Simulation of Temperature Cycling Effects on Electromigration Behavior Under Pulsed Current Stress

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***Abstract*—The temperature cycling effect on electromigration behavior under pulsed current conditions for metallization used in very large scale integrated (VLSI) devices is numerically investigated. This involves the solution of a two-dimensional (2-D) heat-conduction equation and a one-dimensional (1-D) diffusion-drift equation. We find that the characteristic thermal response time for establishing the equilibrium, for a typical VLSI metallization structure, is slightly longer than 1 ms. As a result, the steady-state temperature difference in the metal line between the upper and lower values in response to the pulsed current operation is maximized when the frequency is below 250 Hz with a duty factor of 0.5. The temperature difference decreases with increasing frequency. At frequencies above 10 MHz, the thermal capacity of the metal line inhibits appreciable temperature fluctuation. For a constant line temperature the time-dependent vacancy buildup has been shown to be proportional to r^m with $m = 2$ (where r is the duty factor), consistent with the "average model" for predicting the failure time. In this study, we confirm the speculation that Joule heating due to an elevated current density employed in accelerated life testing can bring about an $m < 2$ dependence at low frequencies. The confirmation is based upon the solution of the electromigration initial and boundary value problem by taking into account the temperature dependence of several relevant physical parameters, particularly the vacancy diffusivity.**

***Index Terms*—Diffusion processes, electromigration, integrated thermal factors, metallization, numerical analysis, transmission line matrix methods.**

I. INTRODUCTION

THE phenomenon of electromigration, or material movement resulting from the passage of an electrical current, continues to be a major reliability concern for the interconnects in very large scale integrated (VLSI) circuits. Longer electromigration lifetimes have been observed for metal lines subjected to pulsed current stress rather than to constantly flowing direct current (dc) stress and various possible mechanisms were proposed by many workers [1]–[12]. As most interconnects carry pulsed signals, it is important to have an improved understanding about the nature of the problem so as to assess adequately the enhancement of the electromigration lifetime.

The Black empirical expression [13] for median time to failure (MTF) is well known as a standard dc electromigration equation. It is convenient to describe the research background of pulsed dc electromigration by using this equation in a modified form

$$\mathrm{MTF} = \frac{A}{j^n r^m} \exp\left(\frac{\Delta E}{kT}\right) \tag{1}$$

where A is a material and geometry dependent constant, j is the current density, r is the duty factor, ΔE is the activation energy, k is the Boltzmann constant, T is the temperature, n is the current density exponent normally assumed to be 2, and m is the duty factor exponent. The value of m is of particular interest because it is employed for characterizing the lifetime enhancement due to pulsed operation. There are two different models generally referred to as "on-time" and "average" models. $m = 1$ is assumed in the on-time model, so that the MTF is inversely proportional to the duty factor r. This means that the current-induced material transport is a function only of the total "on" portions of a repetitive current pulse while there are no effects during the times when the signal is "off." The concept of the on-time model was proposed to give a conservative approach for VLSI interconnect design [14], [15]. Alternatively, the average model [3], [4] assumes $m = n = 2$, so that the dc equivalent current is given by the magnitude of the current averaged over the entire period (i.e., $j \times r$). Clearly, $m > 1$ suggests a relaxation process which occurs during the off times.

Many workers [3]–[6] have found that the results based on $m = 2$ are in good agreement with experimental data. Based on the fundamental diffusion-drift model with the assumption of a constant interconnect temperature, the electromigration initial and boundary value problem under pulsed current conditions has been solved numerically and the conclusion of $m = 2$ was also obtained [8], [12]. Furthermore, we have demonstrated that the "pure" electromigration-induced vacancy buildup (excluding the influence of Joule heating) under a pulsed dc stress can be described accurately by the dc stress scaled according to this duty factor dependence [12]. A recent theoretical investigation [11] has even shown that the MTF is proportional to r^{-2} for an arbitrary periodic stress (unidirectional but not necessarily to be rectangularly-

Manuscript received March 31, 1997; revised August 20, 1997. The review of this paper was arranged by Editor A. H. Marshak. This work was supported by the Natural Sciences and Engineering Research Council of Canada.

