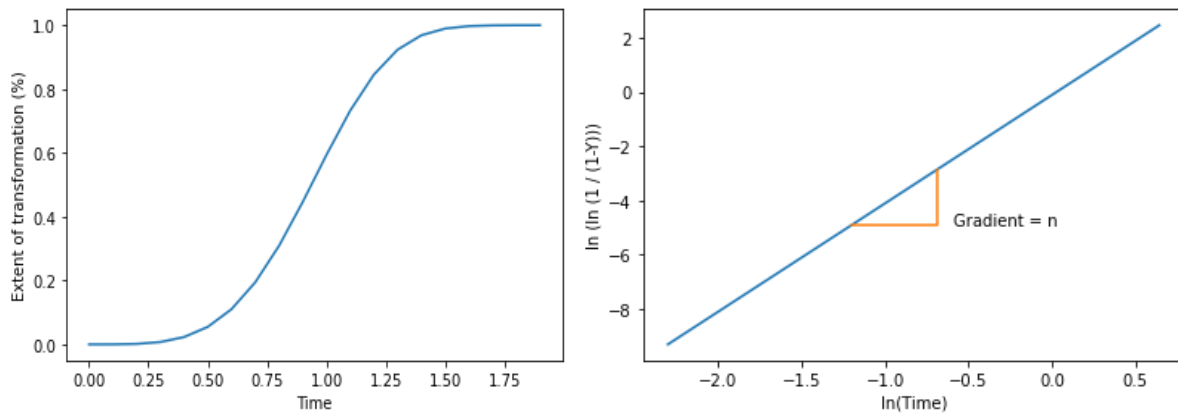

Fig.4. Kolmogorov-Avrami evolution: S-type dependence of transformed volume fraction vs time (a) and the same dependence in double-logarithmic scale (b).

Рис. 4. Еволюція Колмогорова-Аврамі: S-подібна залежність частки перетвореного об'єму від часу (a) і та ж залежність в подвійному логарифмічному масштабі (b).

On the other hand, the times to failure dispersion is often described by Weibull distribution, which in cumulative form (Cumulative function -fraction of failed devices by time t) practically coincides with the Kolmogorov-Avrami equation (Fig. 5):

$$F(x) = 1 - e^{-(x/\lambda)^k}$$

$$-\ln(1 - F(x)) = (x/\lambda)^k$$

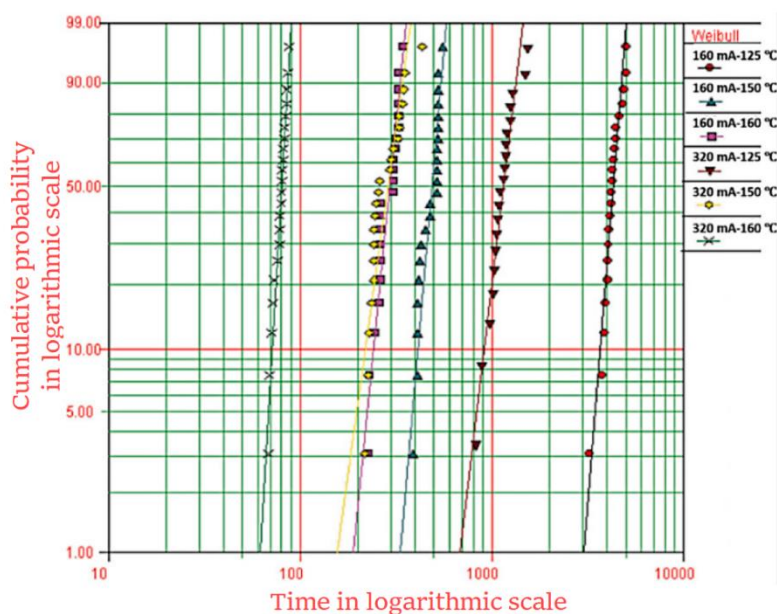$$\ln(-\ln(1 - F(x))) = k \ln x - k \ln \lambda \qquad (39)$$

Fig. 5. Typical Weibull plot (data taken from our recent paper[4])

Рис. 5. Типовий графік Вейбулла (дані взяті з нещодавньої статті авторів [4])

Failure, like phase transformation, usually starts its pre-history by some (1) "nucleation event" - for example, nucleation of nanovoid somewhere at the triple joint of grain boundaries or the interface metal/dielectric, (2) "growth process" (for example, migration of nanovoid to the cathode end, or/and merging or just growth of the voids at the cathode end).

