A model for the effect of line width and mechanical strength on electromigration failure of interconnects with "near-bamboo" grain structures

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(Received 13 July 1990; accepted 12 December 1990)

A simple analytical model for the effect of mechanical strength and line width (for the case of narrow lines) on the electromigration failure of metallic interconnects is presented. Because the line width/grain size ratio and the diffusivity enter differently in the model, application of the resulting failure time equation to published data can provide insight into the mechanisms of enhancement of electromigration resistance by grain structure optimization and alloying.

I. INTRODUCTION

Failure of metallic interconnects ("metallizations") in microelectronic components is generally the result of time-dependent damage accumulation which leads to open or short-circuits. One of the reasons for this degradation involves the phenomenon of electromigration, a mechanism for transport of matter by high electric currents (e.g., Black[1]). The problem of electromigration, which has been under investigation for more than twenty years, is being further aggravated by the continuing trend toward miniaturization and the resulting increase in current densities.

Several strategies for improving the electromigration resistance have been proposed. One involves the addition of alloying elements. In the case of aluminum metallizations, copper,[2] magnesium,[3] nickel,[4] and oxygen,[5] among others, have been described as effective.

A second strategy involves the production of single-crystal[6] or coarse-grain films[7]; also texture formation has been reported as beneficial.[8] A related observation is the strong increase in failure time for metal lines with widths below a critical value,[9,10] an effect which has been ascribed to the formation of a "bamboo" grain structure without grain boundaries running parallel to the line.

These beneficial effects have generally been attributed to a decrease in grain boundary diffusivity and the removal of grain boundaries (which act as fast-diffusion paths), respectively. It is curious, however, that the measures of grain structure optimization, texture processing, and alloying closely parallel the steps taken to achieve high-temperature strength in advanced aluminum alloys for structural applications (e.g., Ref. 11). It might therefore be suspected that mechanical strength is somehow related to electromigration resistance, although the connecting mechanism is not clear. In order to optimize the electromigration resistance of metallizations, a better understanding of this issue is therefore desirable.

In this paper a simple model for the effects of grain structure, width, and mechanical strength of the metal line on electromigration resistance is presented. It is based on earlier formulations of the electromigration phenomenon (to be described in Sec. II). The metal line is assumed to have a grain size which is larger than the line width; this condition, which becomes increasingly realistic with progressing miniaturization, leads to "near-bamboo" grain structures with only a small number of grain boundaries parallel to the line. In order to derive an equation for the failure time distribution, we consider the probability of finding a continuous grain boundary of critical length in the longitudinal direction (Sec. III). This approach leads to a simple analytical expression which, once substantiated, could be useful in analyzing published data (Sec. IV) and could provide a guideline for the development of alternative interconnect materials.

II. THE BACKGROUND

Electromigration is generally considered to be the result of momentum transfer from the electrons, which move in the applied electric field, to the ions which make up the lattice of the interconnect material. This "electron wind" leads to a drift of the metal ions, whose velocity is given by the following expression (e.g., Ref. 1):

$$v = \frac{D}{kT} \cdot eZ^*\rho j \tag{1}$$

where

$$D = D_v + \delta D_b/d .$$

Here j is the electric current density in the line, ρ its resistivity, e the elementary charge, k Boltzmann's constant, and T the absolute temperature. Z^* is an "effective charge" number for the metal ion, which characterizes the momentum transfer; its value, which is not well understood from first principles, can be inferred from experimental data and lies in the range $Z^* = 1 \ldots 40$ for Al. Finally, D is the diffusivity as a result of volume (D_v) and grain-boundary (D_b) diffusion, with δ the grain boundary width and d the grain size. Because of the small grain size in thin films and the relatively low homologous temperatures, grain boundary diffusion usually dominates over volume diffusion, which is to be neglected in this paper.

