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Effect of microstructure on electromigration kinetics in Cu lines

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Abstract. Strong correlation of the modes of electromigration damage and microstructure is reported for Cu films. It is found that changes in the microstructure lead to qualitative variation in electromigration damage kinetics—from the traditional open circuit due to void growth across the line, to damage growing along the line, and not leading to failure. Some of our findings are consistent with the theoretical model based on interplay between surface and grain boundary diffusion. The activation energy E_a = 0.95 eV of electromigration mass transport was measured using a modified electrical resistance method.

1. Introduction

With the development of ultra-large-scale integrated circuits and the scaling down of device geometry, the use of aluminium and its alloys as a material for interconnects becomes a limiting factor in chip performance. Cu is considered to be a possible substitute for Al [1]. Higher resistance to electromigration (EM) and improved reliability may be expected for Cu since it has a higher melting point and therefore higher activation energy of grain boundary diffusion (1.2 eV against 0.6 eV for Al) which is considered as the main mechanism for EM at temperatures of the device operation. However, experiments performed by many authors [2–21] using Cu films fabricated at different conditions have shown large variations in the value of activation energy of EM, E_a, (from 0.5 to 1.25 eV) making questionable the uniqueness of the mechanism for EM in Cu.

Our previous measurements of E_a [22] by life time statistical experiments using 50-lines test geometry [23] showed poor reproducibility of the measured E_a values and often large scattering of the data on the Arrhenius plot, though the samples were obtained and tested at the same conditions. The reason might be some poorly controlled parameters in film preparation, such as exact composition of the residual atmosphere or contaminations on the substrate. Their variations may lead to uncontrollable changes in microstructure (such as micropores and contaminations in grain boundaries) and may influence the processes of void creation and their subsequent growth which determine the time to failure. In addition, because Cu, unlike to Al, does not have a native stable oxide film, the EM process can be complicated by the effect of the surface diffusion, which may also essentially influence the kinetics of damaging by smoothing a film surface [22] and acting as a 'healing' mechanism. It seems reasonable that these features would affect measured values of E_a. The action of surface diffusion has been mentioned in early works on EM [24] to explain thinning of a conductor line in local areas containing many grains. Recently, surface diffusion was considered in [25] as an explanation of the variations in E_a values derived from the drift velocity experiments on the Cu films. It was concluded that such experiments may give some effective E_a value depending on the activation energies for both grain boundary diffusion and surface diffusion. Our comparative life time studies of uncovered Cu lines and Cu lines covered by a thin Ta layer [22] resulted in longer life times for Cu films, implying the importance of surface diffusion in kinetics of EM.

In this work we will demonstrate that different microstructures of Cu film result in different kinetics of voids evolution. We connect the latter with the wide dispersion of E_a values.

2. The experiment

Cu films of 160 nm thickness for use as test structures were deposited in a vacuum onto oxidized Si substrates by means of e-beam evaporation. To obtain films with different microstructures, we varied the deposition parameters: substrate temperature (from 20 to 300 °C), evaporation rate (from 3 to 50 nm s^{-1}), pressure of the residual atmosphere (from 5×10^{-6} to 1×10^{-7} Torr). Both pure Cu films and Cu films covered *in situ* with a Ta layer of 10 nm thick were fabricated.

The sample test geometry was formed by a photolithography technique (lift-off and wet etching for condensation at room and elevated temperatures respectively). The test

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structure contained 50 equal, parallel, periodically spaced Cu lines of 2 μm width and of 1 mm length between two large contact pads. An individual, identical line with four-contacts geometry near the test lines was used as a thin film thermometer and a reference sample (unstressed by high density current). The connection between lines and pads was designed to be gradual, with a relatively small curvature, to minimize current crowding and thermal gradients in these regions. After patterning, the films were annealed in a vacuum at 1×10^{-6} Torr and 450 °C for 1 hour and then cooled down to the test temperature. The test structures were stressed by a direct electrical current with a density of 2×10^6 A cm^{-2} in a vacuum at 1×10^{-6} Torr, at temperatures from 370 to 410 °C. The value of the current density was chosen experimentally for the given parameters of our test structure (lines and pads dimensions, line spacing, thickness of the oxide layer at the silicon substrate, test temperature) and it did not result in any notable temperature gradient problems: typical damages in the form of voids near the cathode and hillocks near the anode were absent. The microstructures of the Cu films before and after EM stressing were investigated by means of scanning and transmission electron microscopy.