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Publisher Item Identifier S 0018-9383(98)00939-3.

pulsed). On the other hand, several experimental studies [6], [7], [9], [10] supported an $m < 2$ or $m \cong 1$ dependence if the pulse repetition frequency is below a certain value. This can be qualitatively explained by nonlinear thermal effects. At sufficiently high frequencies, the interconnect temperature would remain constant because the pulse repetition time is much shorter than the thermal response time. This allows electromigrating material to substantially relax during the off portion of the pulse. In contrast, the fluctuation of temperature at low frequencies might retard the back diffusion during the cooler off portion. Practically, it is extremely difficult, if not impossible, to measure the transient temperature response of the metallization line accurately. Therefore, computer simulation is very desirable to confirm these speculations.

In the present study, we perform a quantitative computation of electromigration behavior under pulsed current stresses, taking into account the effects of frequency dependence of temperature response. In the next section, we determine the maximum difference in interconnect temperature between on and off times at steady state as a function of the pulse repetition frequency for a typical VLSI metallization structure. This requires the solution of a two-dimensional (2-D) time-dependent thermal diffusion equation. In Section III, we incorporate such information into the vacancy supersaturation model for electromigration failure, which involves the solution of the one-dimensional (1-D) electromigration (diffusion-drift) equation in order to evaluate the influence of temperature cycling. The transmission-line matrix (TLM) techniques [12], [16], [17], along with the newly developed boundary treatment [18] are used for numerically solving all these equations. Finally, a summary of the results is given in Section IV.

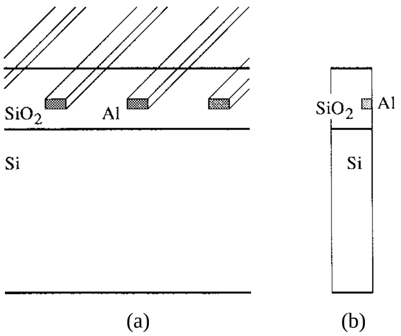
II. THERMAL MODEL: FREQUENCY DEPENDENCE OF TEMPERATURE RESPONSE

In a digital VLSI circuit, a number of fairly long metallization lines are usually arranged in parallel to carry signals. Fig. 1(a) shows such a structure. We assume that the Al lines are 0.75 μm thick by 0.8 μm wide and equally spaced by 4.0 μm between centers. These lines are deposited onto a 1.0-μm thick layer of SiO_2 grown on a 300-μm thick Si wafer. The lines are buried under 1.5 μm of planarized SiO_2 passivation layer. The electrical current flows through the Al lines and creates the Joule heating, $j^2\rho$, where j is the current density and ρ is the electrical resistivity. The temperature dependence of ρ for Al is considered in the model according to

$$\rho(T) = aT \tag{2}$$

with the constant a being equal to $1.10 \times 10^{-8}\ \Omega \cdot \text{cm/K}$ [19]. A 2-D thermal analysis of a cross-sectional element as shown in Fig. 1(b) is conducted to reduce the computational effort. The top surface is approximated to be adiabatic and all sides represent the symmetry faces with zero gradient in temperature across the boundary. The back contact of the chip is held at an ambient temperature of 200 °C.

The model geometry being chosen as such is based on several considerations. First, it is a 2-D model and thereby more accurate and complete (e.g., the inclusion of the heat-conduction paths through passivation material) than can be a 1-D model. Second, the longitudinal temperature distribution perpendicular to the plane of Fig. 1(b) is ignored so as to emphasize the periodic temperature effect itself rather than others originating from temperature gradients. Meanwhile, intensive computer run time can be avoided with the simplified geometry as the calculation for temperature response to a repetitively-pulsed stress could be very time consuming.



(a) (b)

Fig. 1. (a) Parallel Al metallization lines encapsulated with SiO_2 on a Si substrate. (b) Elemental cross section through the structure used in the simulation. Symmetry is exploited to reduce the computation.