Measurements of the current-induced displacement of the near-cathode edge of metal films have shown that Eq. (1) does not apply at low current densities; instead, a threshold current density is found below which no displacement occurs.[12,13] This threshold is found to scale inversely with the length of the line and to decrease at elevated temperatures. Its existence has been attributed to the generation of mechanical stresses in the line: while a tensile stress develops at the near-cathode end because of material depletion, the near-anode end of the line, where ions accumulate, experiences a growing compressive stress. The resulting stress gradient drives back-diffusion of ions, tending to offset the flux due to electromigration. The critical electrical current density j_c at which the net flux vanishes is simply calculated by equating the drift velocity [Eq. (1)] with the velocity of diffusion driven by the stress gradient[14,12]:

$$J_c(L) = \frac{\sigma^* \Omega}{e Z^* \rho L} \tag{2}$$

where σ^* is the maximum stress difference the material can sustain between the tensile and compressive regions, L is the length of the line, and Ω is the atomic volume. This argument explains the observation that the threshold current density is inversely proportional to the length of the line. Because σ^* is related to the mechanical strength of the metallization, also the temperature dependence of j_c can be qualitatively accounted for by the loss of strength with increasing temperature.[12]

In order to calculate failure times, we need to consider the formation of localized damage, usually in the form of voids and hillocks. It is generally accepted that such damage can occur only at sites of flux divergence, such as grain boundary triple lines. Shatzkes and Lloyd[15] have calculated the time for the accumulation of a critical vacancy concentration C_f at an extreme flux discontinuity, i.e., a perfectly blocking grain boundary at which the electromigration flux is required to be zero. By considering both electromigration and back-diffusion in a line of semi-infinite length, they arrive at the following approximate expression for the failure time:

$$t_f = \frac{C_f}{D} \left(\frac{\mathrm{k}T}{e Z^* \rho} \right)^2 j^{-2} \tag{3}$$

The failure time of a line of finite length under concurrent electromigration and diffusion has not yet been analyzed rigorously. We assume for the present paper that an approximate result can be obtained by replacing j in Eq. (3) by $j - j_c$:

$$t_f = \frac{C_f}{D} \left(\frac{\mathrm{k}T}{e Z^* \rho} \right)^2 \frac{1}{(j - j_c)^2} \tag{4}$$

where j_c is given by Eq. (2). This expression will be the basis for our calculation of failure times in the following section.

III. THE STATISTICAL MODEL

The grain structure of the film is simply modeled by an array of brick-shaped grains, with an average size d_1 in the direction of the line and d_2 perpendicular to it (Fig. 1). (Usually the grains in a deposited film will be roughly equiaxed in the plane of the film, i.e., $d_1 = d_2$, but a distinction is made here because the two dimensions have different effects on the statistics of the problem.) For line widths w greater than the (transverse) grain size d_2, there will always be a continuous grain boundary path along the line [Fig. 1(a)]. As the line width drops below d_2, the continuous path of Fig. 1(a) is segmented into shorter paths [Fig. 1(b)]. Hence at a given grain size, the probability of finding a continuous grain boundary segment of a given length along the line decreases as the line becomes narrower. In the following we will consider only this latter case of $w < d_2$ ("near-bamboo structure").

The central assumption of this paper is *that the line will fail at the longest of these continuous grain boundary segments* because there the stress gradient for back-diffusion, and thus the resulting threshold current density, will be smallest. Let $\lambda_{\max,i}$ be the length of the longest grain boundary segment in the i^{th} line. Then for that particular line the failure time would be, using Eq. (4),

$$t_f^i = \frac{C_f}{D} \left(\frac{\mathrm{k}T}{e Z^* \rho} \right)^2 \frac{1}{(j - j_c^i)^2} = \frac{\alpha}{(j - j_c^i)^2} \tag{5}$$

where the critical current density for that particular line is found by replacing L in Eq. (2) with $\lambda_{\max,i}$,

$$j_c^i = \frac{\sigma^* \Omega}{e Z^* \rho \lambda_{\max,i}} \tag{6}$$

Thus the failure time for the i^{th} line may be expressed as

$$t_f^i = \frac{\alpha}{\left(j - \dfrac{\sigma^* \Omega}{e Z^* \rho \lambda_{\max,i}} \right)^2} = \frac{\alpha}{\left(j - \dfrac{\beta}{\lambda_{\max,i}} \right)^2} \tag{7}$$