We used isothermal electrical resistance measurements for determination of the E_a of EM mass transfer. The rate of relative electrical resistance change due to EM is thermally activated and according to [26] can be expressed as $(1/R_0)(\mathrm{d}R/\mathrm{d}t) \sim \exp(-E_a/kT)$, where R and R_0 are the current and original conductor resistances respectively. In our case R represents the net resistance of 50 parallel connected lines. Testing was carried out using a constant voltage source. Measurements were performed at five temperatures in the range of 370–410 °C in a continuous process, without current switching off and vacuum breaking. E_a was determined from the Arrhenius plot of $\ln(1/R_0)(\mathrm{d}R/\mathrm{d}t)$ versus $1/T$.

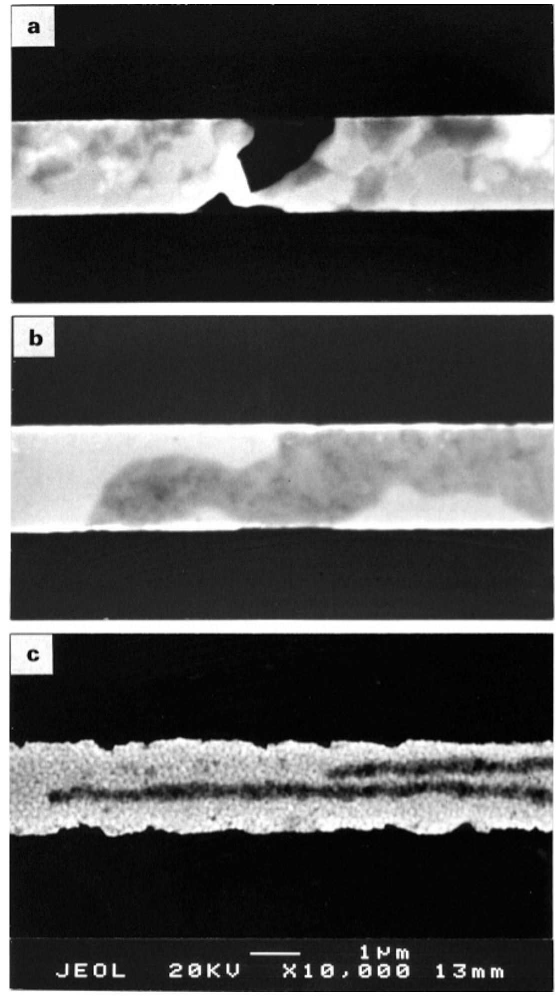

Figure 1. A variety of EM damage kinetics in thin film Cu conductors (SEM images).

3. Results and discussion

Different conditions of fabrication resulted in different microstructures of Cu films. Films obtained at a pressure $p = 1 \times 10^{-7}$ Torr, substrate temperature $T_c = 20$ °C and deposition rate $V_c = 5$ nm s^{-1} after pre test annealing had grains with an average size of $d = 500$ nm. EM damage observed experimentally in such films is shown in figure 1(a).

The degrading of the vacuum conditions, $p = 5 \times 10^{-6}$ Torr, led to a smaller Cu grain size, $d = 150$ nm. Figure 1(b) shows a micrograph of EM damage for this film. The failures in this case appear after a long period of time and are the result of global thinning of large areas rather than evolution of voids across the line as in figure 1(a).

And finally, the films with the smallest grain size, $d = 120$ nm, which were obtained at $p = 1 \times 10^{-6}$ Torr, $T_c = 300$ °C and $V_c = 50$ nm s^{-1}, produced stripe-like voids propagating along the conductor line after EM experiment, see figure 1(c). The length of these voids could reach tens of microns without causing an open circuit.

Specific electrical resistance of the Cu films was measured to be 1.7 $\mu\Omega$ cm in the case of large grains which is close to the value for the bulk material, and 2.8 $\mu\Omega$ cm in the case of small grains, that corresponds well to a resistance increase due to an internal size-effect (grain boundary scattering) [27].

The authors are not aware of any previous reports of such a variety of EM damage morphology in Cu films. It should be emphasized that the three kinds of damage, shown on figure 1, are extreme cases of EM kinetics, but some intermediate cases are also possible. We presume that such a variety of damage kinetics in Cu is due to a structural dependent relationship of grain boundary (GB) transport with the surface diffusion.