TABLE I
SOME PHYSICAL PROPERTIES OF MATERIALS USED IN THE SIMULATION

Parameter	Al	SiO$_2$	Si
Thermal conductivity (W/cm·°C)	2.37	0.014	1.5
Specific heat (J/g·°C)	0.896	1.00	0.70
Density (g/cm^3)	2.707	2.27	2.33

The governing heat-flow equation is given by

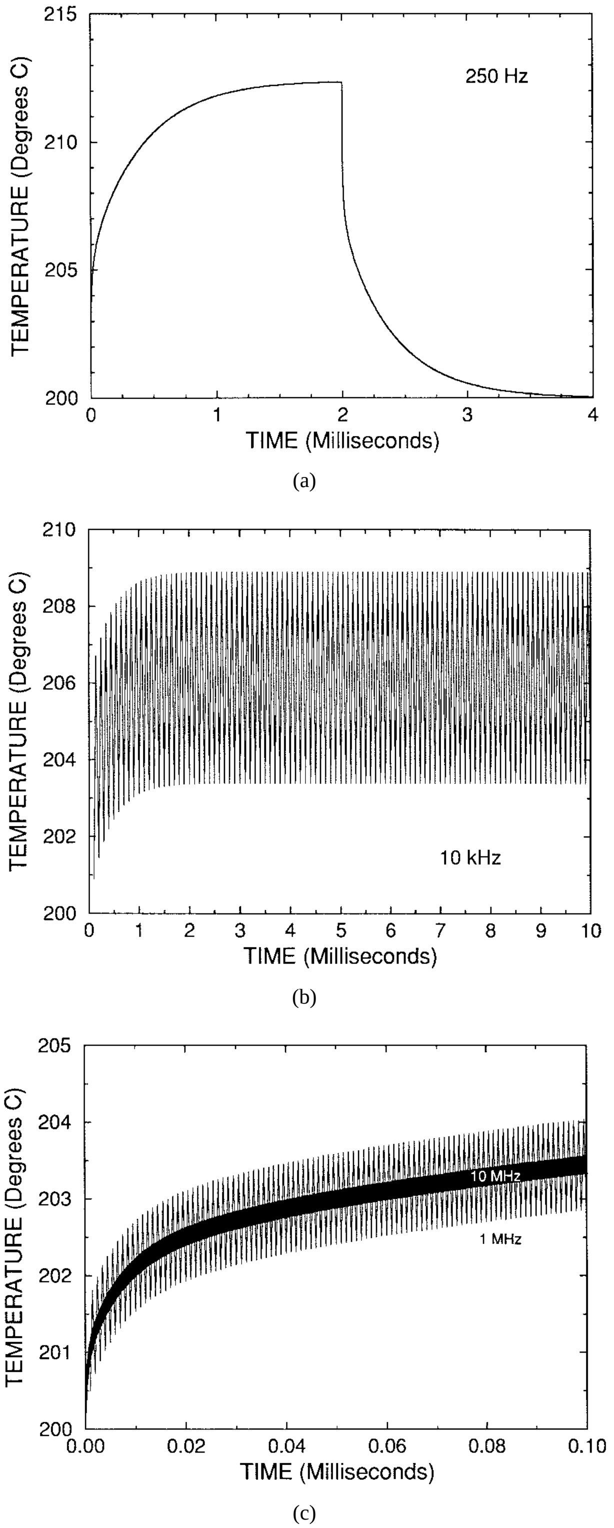
$$\rho_d C_p \frac{\partial T(x,y,t)}{\partial t} = \kappa \nabla^2 T(x,y,t) + j^2 \rho(T) \tag{3}$$

where ρ_d is the density, C_p is the specific heat, κ is the thermal conductivity, and t is the time. The physical parameters for the materials used (Al, SiO_2, and Si) are listed in Table I. Current density j is a constant under the dc condition, and is periodically changed for a pulsed dc stress according to

$$j = \begin{cases} j_p & \text{for } (s-1)p \le t < (s-1)p + t_{\text{on}} \\ 0 & \text{for } (s-1)p + t_{\text{on}} \le t < sp \end{cases} \qquad s = 1, 2, 3, \cdots \tag{4}$$

where t_{on} is the pulse duration, p is the period, and s is the period sequence number. The duty factor is defined as $r = t_{\text{on}}/p$. The temperature response versus time is calculated at a variety of different pulse repetition frequencies for sufficient time to achieve a steady-state cyclical condition.