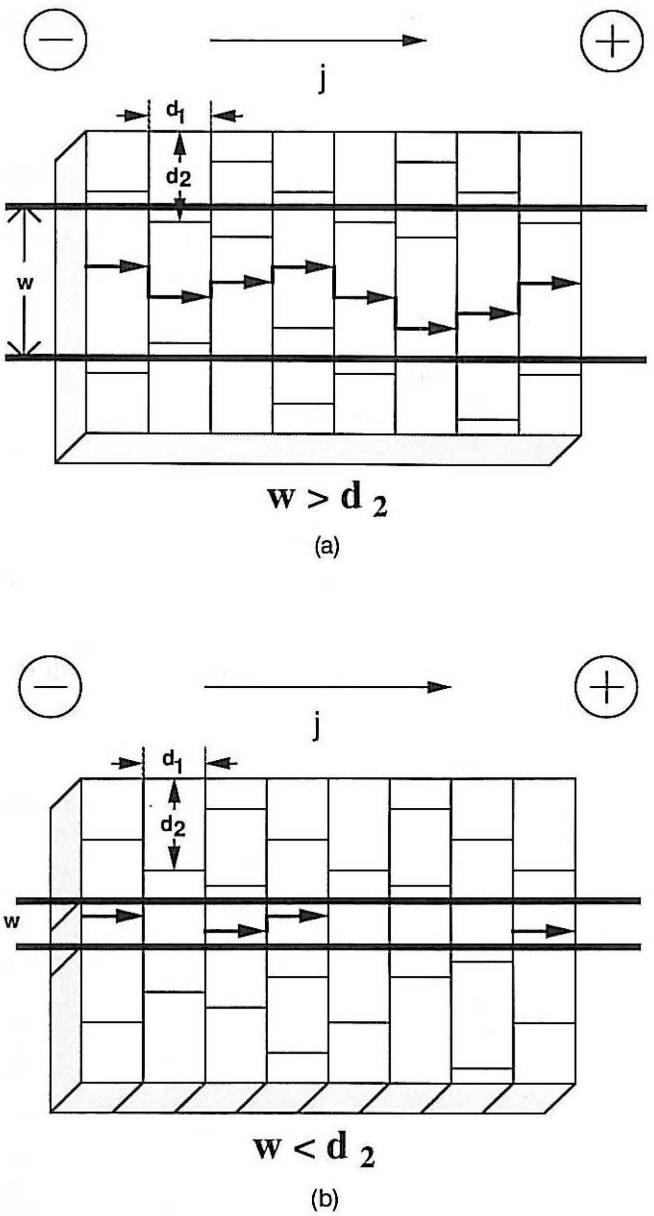

FIG. 1. Schematic illustration of the effect of decreasing the line width w below the transverse grain d_2: for $w > d_2$, a continuous grain boundary path can always be found (a); once $w < d_2$, this path is segmented into shorter parts which are less prone to electromigration damage (b). Large arrow signifies the direction of the electron wind.

Now let $t_f(s)$ be the time required for a given fraction s of the lines to have failed. The failed lines are those for which $t_f^i < t_f(s)$ or, using Eq. (7), those for which

$$\lambda_{\max,i} > \frac{\beta}{\left(j - \dfrac{\sqrt{\alpha}}{\sqrt{t_f(s)}}\right)} = \lambda_c(s) \tag{8}$$

The right side of this equation may be regarded as a critical grain boundary segment length, $\lambda_c(s)$, for this particular failure time. Only those lines with longest grain boundary segments of length $\lambda_c(s)$ or greater will have failed in time $t_f(s)$. But the fraction of failed lines in this time is the same as the probability of finding a particular line with a longest grain boundary segment of length $\lambda_c(s)$ or greater. Thus we need to consider the statistical distribution of grain boundary segment lengths within the lines before we can make failure time predictions.