At that, we should be ready to consider the "growth" process of future failure in the multidimensional space depending on the nature of evolution from nucleating defects to the abrupt change of resistivity (depending on mechanism).

6. Conclusions

1. Failure may be treated as a result of the accumulation of structural entropy beyond some threshold value. Accumulation of structural entropy is calculated as a "non-heating" part of entropy production in the processes of electromigration, thermomigration, and stress migration. Such an approach leads to Black's equation for MTTF with exponent n = 2 for electromigration-induced failure, and to analogous predictions for thermomigration-induced failure, as well as for stress migration-induced failure.

2. Failure may be treated as a result of the incompatibility of steady-states for different processes in an open system. For example, steady-state current under fixed voltage between the cathode and anode ends of interconnect leads to electromigration of atoms and vacancies which, in realistic materials, lead to non-steady-state voiding and hillock formation, and eventual failure. Fully compatible steady-states for all processes would mean "immortality" at least for interconnect.

3. Failure may be treated as a kind of first-order phase transformation in an open system and includes nucleation, growth or migration, and (sometimes) ripening. Moreover, the usually used cumulative Weibull distribution for time to failure (TTF) looks very similar to the Kolmogorov-Avrami equation for crystallization kinetics describing nucleation and growth of the crystalline phase.

4. Some ideas of the present paper may be found in the following books and papers: [1-9].

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НОВІ ТЕРМОДИНАМІЧНІ ПІДХОДИ ДО АНАЛІЗУ ВІДМОВ У МАТЕРІАЛАХ МІКРОЕЛЕКТРОНІКИ

Мета роботи: сформулювати базові ідеї термодинамічного підходу до проблеми надійності матеріалів мікроелектроніки.

Методика: елементи мікроелектронного приладу (у першу чергу металеві з'єднання та припойні контакти) розглядаються як відкриті термодинамічні системи у полях градієнтів електричного потенціалу, температури та напруг.

Результати: Відмову можна розглядати як результат накопичення структурної ентропії, що перевищує деяке порогове значення. Накопичення структурної ентропії розраховується як «нетермічна» частина виробництва ентропії в процесах електроміграції, термоміграції та міграції у градієнті напруг. Нетермічне виробництво

ентропії пов'язане, в першу чергу, з народженням дефектів, зокрема вакансій. Вперше отримані вирази для виробництва ентропії у твердих тілах із стоками та джерелами вакансій. Такий підхід призводить до нової інтерпретації рівняння Блека для середнього часу до відмови з показником n = 2 для випадку відмови, спричиненої електроміграцією, і до аналогічних рівнянь для відмов, спричинених термоміграцією, а також міграцією в полі напруг.

Висновки:

1. Відмову можна розглядати як результат несумісності стаціонарних станів для різних процесів у відкритій системі. Наприклад, стаціонарний струм під фіксованою напругою між катодним і анодним кінцями з'єднання призводить до електроміграції атомів і вакансій, що в реалістичних матеріалах призводить до нестаціонарного утворення пустот і горбків, а також до остаточного виходу з ладу. Повністю сумісні стаціонарні стани для всіх процесів означали б «безсмертя» принаймні для з'єднання. Наприклад, час до відмови повинен прямувати до нескінченності, якщо струм проходить через метал, у якому забезпечується повне пригнічення ефекту Френкеля (пороутворення) ефектом Кіркендалла (зсувом кристалічної гратки внаслідок переповзання крайових дислокацій).

2. Відмову можна розглядати як своєрідне фазове перетворення першого порядку у відкритій системі, яке включає зародження, ріст або міграцію та (іноді) коалесценсію пор або інших причин відмови. При цьому звичний кумулятивний розподіл Вейбулла для часу напрацювання (TTF) виглядає дуже схожим на рівняння Колмогорова-Аврамі для кінетики кристалізації, що описує зародження та ріст кристалічної фази.