For the metallization structure described above, calculated results indicate that the Joule-heating-induced temperature rise is not appreciable for a current density of the order of 10^5 A/cm^2, and is about 2 °C for $j = 1.0 \times 10^6$ A/cm^2 at steady state. For higher current densities, the Joule heating



(a)

(b)

(c)

Fig. 2. Temperature variation of Al lines versus time due to a pulsed dc current stress at different frequencies (current density $j = 2.5 \times 10^6$ A/cm^2, duty factor $r = 0.5$). (a) 250 Hz. (b) 10 kHz. (c) 1 MHz and 10 MHz.

increases rapidly. Therefore, we choose 2.5×10^6 A/cm^2 as a plausible value to show our results, which is also typical in many traditional accelerated electromigration tests.

Displayed in Fig. 2(a)–(c) are the simulation results of the temperature response within the Al lines at various frequencies. The magnitude of the thermal time constant is found to be of the order of ms. For longer heating or cooling times we can expect to obtain a maximum difference in line temperature under steady-state pulsed excitation. If we consider a factor of 90 per cent of the temperature rise or decay, then the time scale for both on and off intervals can be approximated by 1 ms, corresponding to a repetition frequency of 500 Hz with a duty factor $r = 0.5$. This steady-state establishing time is consistent with that in an early report [20], where the 1-D calculation of temperature distribution along the metallization line under dc stress is performed. Our more accurate calculations with respect to the 2-D structure indicate that 2 ms [or a frequency of 250 Hz with $r = 0.5$, see Fig. 2(a)] would allow the upper and lower line temperatures to approach the equilibrium value for a continuous current stressing and to return to the ambient temperature when the current is switched off. Consequently, the temperature difference is maximized and will remain as a constant for even lower frequencies. In the present case, this temperature difference is slightly greater than 12 °C. In other words, the line temperature varies between 200 and 212 °C periodically at any frequency below 250 Hz. Fig. 3 shows the maximum temperature difference between on and off times as a function of the pulse repetition frequency. There is a large temperature drop in the frequency range from 250 Hz to about 10 kHz and the temperature variation decreases steadily as the frequency further increases. Eventually, after the frequency is above 10 MHz, the thermal capacity of the metal line inhibits any obvious change in the line temperature. As a result, the line temperature is stabilized to an average value, and the relevant temperature fluctuation effects would be negligible.

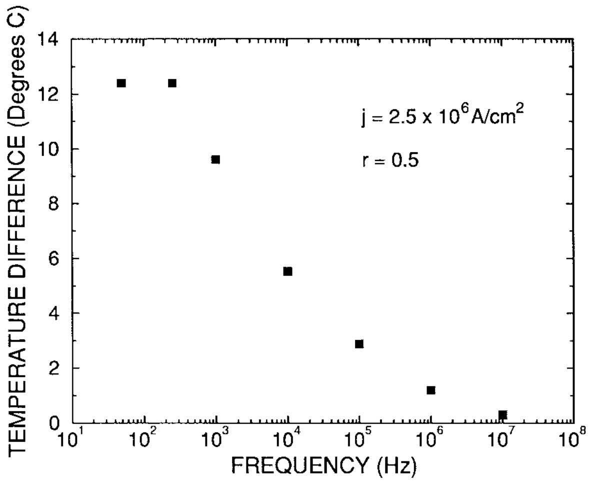


Fig. 3. Maximum temperature difference between on and off portions of the pulse at steady state versus the pulse repetition frequency (current density $j = 2.5 \times 10^6$ A/cm^2, duty factor $r = 0.5$).