For our model grain structure, the probability of finding, in a line of width w, a longitudinal grain boundary between two given transverse boundaries is simply

$$p_1 = \frac{w}{d_2} \tag{9}$$

It follows that the cumulative probability of finding, in a line of length L, at least one continuous segment of length equal to, or greater than, λ is given by combined probabilities in the following way:

$$p_\lambda = 1 - \left[1 - \left(\frac{w}{d_2}\right)^{\lambda/d_1}\right]^{L/d_1}$$
$$\approx 1 - \exp\left[-\frac{L}{d_1}\left(\frac{w}{d_2}\right)^{\lambda/d_1}\right] \tag{10}$$

The approximation by an exponential, which is convenient for further calculations, applies only for long lines. As discussed above, for a given fraction, s, of failed lines, there is a corresponding failure time $t_f(s)$ and a critical grain boundary segment length $\lambda_c(s)$. By setting $p\lambda = s$ and $\lambda = \lambda_c(s)$ in Eq. (10), we can find the relationship between $\lambda_c(s)$ and s,

$$\frac{\lambda_c(s)}{d_1} = \frac{\ln\left(-\dfrac{L}{d_1 \ln(1 - s)}\right)}{\ln\left(\dfrac{d_2}{w}\right)} \tag{11}$$

The corresponding failure time can then be found by combining this with Eq. (9),

$$t_f(s) = \frac{\alpha}{j^2\left[1 - \dfrac{j^*(s)}{j}\ln\left(\dfrac{d_2}{w}\right)\right]^2} \tag{12}$$

where

$$j^*(s) = \frac{\beta}{d_1 \ln\left(-\dfrac{L}{d_1 \ln(1 - s)}\right)} \tag{13}$$

Further, the effective diffusivity due to a grain boundary running along a line of width w is:

$$D = \delta D_b / w \tag{14}$$

Also, the critical vacancy concentration C_f at which failure of the line is assumed to occur will scale with the product of line width and film thickness h; assuming w to be proportional to h, we set:

$$C_f = A\frac{w^2}{d_2^2} \tag{15}$$

where A is a dimensionless constant.

The final result for the failure time of a fraction s of lines can be conveniently expressed in the following way:

$$t_f(s) = \frac{B}{j^2}\frac{\left(\frac{w}{d_2}\right)^3}{\left\{1 - \frac{j^*(s)}{j}\ln\frac{d_2}{w}\right\}^2} \tag{16}$$

where

$$B = \frac{Ad_2}{\delta D_b}\left(\frac{kT}{eZ^*\rho}\right)^2$$

and

$$j^*(s) = \frac{\sigma^*\Omega}{eZ^*\rho d_1}\frac{1}{\ln\left[\frac{-L}{d_1\ln(1-s)}\right]}.$$

The theoretical median time to failure (MTF) is obtained for $s = 0.5$, but also lower failure probabilities, e.g., $s = 0.001$ (0.1%), are readily calculated. Typical curves of failure time t_f vs w/d_2 according to Eq. (16) are shown in Fig. 2 for the two failure probabilities $s = 50\%$ (MTF) and $s = 0.1\%$ and for two values of j^*.

IV. DISCUSSION

The main assumption in this paper is that electromigration failure in "near-bamboo" structures is indeed related to grain boundaries. While recent metallographic evidence suggests that this may not be true under certain circumstances,[16] similar suggestions have been made by Kinsbron[10] and Cho and Thompson.[17] The statistical aspects of the latter model exhibit some similarities with the present model, but the link with kinetics and strength considerations is developed only here. We now examine the consequences and possible merits of this approach.