Below we will analyse our experimental observations in a framework of a theoretical model of EM [28–30] which considers coupled GB mass transport and surface diffusion. We will show that according to the model the kinetics leading to the type of damages, shown in figure 1(a) should occur for the large grained Cu films, whereas global thinning of Cu film should occur in the case of small grains.

The model describes the case of Blech–Kinsbron sample geometry [31] when a metal stripe lie on the conductive substrate and EM causes displacement of the cathode end of the stripe. This model takes into account surface diffusion on the side face of the cathode end of the film, but it can be also applied to explain the first and second kind of EM kinetics in our experiments. According to the theory, two different modes of surface evolution can exist depending on the value of the dimensionless parameter $\alpha = Id^2/8B$, where $I = D_{gb}\delta j\rho Ze/kT$ is the GB mass flux induced by EM, and $B = D_s\gamma_s\omega^2 N_s/kT$ is known as the Mallins constant. D_{gb} and D_s are the GB and the surface self-diffusion coefficients. δ is the GB width, j is the current density, ρ is the specific resistivity, Ze is the effective charge of diffusing atoms, k is the Boltzmann constant, T is the absolute temperature, γ_s is the surface tension, ω is the atomic volume, N_s is the surface atomic density and d is the grain diameter. For large α, surface diffusion can not maintain the homogeneous surface motion: voids or hillocks must form at GBs. As a result, the usual morphology of damage, as shown in figure 1(a), occurs.

However, for small α, surface diffusion becomes important and a global steady state regime of thermal grooving takes place when the surface moves homogeneously. In this case, sink or source of atoms at the GB can only slightly change the shape of GB grooves. This means that surface flux occurring due to a curvature gradient along the surface, may redistribute material between the GBs. Such kinetics will result in global thinning as shown in figure 1(b).

Considering the GBs as the source of vacancies (sink of atoms) and substituting in the expression for α typical values of parameters: $D_s/D_{gb} \simeq 1$, $\delta \simeq 0.5$ nm, $j\rho = 1$ V cm^{-1}, $Ze \simeq 3 \times 10^{-19}$, $\omega = 1.18 \times 10^{-29}$ m^3, $N_s \simeq 10^{19}$ m^{-2}, $\gamma_s \simeq 1.5$ N m^{-1}, we obtain that for $d = 500$ nm (as in the first case of the EM damage) parameter $\alpha \simeq 25$, whereas for $d = 150$ nm (as in the second observed case) $\alpha \simeq 1$. Thus, the theoretical model [28–30] can explain observed damage across the line in the first case and thinning of the film in the second case.

While the first and the second kind of damage (figures 1(a) and (b)) have quite plausible explanations, the origin of the third kind of damage (stripe-like voids along the conductor line, figure 1(c)) is still not clear. However, it seems reasonable, that stripe-like voids have the same nature that thinning has. TEM investigations indicated that these voids arise from lengthwise thinning localized on the width of several grains (figure 2). We think that the latter phenomenon is related to tensile thermal stresses which should arise in the Cu film on the Si substrate due to cool down from the temperature of pre-annealing (450 °C) to the temperature of EM test (370–410 °C). As was shown in [32] for the films of 1 μm thick, the level of these stresses is negligible. However, it is known that the amount of stress depends on the film thickness [33] and on the grain size [34], and in our case of small thickness and small grain size, the films might sustain notable tensile stress at the test temperature.

These stresses relax at the line borders [35] at the width of the order of the film thickness that lead to a stress gradient across the line and, therefore, to a gradient of vacancy equilibrium concentration [36]. The chemical potential of vacancies in the tensile film depends on

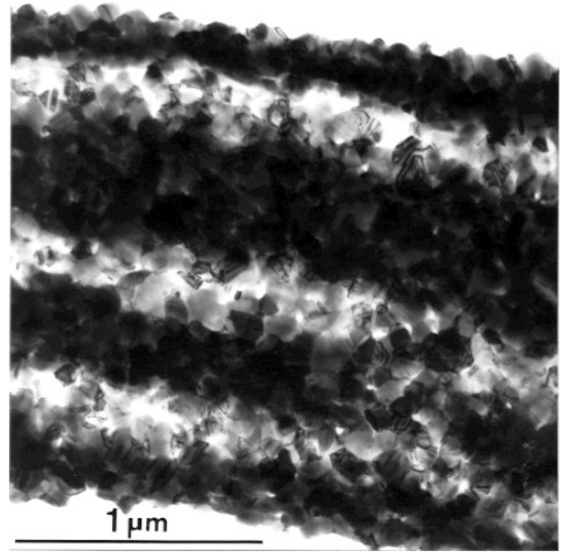

Figure 2. TEM image (plan view) of a section of a Cu line with three parallel stripe-like voids.