Although a particular metal line geometry is employed in this study, the conclusions drawn above regarding the frequency dependence of temperature response do not appear to be significantly different for other realistic line sizes used in VLSI metallization. From the thermal point of view, current density is the most important parameter in determining the temperature rise within the metal line. For carrying the same current, a more “aggressive” design using a smaller line dimension (e.g., in the deep sub-micron range) will increase current density and temperature rise. On the other hand, when the current density is the same, a smaller cross-sectional area represents a less power dissipation and will alleviate heat generation. A further relevant factor in thermal considerations is the SiO_2 layer between the metal line and the Si wafer. A thinner SiO_2 layer would be helpful to reducing the metallization thermal resistance and heat dissipation [21].

III. DIFFUSION-DRIFT MODEL: VACANCY SUPERSATURATION BEHAVIOR WITH NONLINEAR HEATING

The electromigration initial and boundary value problem can be examined by the following continuity equation [22] for a diffusion-drift system

$$\frac{\partial C(x,t)}{\partial t} = D\left[\frac{\partial^2 C(x,t)}{\partial x^2} - \alpha\frac{\partial C(x,t)}{\partial x}\right], \qquad 0 < x < l \quad (5)$$

with

$$\alpha = \frac{Z^* e\rho j}{kT} \quad (6)$$

where C is the vacancy concentration, $Z^* e$ is the effective ionic charge, D is the grain-boundary self-diffusivity which has an Arrhenius temperature dependence with D_0 being the preexponential factor

$$D = D_0 \exp\left(-\frac{\Delta E}{kT}\right). \quad (7)$$

The parameter α, whose reciprocal is directly related to the Blech length [23], characterizes the reduced electromigration driving force. Equation (5) is subject to an initial uniform vacancy concentration

$$C(x,0) = C_0, \qquad 0 \leq x \leq l \quad (8)$$

along with the completely blocking (zero diffusion flux) boundary condition at $x = 0$

$$D\left[\frac{\partial C(0,t)}{\partial x} - \alpha C(0,t)\right] = 0, \qquad t \geq 0 \quad (9a)$$

and a constant vacancy concentration at $x = l$

$$C(l,t) = C_0, \qquad t \geq 0. \quad (9b)$$

Equations (9a) and (9b) represent a set of standard boundary conditions with reasonable physical meaning [24]. Vacancies would migrate from the supplying end at $x = l$ (such as a bonding pad) to the blocking end at $x = 0$ (a contact) and accumulate there with the elapsed stressing time. The vacancy concentration will be saturated ultimately at the blocking boundary. If the quantity αl is sufficiently large (Blech length effect [23]), a critical value of the vacancy concentration C^* may be reached before the occurrence of the saturation and a void formation will be initiated. Otherwise, the metallization line would be virtually immune to the electromigration damage. Clearly, the variation of vacancy concentration at the blocking boundary $C(0,t)$ is of special interest for predicting failure time.

Based on the above formulation, there is no macroscopic diffusion phenomenon at the very beginning owing to the initial uniformity of the background vacancy concentration. However, the current-induced electromigration quickly changes the distribution of the vacancy concentration, and both drift (due to the electric field) and diffusion (due to the concentration gradients) come into play. In the off portion of the current pulse, there is only the diffusion process which tends to restore the migrated vacancies toward their original position and balance the vacancy distribution.