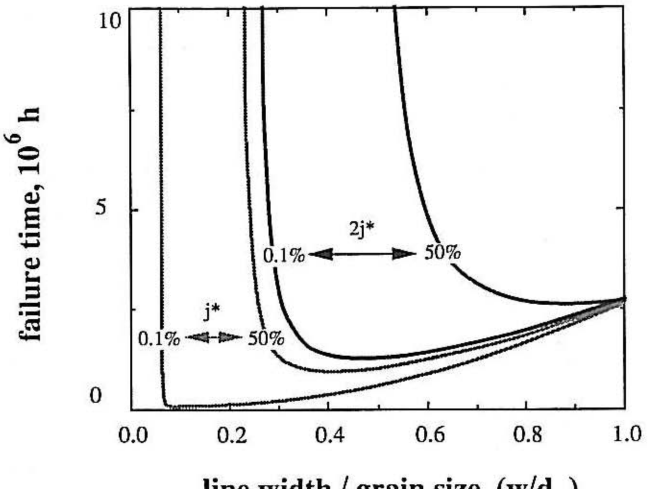

FIG. 2. Model predictions for the effects of mechanical strength (proportional to j^*) and of failure probability on failure time versus line width over transverse grain size. (Absolute values in failure time are for the conditions in Fig. 3.)

It is seen in Fig. 2 that qualitatively the same initial decrease and subsequent rapid increase in mean failure time, as has been measured for progressively narrower lines, are reproduced. The model predicts a singularity at

$$w_\infty(s) = d_2\exp\left(-\frac{j}{j^*(s)}\right) \tag{17}$$

and a minimum at

$$w_{\min}(s) = d_2\exp\left(\frac{2}{3} - \frac{j}{j^*(s)}\right) \tag{18}$$

In practice, of course, there will not be a true singularity because even perfect bamboo structures, while being much more electromigration resistant, have finite failure times. In such structures, additional failure mechanisms, which are not considered here, will become dominant. Also, the singularity arises in the present treatment because of the simple correction to the Shatzkes–Lloyd expression in Eq. (4). Further work will be necessary to establish the details of the vacancy kinetics in a finite line element. The comparison with experimental data (below), however, shows that the correction appears to be reasonable.

It is clear from Fig. 2 that the assumed probability s is critical for the failure time. The curve for failure of the first 0.1% of all lines continues to fall to lower lifetime values than the MTF before showing a similar sharp increase. This continuous drop in t_f (0.1%) corresponds to a sharply increasing variance of the lifetime distribution, which is in qualitative agreement with experimental data.[10,17]

Figure 2 furthermore suggests that raising the mechanical strength (proportional to j^*) can produce substantial gains in both t_f (50%) and t_f (0.1%) by shifting the "singularity" to higher w/d_2 values.

In addition, the model can be made to fit experimental data with good accuracy. Figure 3 shows the MTF measured by Vaidya *et al.*[9] for Al–0.5% Cu lines of different widths. The theoretical line was obtained by fitting the constants B and j^* (50%) such that the location and numerical value of the minimum coincided with the experimental results. Because of their physical significance, these parameters are, however, not merely fitting constants, but can in principle be calculated from Eq. (16). It turns out that the material parameters which have to be assumed to obtain these constants have reasonable magnitudes: $\delta D_b/A = 10^{-23}$ m^3/s and $\sigma^*/Z^* = 12$ MPa (or $Z^* = 8$ for an assumed yield stress of 100 MPa). In view of the simplicity of the model, the agreement with experiment must be considered extremely good.