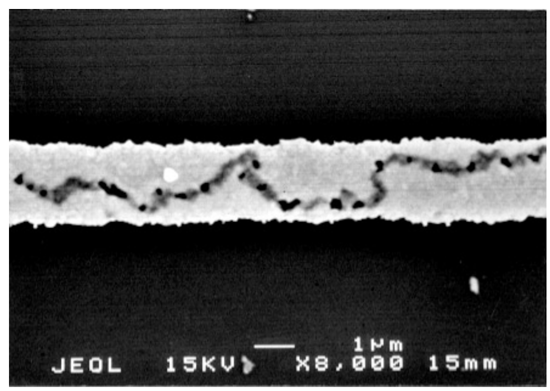

Figure 3. Ribbon-like void 'locked up' inside the line.

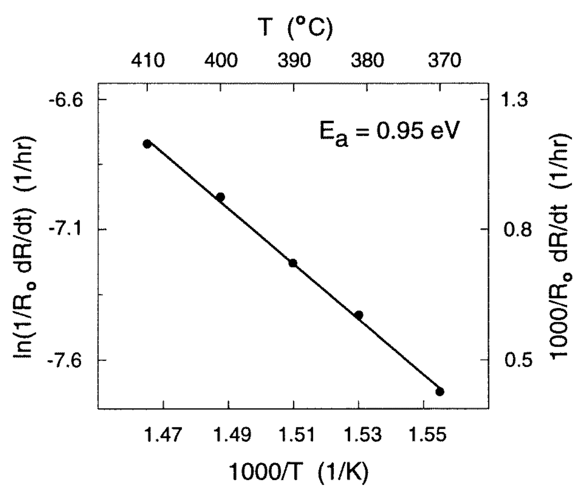

Figure 4. Arrhenius plot of the time rate of change in resistance of the Cu test structure containing fifty lines.

the distance from the borders according to the relation, $\mu_v(y) = \mu_v^0 - \sigma(y)\omega$, where μ_v^0 is the chemical potential of vacancies without stresses and $\sigma(y)$ is the stress distribution across the line. EM mass transport is a vacancy sensitive process and it should be faster inside the line where the vacancy concentration is higher. Some experimental observations of stripe-like voids morphology may serve in favour of such an assumption. Firstly, they arise inside the line, but not at the line borders. As the stripe-void growth is accompanied by stress relaxation at its borders, the next void would be formed between the first void and the border of the line. Indeed, sometimes we observed two and even three parallel stripe-voids, as shown in figure 2. Secondly, whenever they grow not exactly parallel to the line axis and start to approach the line side, they do not touch it but 'push off' from it changing their direction (see figure 3).

It should be noted that small grain size leads to a high specific electrical resistance of the film and to a large number of paths for EM that sets limits for use of such a film as an interconnect material. However, as model objects, small-grained films may serve for the deeper understanding of the EM processes.

We believe that the large diversity of EM kinetics is related to the observed poor reproducibility in our previous measurements [22] of E_a. Previously we employed a widely used method for E_a determination based on Black's formula [37] for median time to failure $\mathrm{MTTF} = Aj^{-n}\exp(E_a/kT)$, where A and n are constants. A pre-exponential factor A might be a large source of errors for samples having different microstructure and different damage morphology. Therefore, in the present work we monitored changes of the electrical resistance at early stages of EM for E_a measurements as an alternative method. Obviously, in the early stages the final morphology of the damage is of no importance and it is not revealed in $\mathrm{d}R/\mathrm{d}t$ measurements [26]. Moreover, this method allows measurements to be performed at several different temperatures on the same sample and to eliminate the dependence arising from structural variations. The value of the activation energy was found to be 0.95 eV (see figure 4) for the samples with the microstructure as in figure 1(b). This value is close to the value of E_a for GB diffusion, indicating that GB diffusion is the limiting mechanism of mass transport.

4. Conclusion

We demonstrated that different microstructures in Cu films result in a large diversity of kinetic processes of EM mass transfer. In some extreme cases voids in the form of long narrow stripes along the Cu line were observed. Such types of EM damage have never been reported in Cu or any other material. Within the framework of the existing theoretical models our findings suggest that surface diffusion plays an essential role in EM kinetics.

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