One of the problems with simulations applied to the pulsed electromigration phenomena is that the modeler must consider two incompatible time scales simultaneously as the pulse period is very short compared with the time to failure. For high frequencies both the time step and the spatial resolution of a numerical method have to be made very small, which could bring about a prohibitive computational cost. However, there are appropriate ways to get round this difficulty. We have shown in [12] that the monotonical convergence of the vacancy concentration with increasing frequency allows reasonable conclusions to be drawn before the computation becomes intensive. Section II shows that above 10 MHz and below 250 Hz represent two distinct regions from the thermal point of view. In the present model, the parameter α is a function of current density j, electrical resistivity ρ, and temperature T. Notice that j is varied with time t according to the signal frequency and duty factor, D and ρ change at different T, and T depends on the created Joule heating. In order to highlight the temperature cycling effect, we calculate the vacancy concentration $C(0,t)$ versus time at a very low frequency of 1 mHz with a duty factor of $r = 0.5$. Although this frequency itself may not be so interesting in practical circuits, it is of assistance in characterizing the low-frequency behavior due to temperature effects. As the steady-state temperature field can be established in the order of 10^{-3} s, it would be appropriate to assume two constant temperatures, a high one (T_{on}) and a low one (T_{off}), for the on and off portions of the waveform. Such treatment only very slightly enhances the effect to be simulated but greatly simplifies the matter. According to the solution of temperature response presented in the preceding section, T_{on} and T_{off} are 212 and 200 °C, respectively, when $j = 2.5 \times 10^6$ A/cm^2. In the calculation, $Z^* = 1, D_0 = 1 \times 10^{-4}$ cm^2/s, and $\Delta E = 0.67$ eV [23], [25] are assumed.

The results are shown in Fig. 4. Here, the power is cycled a very large number of times to reach the steady state, with the temperature T and associated parameters (D and ρ) varying periodically. We have also plotted the high frequency ($>$10 MHz) curve in the same diagram for comparison, which is produced under an equivalent dc current stress scaled down by the pulsed current and duty factor $(j_{dc} = j \times r = 2.5 \times 10^6 \times 0.5 = 1.25 \times 10^6$ A/cm^2) [12]. As expected, the low-frequency curve with the temperature fluctuation is situated above the high-frequency curve where a constant average temperature of 206 °C is assumed, giving rise to a higher vacancy concentration at the same stressing time. It has been shown [26] that the failure time is normally dominated by the void incubation process described by the vacancy supersaturation model instead of its subsequent rapid growth. As an example, one may assume that the ratio between

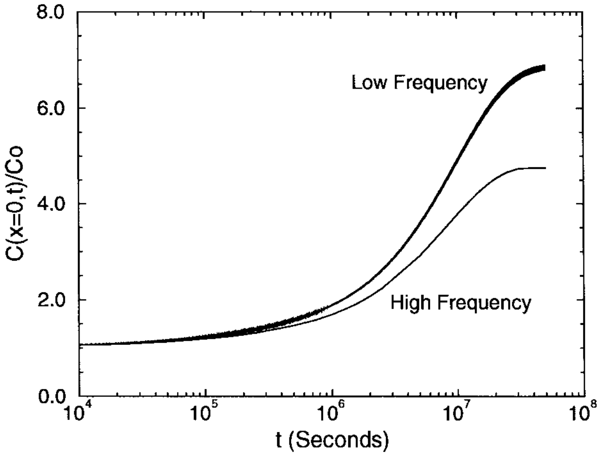


Fig. 4. Vacancy buildup as a function of time at frequencies above 10 MHz and below 250 Hz (current density $j = 2.5 \times 10^6$ A/cm^2, duty factor $r = 0.5$).

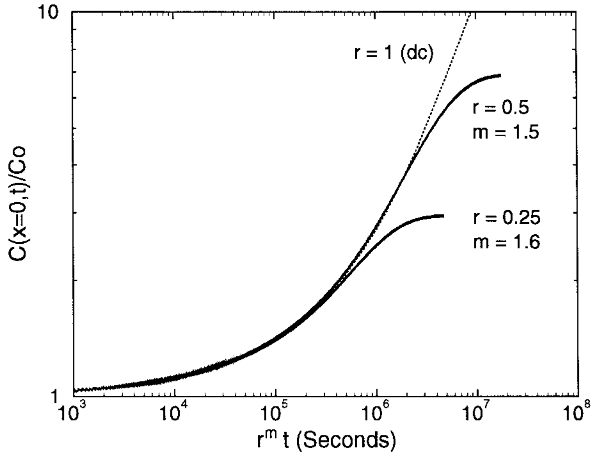


Fig. 5. Vacancy buildup as a function of time for several values of r (current density $j = 2.5 \times 10^6$ A/cm^2). The curves for the pulsed cases correspond to a frequency lower than 250 Hz. Notice that the time axis is scaled by multiplying a factor r^m. In the region below saturation, the vacancy buildup with time is proportional to r^m with $m < 2$.

the critical vacancy concentration and the initial background value (C^*/C_0) is equal to four. With this ratio, the failure time at the low frequency is found to be approximately 6×10^6 s and that at the high frequency is doubled. Furthermore, if C^*/C_0 is equal to five, then the metallization line can survive for about 10^7 s at the low frequency while it will never fail under high-frequency operation.