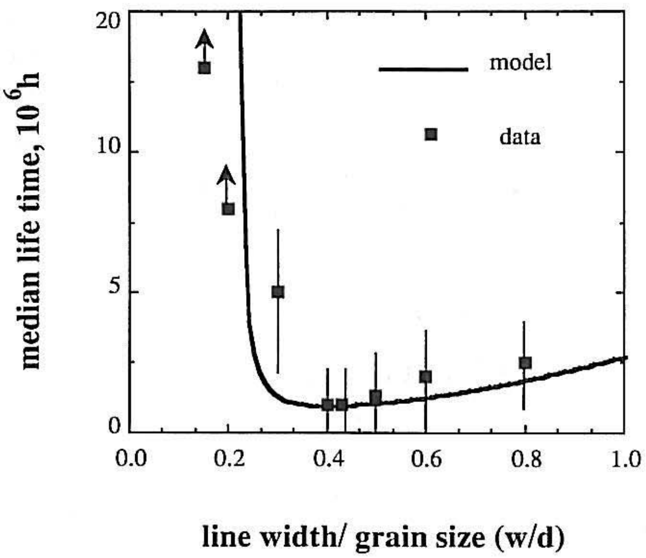

FIG. 3. Median lifetime versus ratio of line width to grain size for Al–0.5% Cu metallizations. Data points and error bars are for accelerated tests by Vaidya *et al.*,[9] who extrapolated their values to operating conditions (80 °C, 10^9 A/m^2). Full line corresponds to the present model.

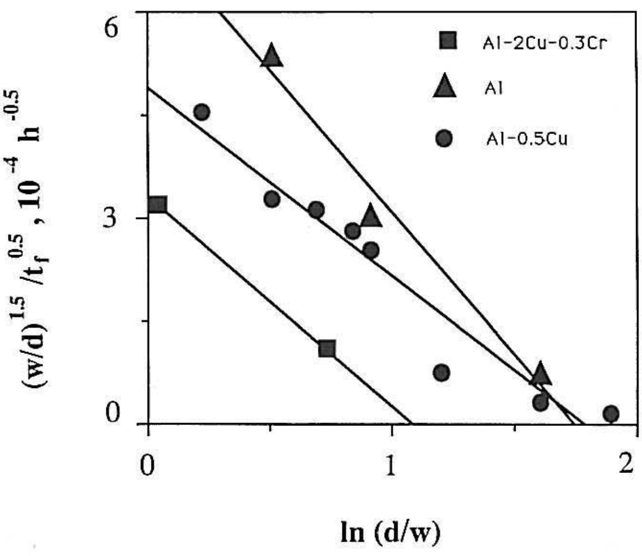

FIG. 4. Result of replotting failure time data for different alloys according to Eq. (10): Data from Vaidya *et al.*[9] (Al and Al–0.5% Cu) and Cho and Thompson[17] (Al–2Cu–0.3Cr). In such a plot the x-axis intercept is inversely proportional to the mechanical strength, while the y-intercept scales as the square root of the diffusivity.

Mechanical strength and diffusivity enter in the model in different ways: while σ^* affects the threshold current density, D_b determines the kinetic factor B. Therefore Eq. (16) suggests that by replotting electromigration data as $x = \ln(d_2/w)$ and $y = (w/d_2)^{3/2}/(t_f^{1/2})$, the parameters B and j^* can be obtained graphically from the x-axis and y-axis intercepts $x(0)$ and $y(0)$:

$$x(0) = j/j^*$$
$$y(0) = j/\sqrt{B} \tag{19}$$

Thus the x-axis intercept scales inversely with the mechanical strength, while the y-axis intercept is proportional to the square root of the diffusivity. By plotting data in this way, the effects of alloying additions on diffusivity and on mechanical strength can in principle be separated. This procedure, however, requires reliable failure time data as a function of w/d_2, preferably from the same experimental source.