In Fig. 5, the vacancy buildup behavior is shown as a function of time scaled by the duty factor and its exponent, $r^m t$, for $r = 1.0$, 0.5, and 0.25. All the curves are obtained under an identical peak current density of 2.5×10^6 A/cm^2. As already mentioned, a low frequency of 1 mHz is used for the pulsed current, and the dc stress $(r = 1)$ is applied at a constant average line temperature of 206 °C. One can see that the level at which the vacancy concentration saturates increases with increasing r since a greater r means a longer time to apply the current stress for the same value of period. In this simulation, we tried different values of m for the various r in such a way that all the curves become coincident below saturation. The coincidence with assuming the same critical concentration implies that the vacancy buildup is proportional to r^m, or an r^{-m} dependence can be seen to initiate electromigration failure. It has been shown that $m = 2$ gives the best fit to the coincidence at a constant line temperature (high-frequency case) for different values of r [8], [12]. An $m < 2$ dependence in the lifetime enhancement would be expected at low frequencies due to the temperature cycling effect. As shown in Fig. 5, such a dependence is indeed obtained. For the reason of thermal nonlinearity, m is found to be 1.5 for $r = 0.5$, and a somewhat greater value of 1.6 is exhibited for $r = 0.25$.

Fig. 6 is a more complete diagram, showing the temperature difference between on and off states and the resultant m-value variation for a frequency below 500 Hz with $r = 0.5$. These calculations under a typical range of accelerated current-density stress conditions are performed by using the same approach as detailed above. We find that the value of m decreases with the increase of the current density from 1×10^6 A/cm^2 onwards. A current density of 3.5×10^6 A/cm^2 leads to a temperature difference near 25 °C and $m \cong 1$ can be deduced from these data, which follows the on-time model. It is thus clear that the $m < 2$ or $m = 1$ dependence is observable experimentally and that the concrete value of m depends strongly upon the temperature difference, which in turn varies with current density, test (oven) temperature as well as sample structure. This could be one reason why the reported transition region of frequency between the average and on-time models is far from consistent [6], [7], [9], [12]. On the contrary, the frequency value above which the average model holds true is comparatively independent of the strength of the applied stress because of the attainment of a stable temperature within the metal line. The frequency of greater than 10 MHz obtained in this study is in the same range as that reported elsewhere [9], [10]. The variance of the m value with current stress and operating frequency can be shown by a numerical example based on our calculation. As already seen, a temperature difference of 12 °C induced by $j = 2.5 \times 10^6$ A/cm^2 and 25 °C by $j = 3.5 \times 10^6$ A/cm^2 at low frequencies with $r = 0.5$ result in $m = 1.5$ and 1, respectively. However, the temperature difference is negligibly small $(<0.5\ °\mathrm{C})$ at both current densities if the pulse repetition frequency is above 10 MHz with the same duty factor, resulting in an identical $m = 2$ dependence.