For illustration purposes (Fig. 4), we have analyzed three sets of data for unpassivated Al and Al–0.5Cu (Vaidya *et al.*[9]) and Al–2Cu–0.3Cr (Cho and Thompson[17]). The results of this exercise, which are tabulated in Table I, show that adding Cu to pure Al did not change its strength (the x-axis intercept is the same), but reduced its diffusivity by about a factor of 2; this conclusion is in keeping with the generally reported effect of Cu. By contrast, the addition of Cr, which is used to impart high-temperature strength to structural Al alloys (e.g., Ref. 18), improved both the mechanical strength (smaller x-intercept) and the diffusivity (smaller y-intercept).

Such preliminary conclusions should still be considered with caution; detailed microstructural investigations coupled with independent measurement of film strength are necessary to check the validity of this concept. It must also be realized that in an actual component the passivation will greatly influence the mechanical strength of the system. In any case, due to the exponential dependences in Eqs. (17) and (18), small changes in mechanical strength of the metallization/passivation system have the potential of greatly affecting electromigration lifetimes. It remains to be seen whether the success of introducing virtually insoluble elements, which precipitate to form obstacles for lattice dislocations, can be rationalized in this way.

In comparison to these potential strength effects, grain size effects seem to be more subtle. The grain dimension perpendicular to the line (d_2) should be as large as possible, but its value enters only logarithmically. Along the line, the grain dimension (d_1) should

TABLE I. Analysis of the material constants j^* and B using the graphical procedure of Fig. 4.

	j^*/j	B[a]	Reference	Remark
Al	0.571	1.9	9	b
Al–0.5% Cu	0.561	4.2	9	c
Al–2Cu–0.3Cr	0.916	9.1	17	d

[a](in 10^{24} sm^4/A^2).
[b,c]$j = 2 \times 10^{10}$ A/m^2, $T = 250$ °C, extrapolated to 10^9 A/m^2, 80 °C, assuming $t_f \sim j^{-2*} \exp(0.5 \text{ eV}/kT)$.
[d]$j = 1.2 \times 10^{10}$ A/m^2, 275 °C, same extrapolation.

be small in order to reduce the length of a statistically occurring longitudinal boundary. It could therefore be desirable (if at all practical) to produce a grain shape which is elongated in the direction perpendicular to the line. However, the model also shows that such grain structure optimization is less effective for the failure of the first few lines, which of course is much more relevant to applications than the mean time to failure. It is suggested in the light of this model that only by raising the mechanical strength at the same time can a significant and useful improvement in electromigration resistance be achieved.

V. CONCLUSIONS

(1) A simple analytical model for the effect of grain structure and line width on the failure time of metallization lines has been developed. It rests on the assumption that failure will take place at the longest statistically occurring longitudinal grain boundary and uses earlier derived expressions for the threshold current density.

(2) Although many refinements of the present model are still possible, good agreement between the theory in its present form and previously published experiments has been obtained by choosing physically reasonable material parameters.

(3) Application of the model to different sets of data reveals that alloys used in metallizations may derive their increased electromigration resistance from both a decrease in diffusivity and an increase in mechanical strength. The model suggests strongly that mechanical strength could be an important variable in the search for better interconnect materials.

(4) Grain structure optimization, by contrast, seems to be a less efficient means for improving electromigration resistance because it affects calculated times to failure of the first few lines in an ensemble to a much smaller extent than the (usually irrelevant) mean time to failure.

ACKNOWLEDGMENTS

It is a pleasure to acknowledge many interesting and valuable discussions with Professor P. Flinn at Stanford University and INTEL. One of the authors (EA) is grateful to the Department of Materials Science and Engineering at Stanford University for the hospitality and stimulating environment provided during his time there as Visiting Professor. The financial support for this stay by the Alfred Krupp von Bohlen und Halbach-Stiftung, Essen, Germany, is gratefully acknowledged. The other author (WDN) wishes to gratefully acknowledge support of the Air Force Office of Scientific Research under AFOSR Grant 89-0185 and of the Defense Advanced Research Projects Agency through the University Research Initiative program at the University of California at Santa Barbara under ONR contract N00014-86-K-0753.

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