Based on the present electromigration model, the vacancy concentration at the blocking boundary depends on the integrated current density which tends to the average value at a constant line temperature for commonly-used frequencies. The time to failure, as a result, scales as $m = 2$. It is worthwhile to note that an $m \cong 1$ dependence at sufficiently low frequencies may possibly be found even in the absence of the temperature cycling effects. This has been illustrated by a similar model within the diffusion-drift framework [27] and may also be produced by a totally different vacancy relaxation model where a fitting parameter based on experimental data is used [28]. However, a large deviation of the vacancy concentration from the average level to reach the critical ratio C^*/C_0 is observable only when there is a small number of vacancy-concentration

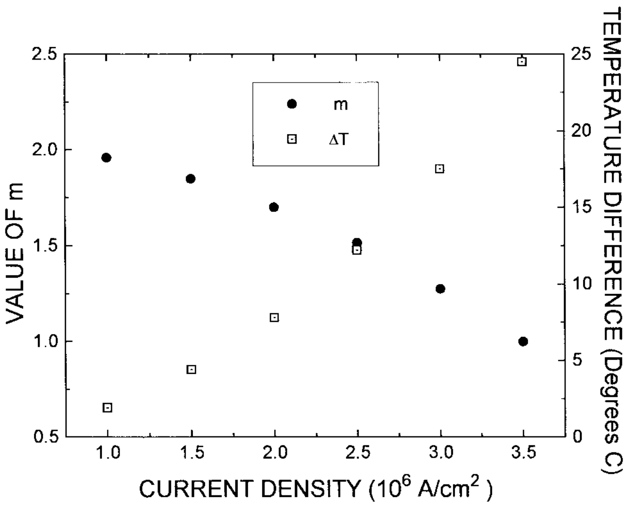


Fig. 6. The value of m and the temperature difference as a function of current density at frequencies below 250 Hz with a duty factor of 0.5.

oscillations in response to the pulsed current waveform up to the time of failure. The corresponding frequencies have been shown to be very much lower than 1 mHz for Al metallization [12]. Careful inspection of Figs. 4 and 5 reveals that such an oscillatory behavior (tightly around the average level) at a frequency of 1 mHz is actually exhibited while its apparent smallness is also demonstrated. As a frequency greater than 1 mHz would result in even smaller vacancy-concentration oscillations, the use of this value as an example frequency to show the temperature cycling effects can be justified. The deduced m-value variation has therefore been attributed solely to the temperature cycling effects which are the main subject of the present study.

Finally, we emphasize that the conclusions drawn in this section are only strictly valid under two basic assumptions of the vacancy supersaturation model. First, the void incubation process dominates the entire failure time. Additional studies would be necessary if this assumption were not used for the application of the on-time and average models at different operating frequencies. Second, the present model, which is based on the fundamental diffusion-drift transport mechanism, essentially incorporates grain-boundary kinetic parameters in a continuum form but does not take into account microstructural details of the thin metal film. For narrow VLSI interconnect lines with a near-bamboo microstructure, the responsible failure mechanism may be complicated by the coexistence of polycrystalline clusters and bamboo segments. Relevant implications on both the m and n values are still under further assessment and investigation.

IV. Concluding Comments

In summary, we have investigated the temperature cycling effect on electromigration behavior under pulsed current stresses by numerically solving two partial differential equations governing the physical processes. The temperature fluctuation has been given as a function of the pulse repetition frequency. We found that the metallization temperature remains at an average constant value at an operating frequency above 10 MHz for a representative system. Under the condition of a constant temperature, the average current density model with $m = 2$ for the duty factor is valid. On the other hand, the temperature oscillation in metallization lines reaches a maximum amplitude when the frequency is lower than 250 Hz. In this study, we confirmed the speculation that an $m < 2$ dependence can be obtained at a low frequency due to the temperature dependence of several physical parameters, including the vacancy diffusivity and electrical resistivity of the metal lines.

In addition, we found that a current density of the order of 10^5 A/cm^2 does not create appreciable Joule heating within the metallization. Therefore, the temperature cycling effects (and the deviation from the $m = 2$ dependence) may only be of much concern in accelerated life testing. Moreover, it should be noted that significant heat generation due to a high current density stressing can alter the value of n in (1) as well. In order to obtain more reliable data that would be extrapolated to normal working conditions for lifetime estimation, a current density not excessively greater than that used in the real-life operation (e.g., below 1×10^6 A/cm^2) is recommended for those tests whenever possible. Finally, test structures should be designed appropriately to minimize severe Joule heating effects that may not be a factor under normal device operation.

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